Lattice Boltzmann approach to fluid flow in a lid-driven cavity bounded by coaxial cylinders

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Diffuse reflection boundary conditions

- Boltzmann equation with the BGK approximation of the collision term :

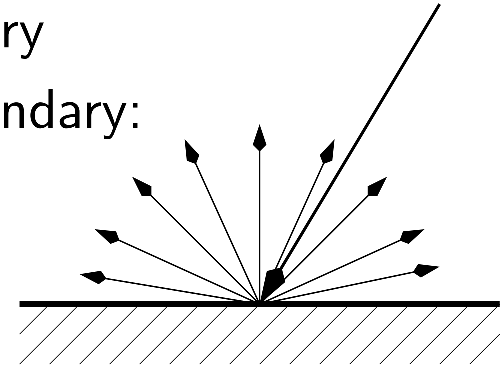
$$\partial_t f + \frac{1}{m}\mathbf{p}\cdot\nabla f + \mathbf{F}\cdot\nabla_{\mathbf{p}} f = -\frac{1}{\tau}[f - f^{(\mathrm{eq})}]$$

  where $\tau \sim \mathrm{Kn}$ and $f^{(\mathrm{eq})}$ is the Maxwellian distribution
- The hydrodynamic variables are given as moments of f up to order N
- The diffuse reflection boundary conditions require:

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

  where χ is the outwards-directed normal to the boundary
- n_{w} is fixed by requiring zero mass-flux through the boundary:

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



- $\Rightarrow$ implementation of the diffuse reflection boundary conditions requires the computation of integrals of f and $f^{(\mathrm{eq})}$ over half of the momentum space

Discretization of the momentum space

$$1D: \quad f(p) \simeq f^N(p) = \omega(p) \sum_{\ell=0}^{N} \mathcal{F}_\ell \phi_\ell(p) \qquad \int_{\mathcal{D}} dp\, \omega(p)\, f^N(p)\, p^s = \sum_{k=1}^{Q} f_k\, p_k^s$$

- The polynomials $\{\phi_\ell\}$ are orthogonal over the domain $\mathcal{D}$ with respect to the inner product defined by the weight function $\omega(p)$ and $0 \le s \le N < Q$
- Full-range Gauss-Hermite Lattice Boltzmann models HLB(Q) :

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

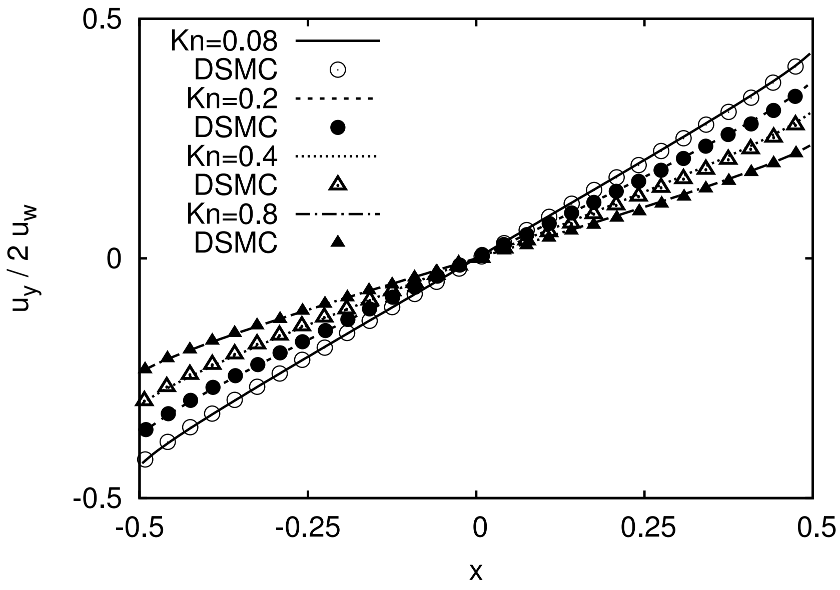
- Half-range Gauss-Hermite lattice Boltzmann models HHLB(Q) :

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

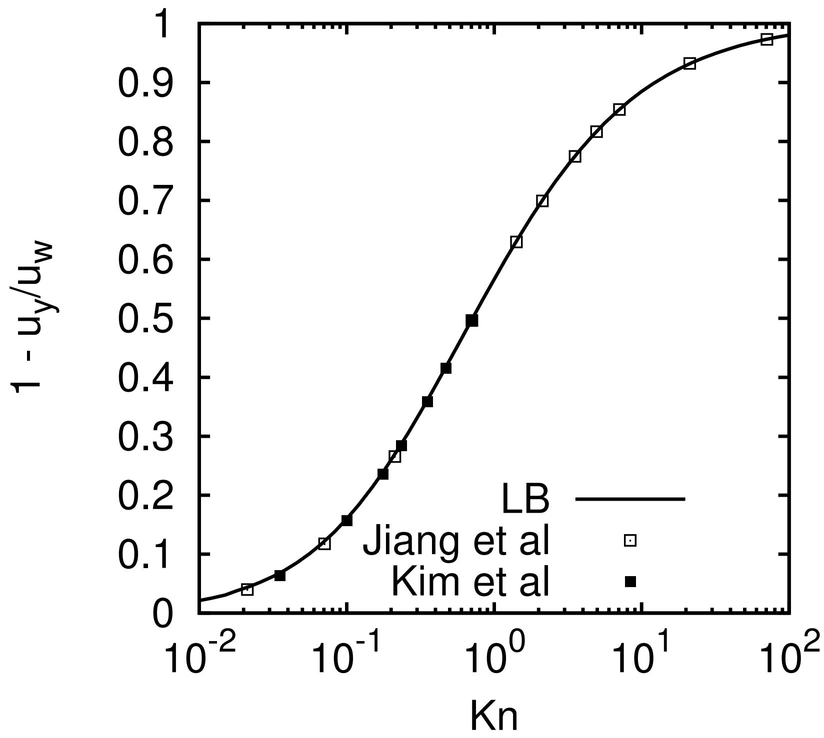
- $f_k = w_k f^N(p_k)$, where p_k are the Q roots of $\phi_Q(p)$ and w_k are the associated quadrature weights
- Microfluidics : LB models of high order N and half-range capabilities
- $3D$ models are built using Cartesian products: $3D = 1D \times 1D \times 1D$

V.E.Ambruș and V.Sofonea, J.Comput. Phys. **316** (2016) 760 / J. Comput. Sci. **17** (2016) 403

Couette flow : velocity slip



(1)

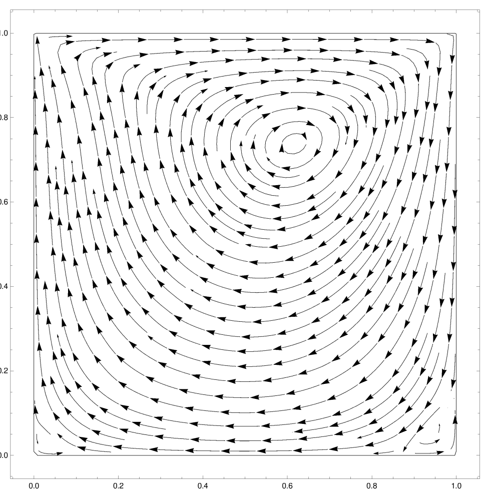


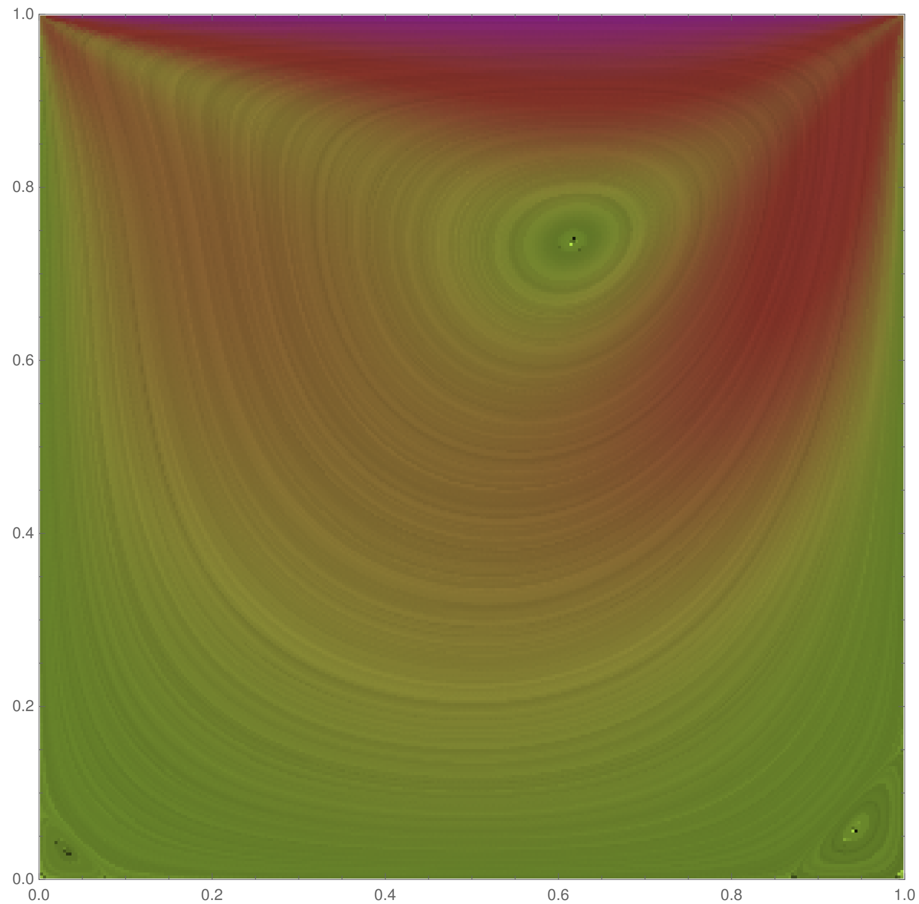
(2)

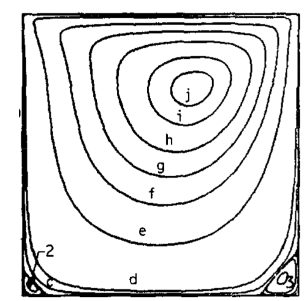
1. Comparison of the LB velocity profiles at $u_w = 0.63$ with the DSMC results in [1]
2. Comparison between the slip velocity values obtained with the LB model $HHLB(21) \times HLB(4) \times HLB(4)$ and the linearised Boltzmann results in [1] and [2].

[1] S.H.Kim, H.Pitsch and I.D.Boyd, J.Comput. Phys. **227** (2008) 8655
[2] S.Jiang and L.S.luo, J.Comput.Phys. **316** (2016) 416

lid cavity : Navier - Stokes regime (streamlines) $Re = 100$





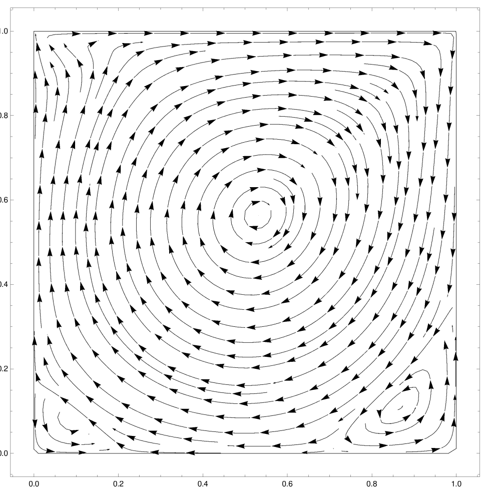


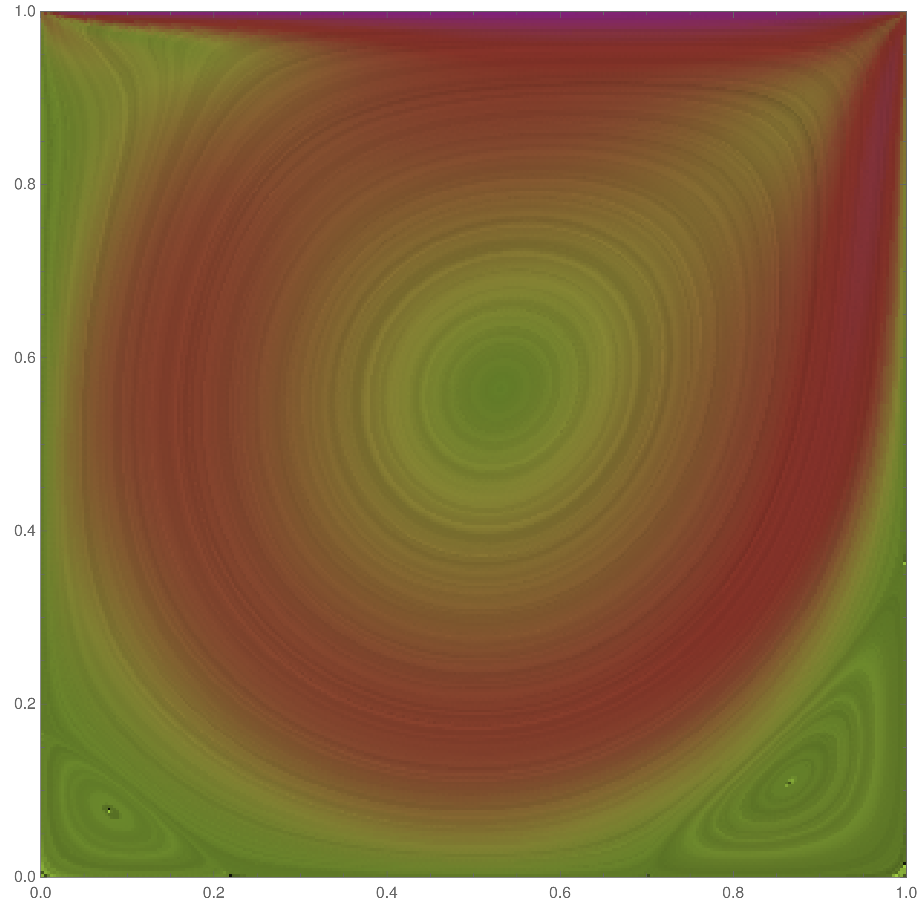
LB : 60×60 nodes, $HLB(5) \times HLB(5)$

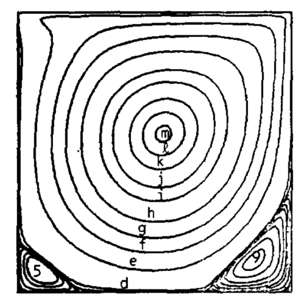
Ghia et al. (1982)

[1] Ghia et al., J. Computational Physics 48 (1982) 387

lid cavity : Navier - Stokes regime (streamlines) $Re = 1000$







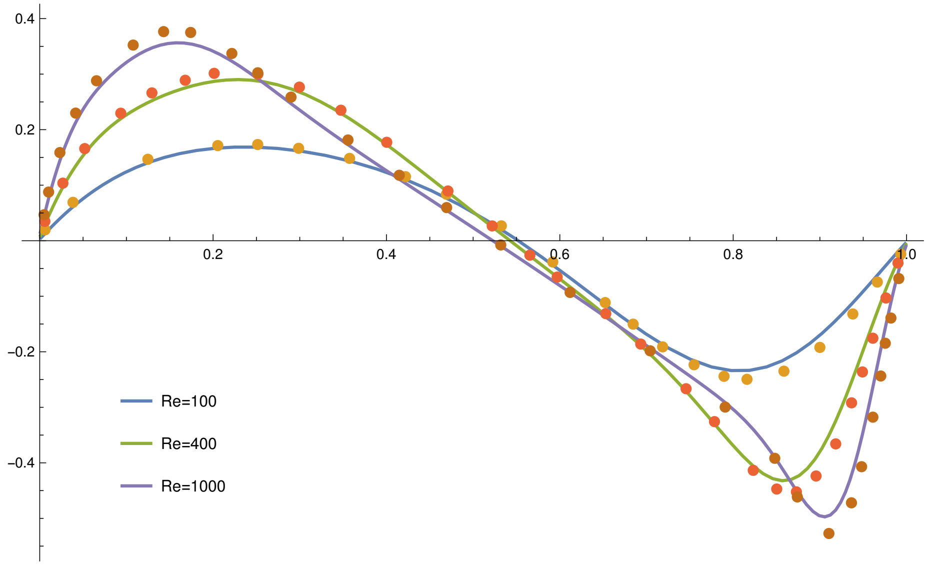
LB : 120×120 nodes, $HLB(5) \times HLB(5)$

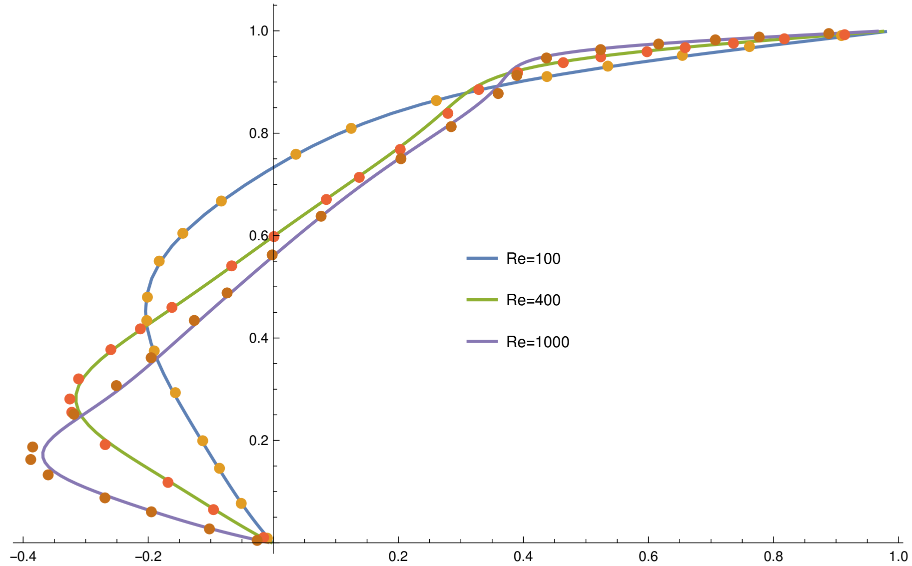
Ghia et al. (1982)

[1] Ghia et al., J. Computational Physics 48 (1982) 387

lid cavity : Navier - Stokes regime (velocity profiles)

LB velocity profiles (lines) through the horizontal and vertical centerlines of the square cavity, for various values of Re





$u_y(x, y = L/2)$ $u_x(x = L/2, y)$

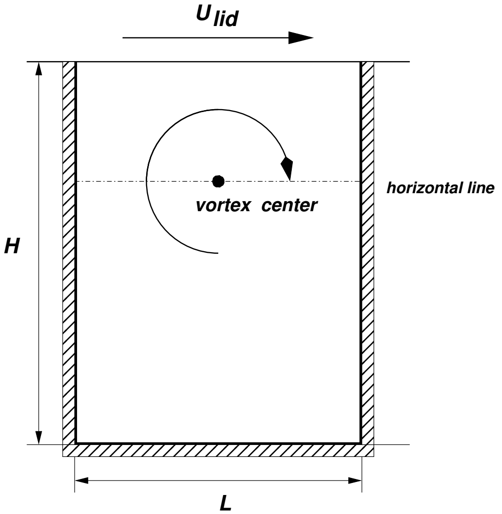
[1] Hu et al., Computers and Fluids (2017) http://dx.doi.org/10.1016/j.compfluid.2017.06.008
LB simulation (D2Q9) with 100×100 nodes

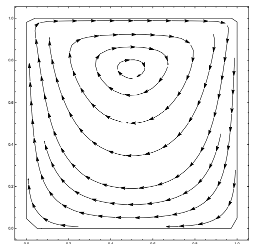
[2] Ghia et al., J. Computational Physics 48 (1982) 387

Lid cavity: comparison with Naris and Valougeorgis (2005)

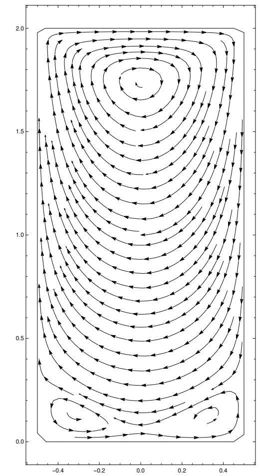
S.Naris and D.Valougeorgis
Physics of Fluids **17** (2015) 097106

DVM simulations – rarefied gas
rarefaction parameter $\delta \propto 1/Kn$



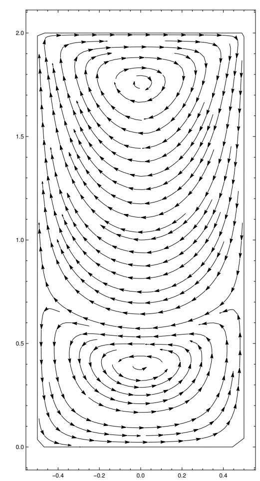


A=1
$\delta = 100$

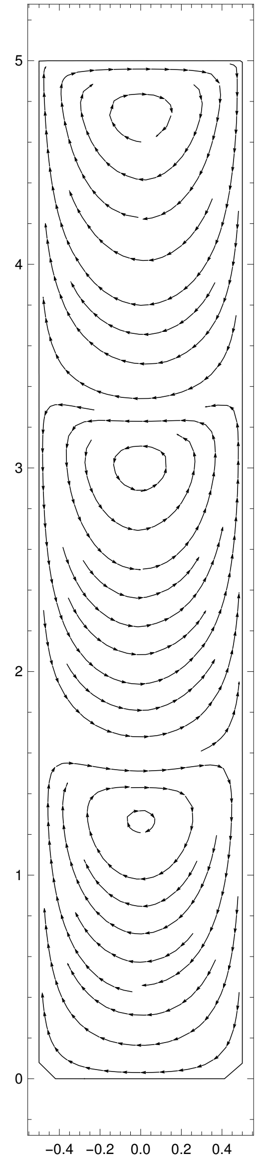


A=2
$\delta = 10$

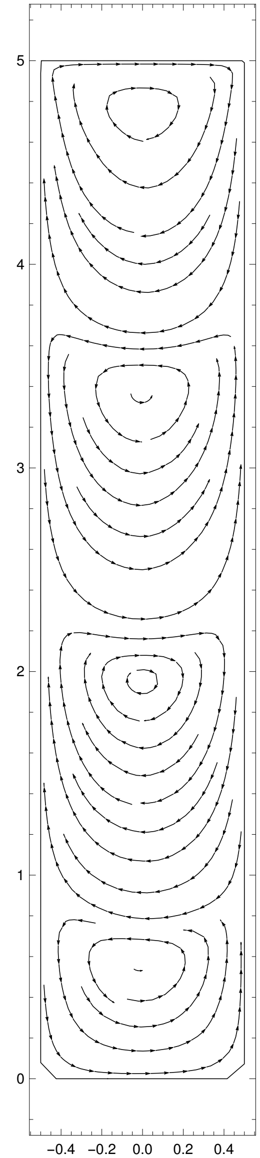
$A = 1$: single vortex also
for $\delta \in \{0.5, 1, 10\}$



A=2
$\delta = 100$



A=5
$\delta = 10$



A=5
$\delta = 100$

nondimensionalized quantities :

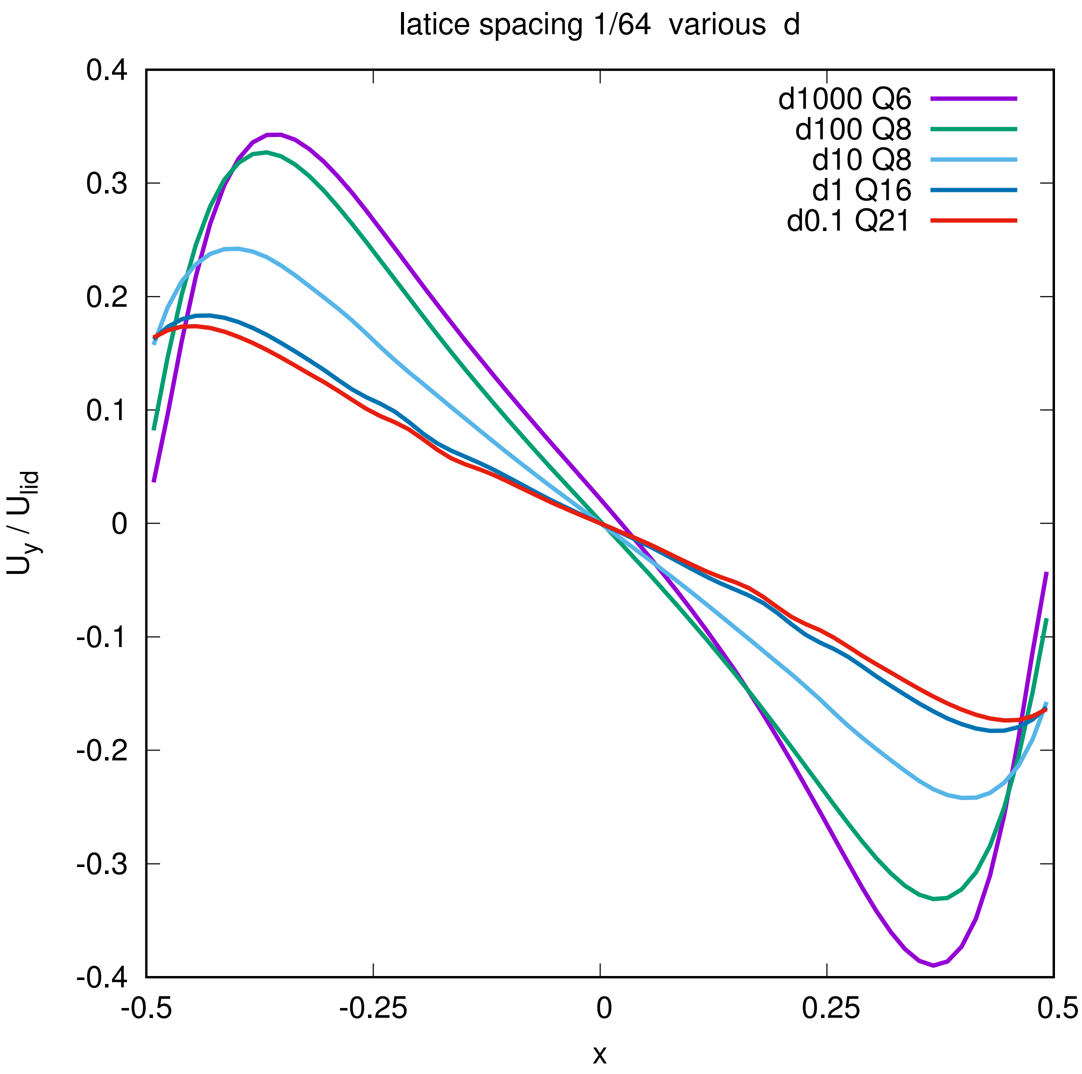
$U_{lid} = 0.01$ aspect ratio $A = H/L$

Lattice Boltzmann : relaxation time τ

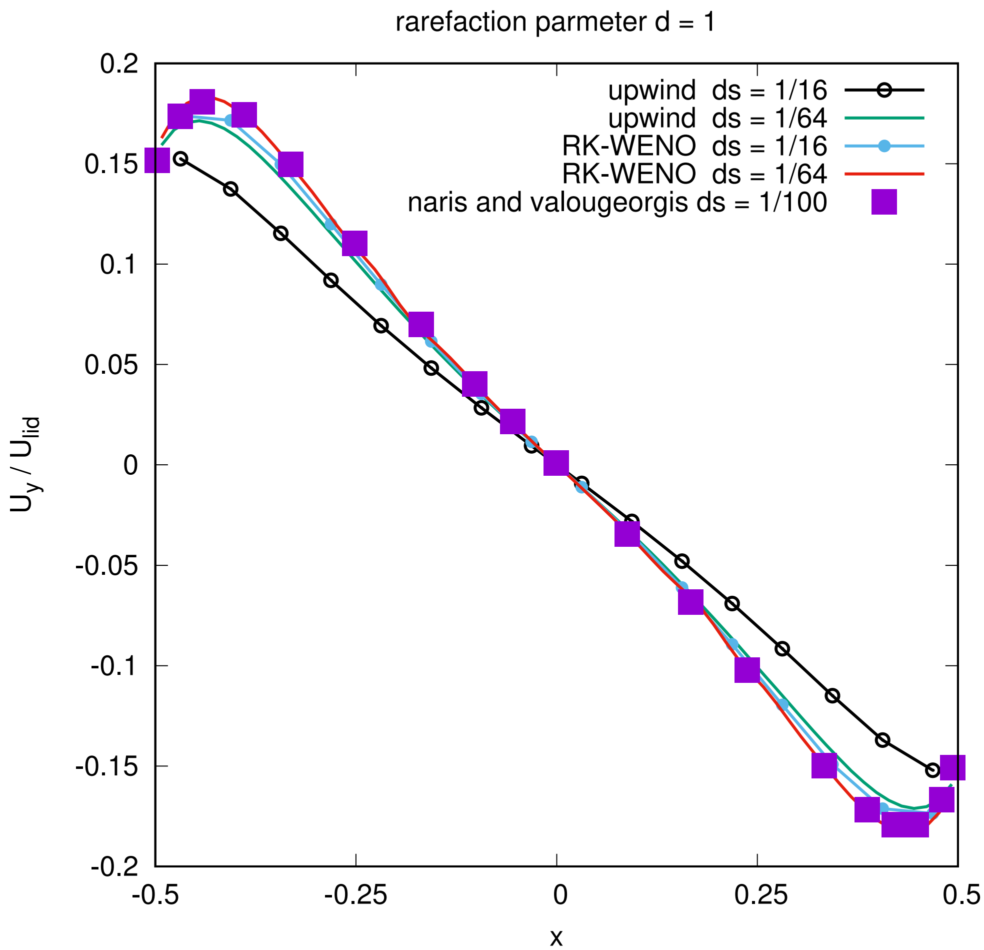
Naris and Valougeorgis : rarefaction parameter δ

$$\tau = 1/\delta\sqrt{2}$$

Lid cavity: $U_y(x)$ for $A = 1$ and various values of δ



Lid cavity: $U_y(x)$ for various numerical schemes $(A = 1)$



Comparison with S.Naris and D.Valougeorgis, Physics of Fluids **17** (2005) 097106

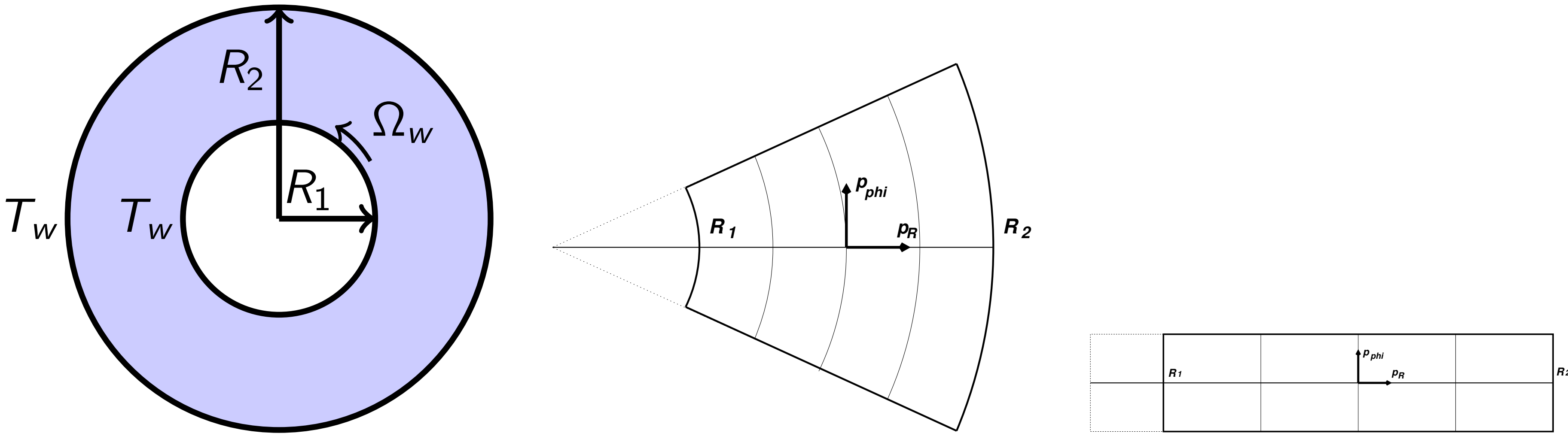


Figure: Circular Couette flow of angular velocity $\Omega_w = u_w^{\varphi}/R$.

In cylindrical coordinates, for homogeneous flow along the φ and z directions (where periodic boundary conditions apply), the Boltzmann equation reduces to:

$$\partial_t f + \underbrace{\frac{2p^{\hat{R}}}{m}\frac{\partial(fR)}{\partial R^2} + \frac{p^{\hat{\varphi}}}{mR}\frac{\partial f}{\partial \varphi}}_{\text{advection term}} = \underbrace{\overbrace{-\frac{1}{\tau}[f - f^{(\mathrm{eq})}]}^{\text{relaxation term}} \overbrace{- \frac{1}{mR}\left[(p^{\hat{\varphi}})^2 \frac{\partial f}{\partial p^{\hat{R}}} - p^{\hat{R}} \frac{\partial(f p^{\hat{\varphi}})}{\partial p^{\hat{\varphi}}}\right]}^{\text{inertial term}}}_{\text{source term}} \tag{1}$$

The advection term is implemented following Falle et al., Mon.Not.R.Astron.Soc. 278, 586-602 (1996).

Time stepping and advection

- The time stepping is implemented using the third order Runge-Kutta method (RK-3)[1] :

$$f(t+\delta t) = \frac{1}{3} f(t) + \frac{2}{3} f^{(2)} + \frac{2}{3} \delta t L[f^{(2)}] \qquad (L[f] = \partial_t f)$$

where $L[f] = \partial_t f$, $\quad f^{(1)} = f(t) + \delta t L[f(t)]$, $f^{(2)} = \frac{3}{4} f(t) + \frac{1}{4} f^{(1)} + \frac{1}{4} \delta t L[f^{(1)}]$

- The fluid domain is discretised using $N_R \times N_\varphi$ equidistant points:

$$R_s = R_1 + \left(s - \frac{1}{2}\right) \frac{R_2 - R_1}{N_R}, \qquad \varphi_\ell = \varphi_1 + \left(\ell - \frac{1}{2}\right) \frac{\varphi_2 - \varphi_1}{N_\varphi}, \tag{2}$$

- Implementation of the advection term involves radial / azimuthal WENO-5 fluxes[2]:

$$\begin{aligned} \left[\frac{2p^{\hat{R}}}{m} \frac{\partial (fR)}{\partial R^2}\right]_{s,\ell} &= 2 \frac{R_{s+1/2} \mathcal{F}^R_{s+1/2,\ell} - R_{s-1/2} \mathcal{F}^R_{s-1/2,\ell}}{R^2_{s+1/2} - R^2_{s-1/2}}, \\ \left[\frac{p^{\hat{\varphi}}}{mR} \frac{\partial f}{\partial \varphi}\right]_{s,\ell} &= \frac{1}{R_s} \frac{\mathcal{F}^{\varphi}_{s,\ell+1/2} - \mathcal{F}^{\hat{\varphi}}_{s,\ell-1/2}}{\varphi_{\ell+1/2} - \varphi_{\ell-1/2}}. \end{aligned} \tag{3}$$

[1] C.-W. Shu, S. Osher, J. Comput. P hys. **77** (1988) 439-471.
[2] G. S. Jiang and C. W. Shu, J. Comput. Phys. **126**, 202 (1996).

WENO-5 flux

- The fluxes are implemented using WENO-5:[3]

$$\mathcal{F}_{s+1/2} = \overline{\omega}_1 \mathcal{F}^1_{s+1/2} + \overline{\omega}_2 \mathcal{F}^2_{s+1/2} + \overline{\omega}_3 \mathcal{F}^3_{s+1/2}. \tag{4}$$

- The interpolating functions $\mathcal{F}^q_{s+1/2}$ are given by:

$$\begin{aligned}
\mathcal{F}^1_{s+1/2} =& V\left(\frac{1}{3}F_{s-2} - \frac{7}{6}F_{s-1} + \frac{11}{6}F_s\right), \\
\mathcal{F}^2_{s+1/2} =& V\left(-\frac{1}{6}F_{s-1} + \frac{5}{6}F_s + \frac{1}{3}F_{s+1}\right), \\
\mathcal{F}^3_{s+1/2} =& V\left(\frac{1}{3}F_s + \frac{5}{6}F_{s+1} - \frac{1}{6}F_{s+2}\right),
\end{aligned} \tag{5}$$

where $V = p^{\hat{R}}/m$ or $p^{\hat{\varphi}}/m$.

- The weighting factors $\overline{\omega}_q$ are defined as:

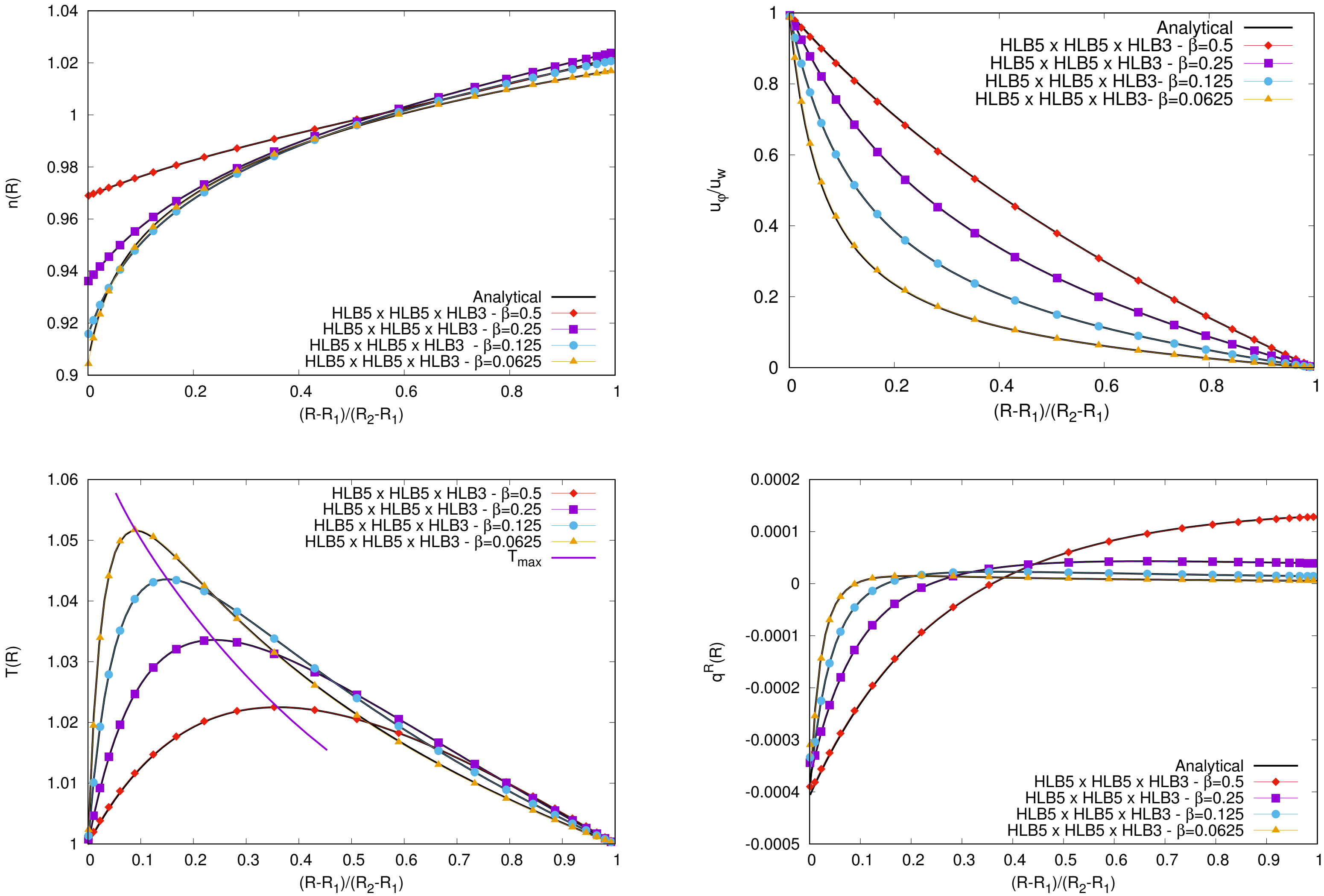
$$\overline{\omega}_q = \frac{\widetilde{\omega}_q}{\widetilde{\omega}_1 + \widetilde{\omega}_2 + \widetilde{\omega}_3}, \qquad \widetilde{\omega}_q = \frac{\delta_q}{\sigma_q^2}. \tag{6}$$

- The ideal weights δ_q are:

$$\delta_1 = 1/10, \qquad \delta_2 = 6/10, \qquad \delta_3 = 3/10, \tag{7}$$

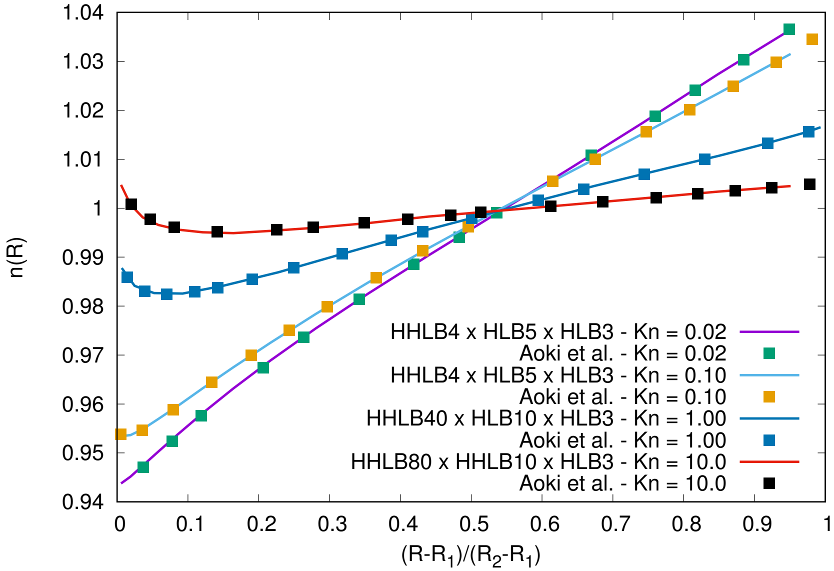
[3] G. S. Jiang and C. W. Shu, J. Comput. Phys. **126**, 202 (1996).

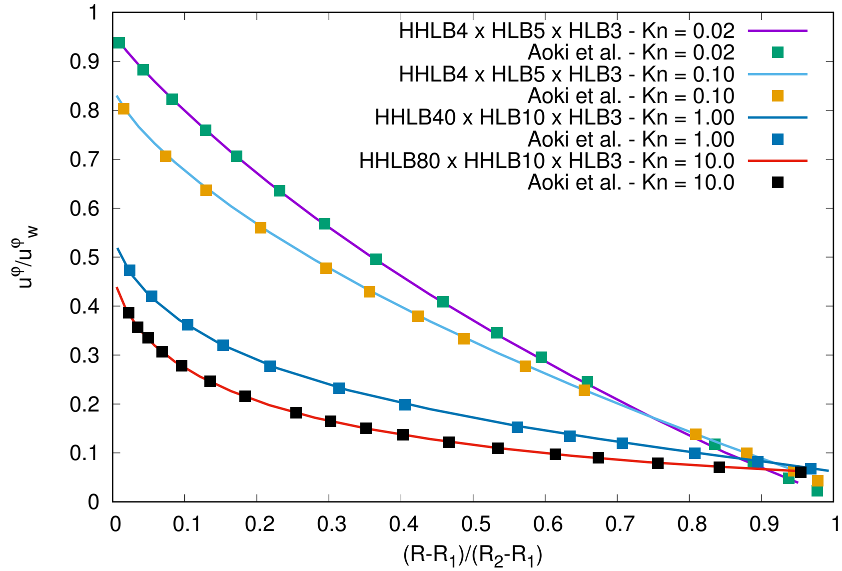
Hydrodynamic regime - $Kn \to 0$

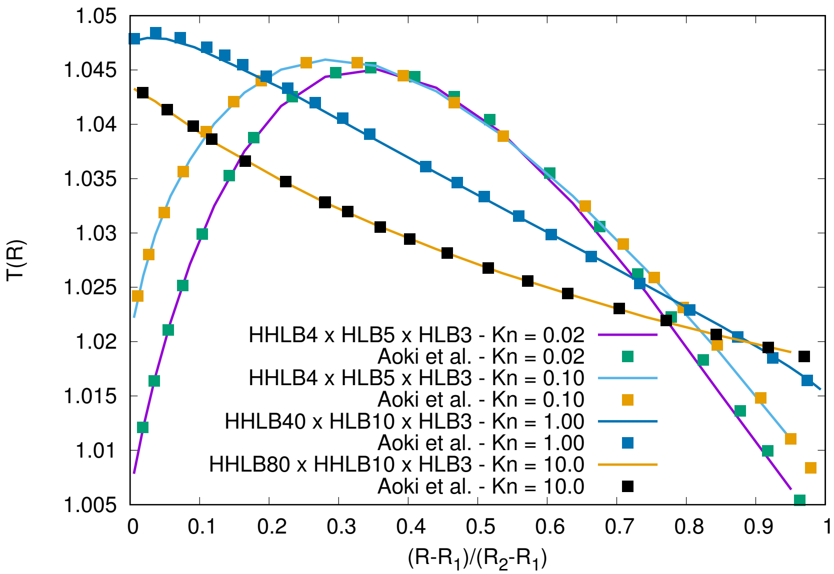


Profiles of number density, velocity, temperature and radial heat flux for the inner wall azimuthal velocity $u_w = 0.5$, wall temperature $T_w = 1.0$ and various values of $\beta = R_1/R_2$, $\delta t = 5 \times 10^{-4}$, number of nodes in the radial direction $N_R = 48$.

Circular Couette flow : transition regime

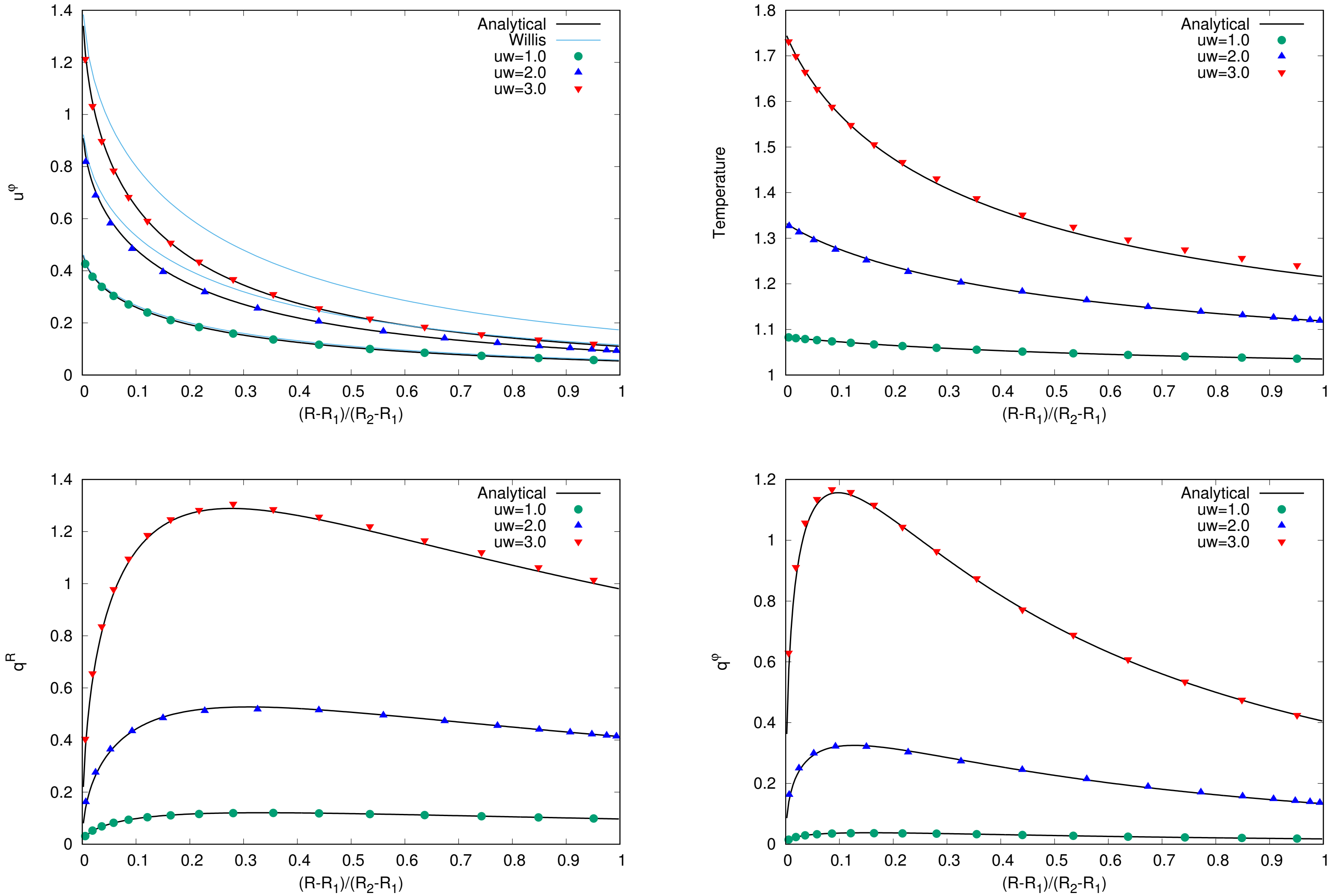






Comparison between our simulation results and those reported in K.Aoki, H.Yoshida, T.Nakanishi, and A. L. Garcia, Phys. Rev. E 68, 016302 (2003): number density $n(R)$; temperature $T(R)$; (c) normalised azimuthal velocity $u^{\hat{\varphi}}(R)/u^{\varphi}_{w}$. The angular velocity of the inner cylinder was set to $\Omega_{\rm in} = 0.5\sqrt{2}$, while the relaxation time was set to $\tau = {\rm Kn}\sqrt{\pi}/nT\sqrt{8}$ in order to conform with the parameters used by Aoki et al.

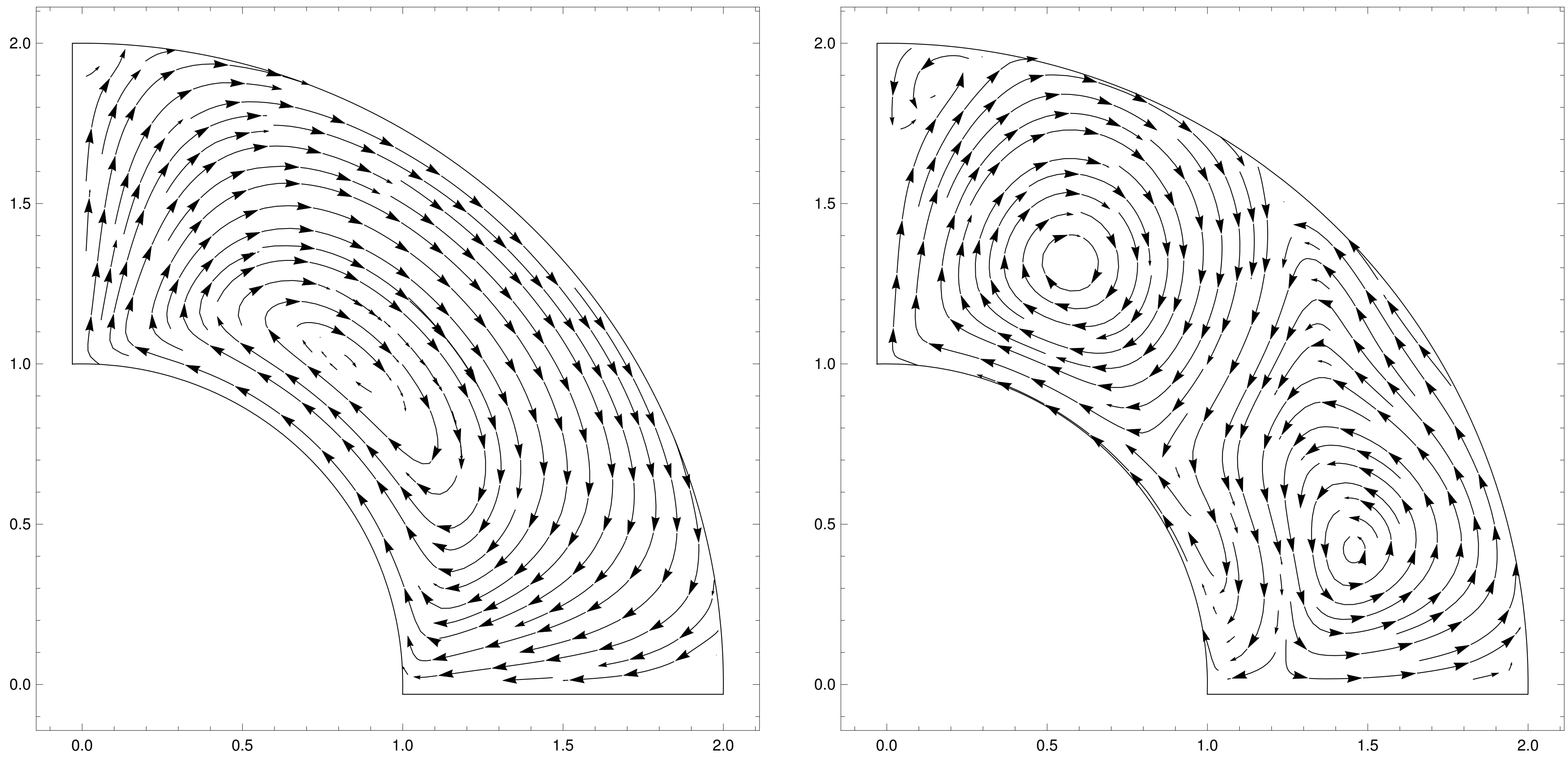
Free molecular flow regime - $Kn \to \infty$



Comparison between the results obtained with the model $HHLB(200) \times HHLB(10) \times HLB(3)$ and the analytic predictions in the ballistic regime, for various values of the azimuthal velocity u_w ($\beta = R_1/R_2 = 0.5$, $\delta t = 2 \times 10^{-5}$, number of nodes in the radial direction $N_R = 16$).

cylindrical Couette cavity $\varphi = 90^o$ $\tau = 10^{-3}$

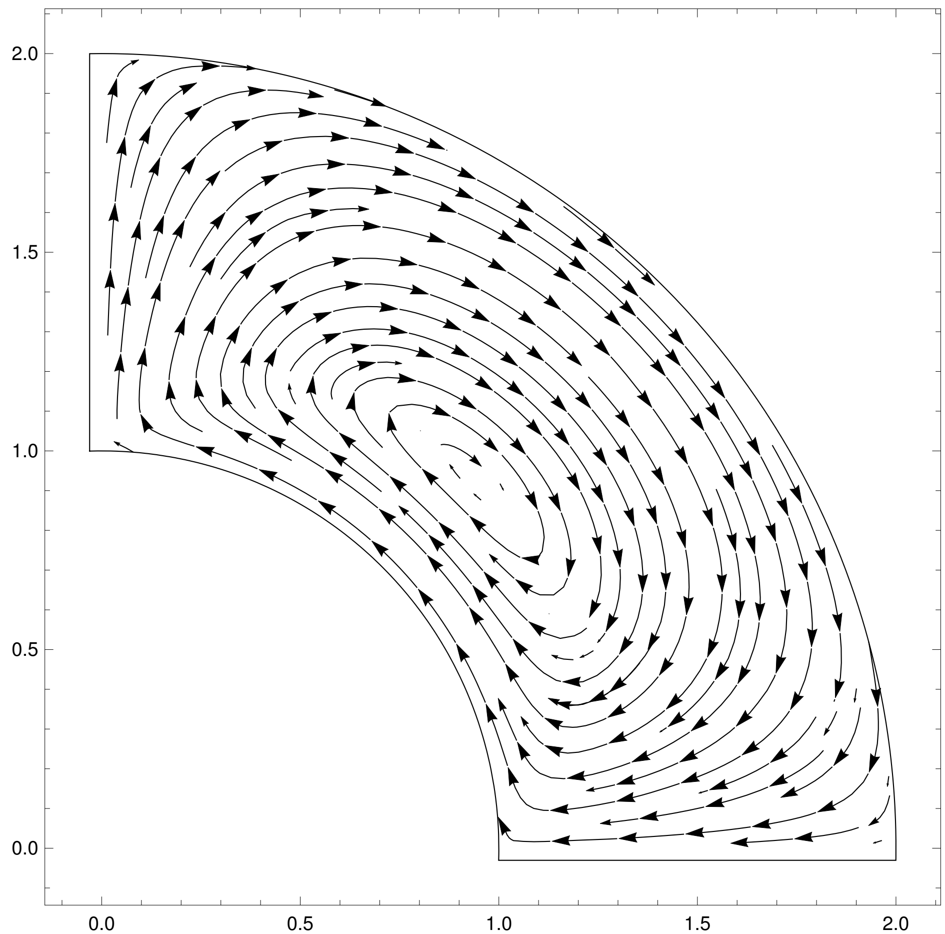
$R_1 = 1$ $R_2 = 2$ $u_\varphi(R_2) = 0$ $HLB(5) \times HLB(5)$

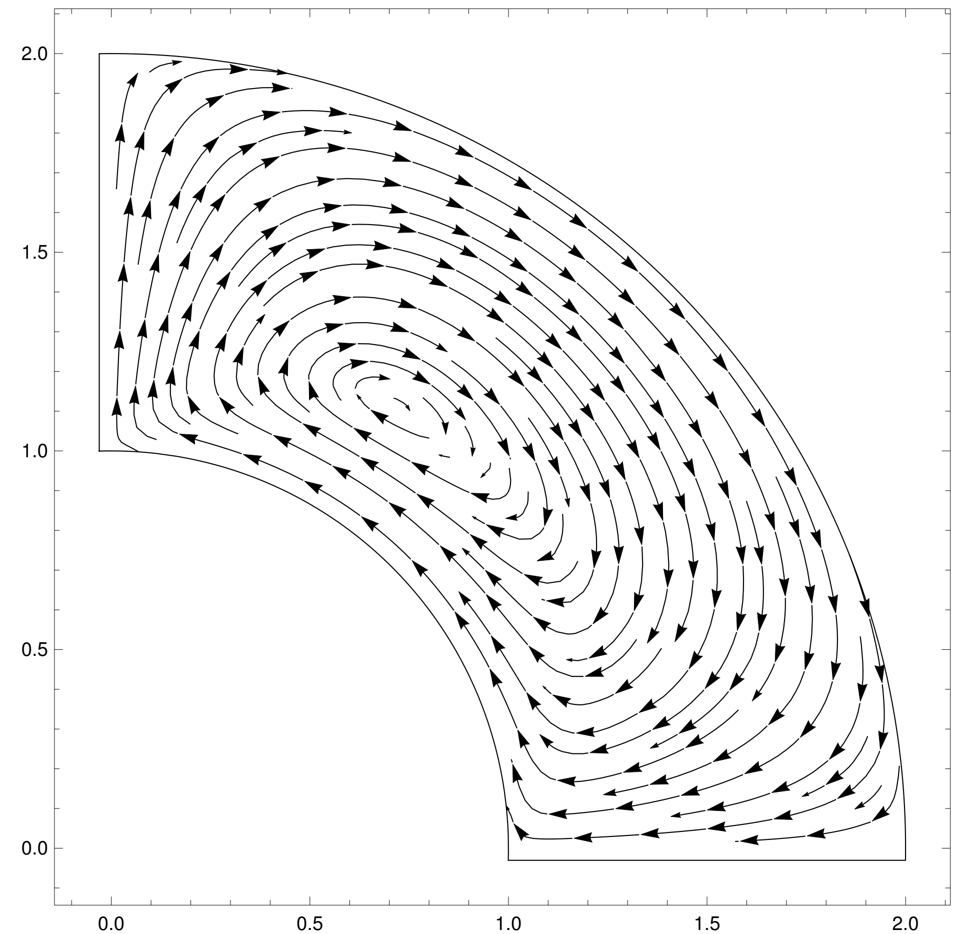


$u_\varphi(R_1) = 0.01$ $u_\varphi(R_2) = 1$

cylindrical Couette cavity $\varphi = 90^o$ $\tau = 10^{-1}$

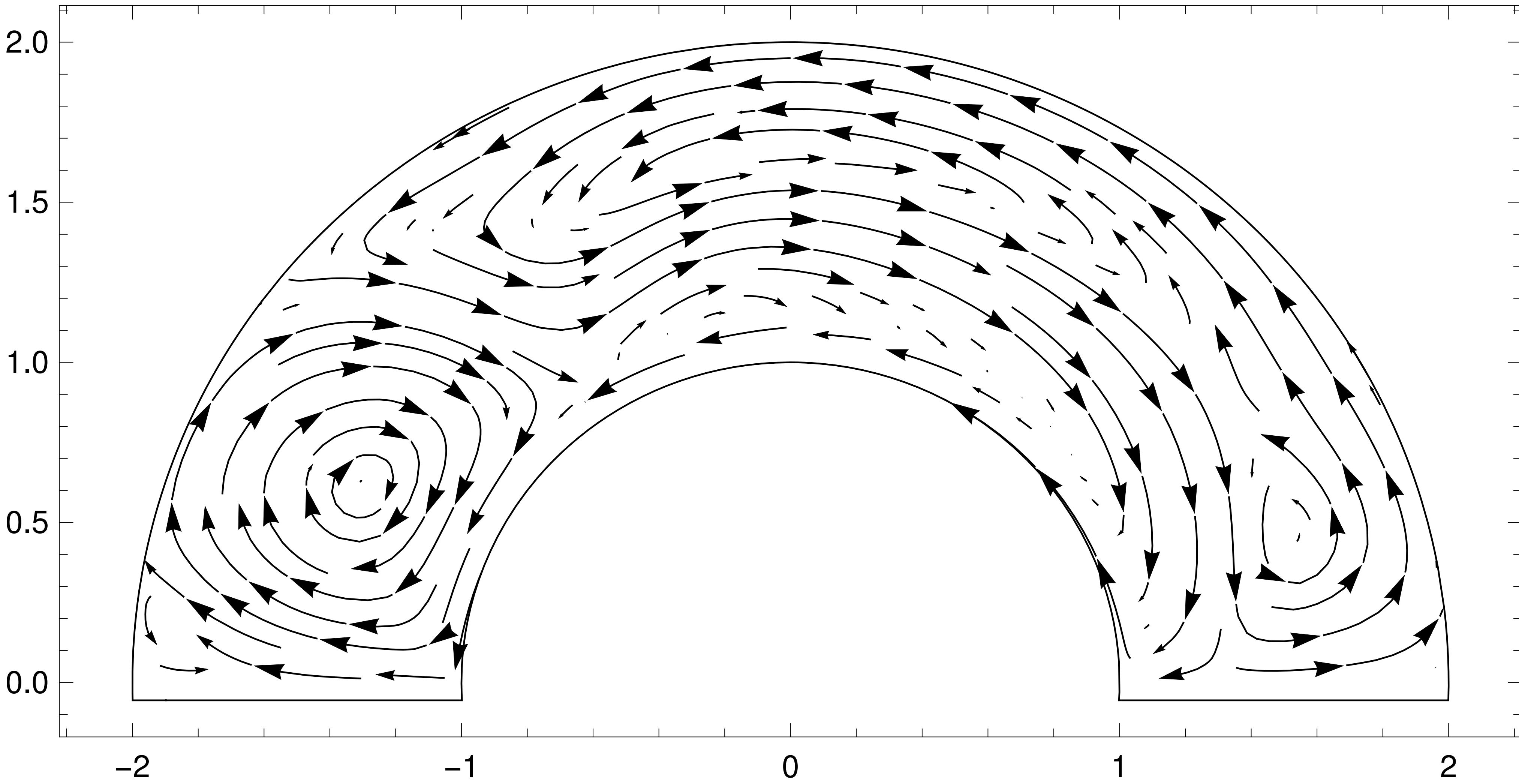
$R_{int} = 1$ $R_{ext} = 2$ $u_\varphi(R_2) = 0$ $HHLB(5) \times HHLB(5)$



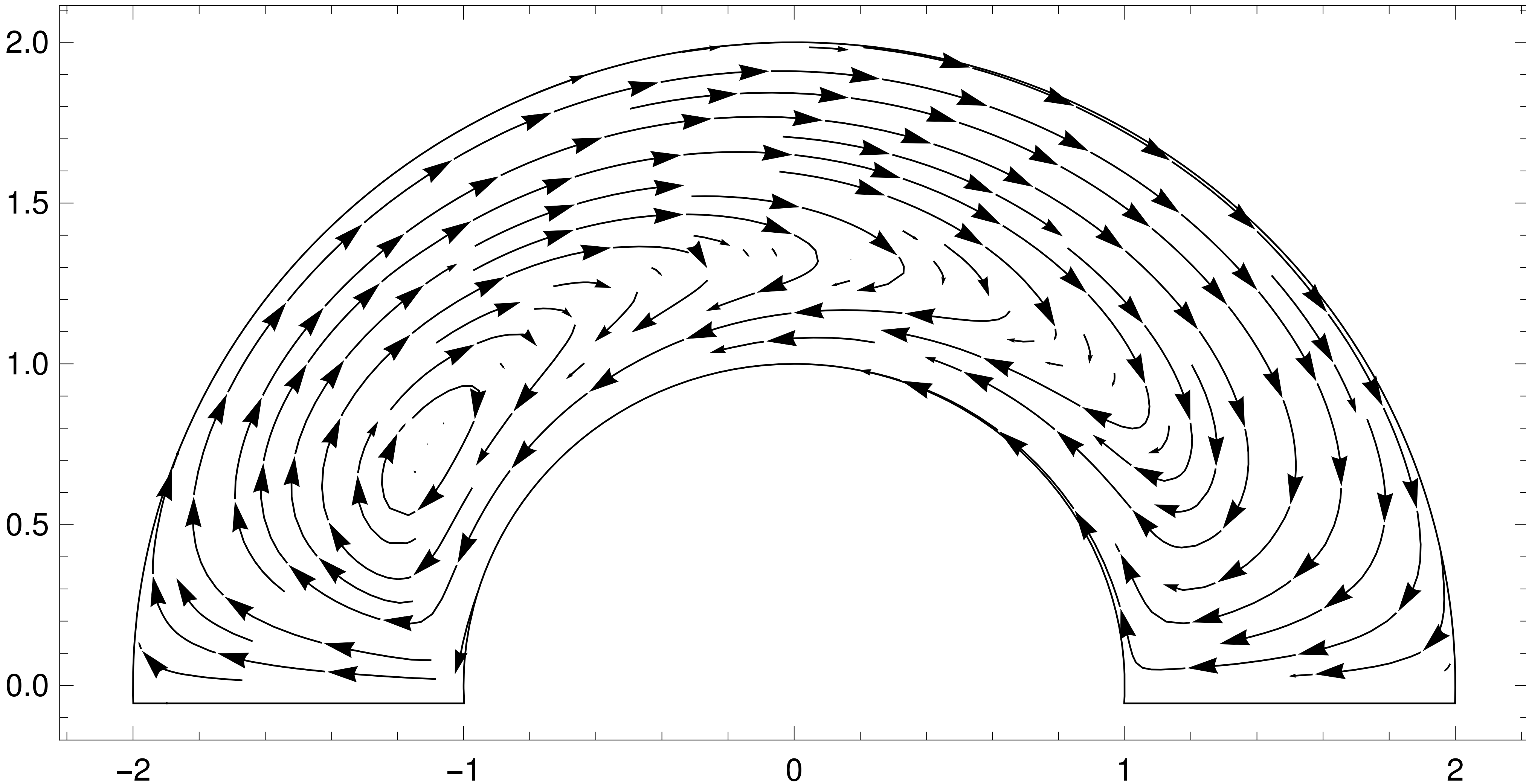


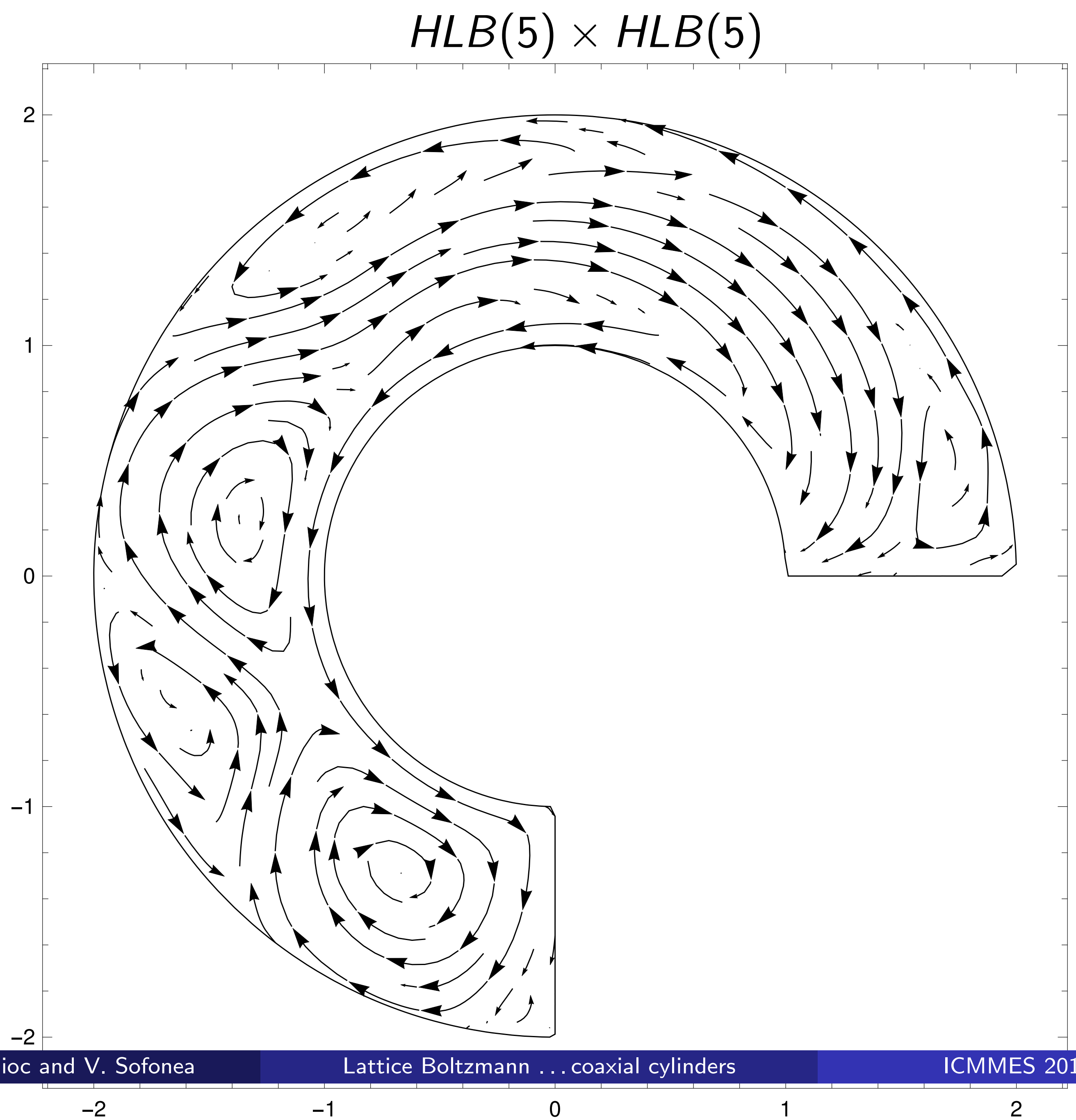
$u_\varphi(R_{int}) = 0.01$ $u_\varphi(R_{int}) = 1$

$$HLB(5) \times HLB(5)$$

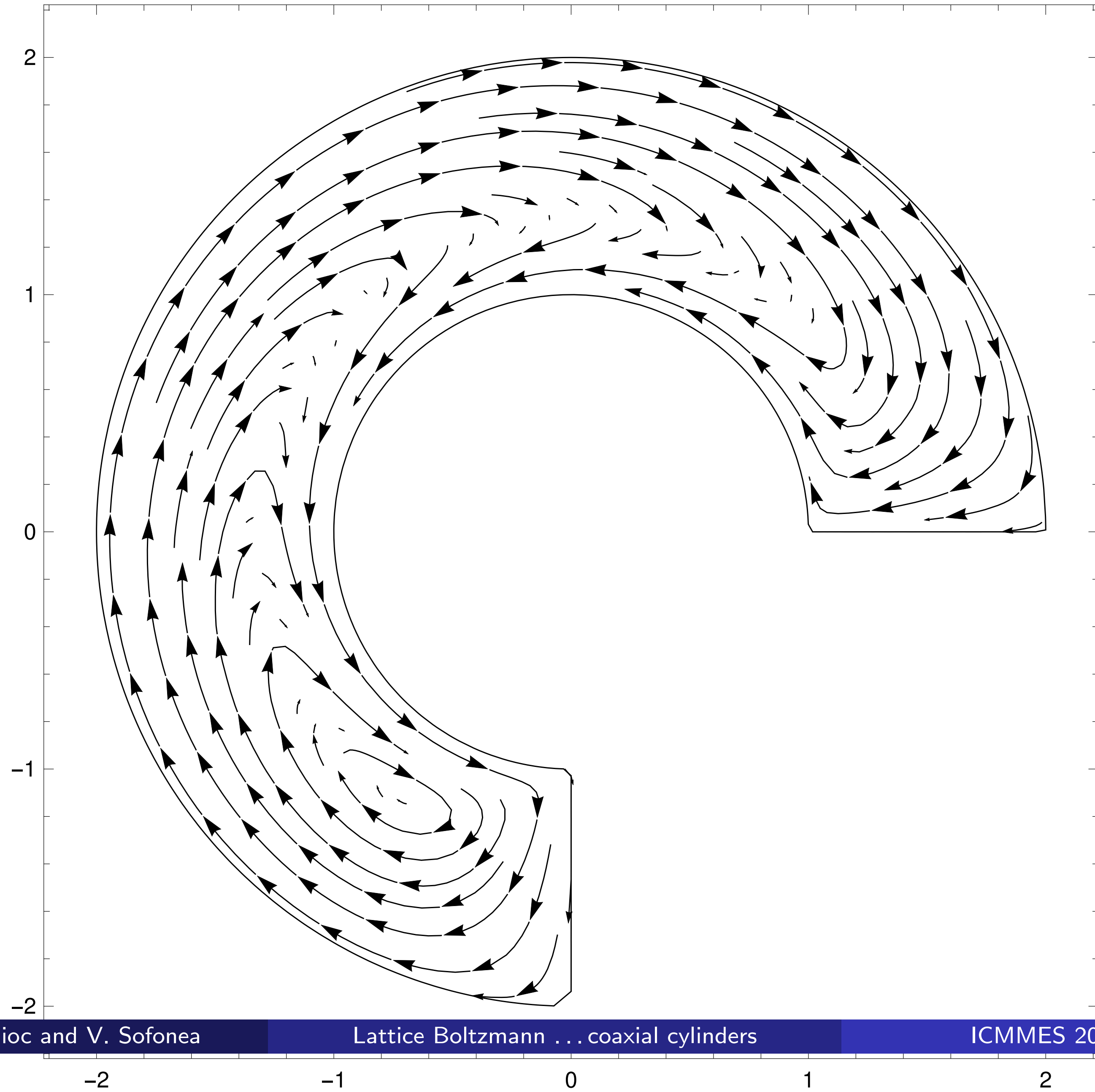


$$HHLB(5) \times HHLB(5)$$




$HLB(5) \times HLB(5)$
2
1
0
−1
−2
−2
−1
0
1
2

$HHLB(5) \times HHLB(5)$



Conclusion

- The use of the half-range Gauss Hermite quadrature in Lattice Boltzmann models allows one to ensure the recovery of the incoming and outgoing mass fluxes in the normal direction to a solid wall
- Half-range Lattice Boltzmann models (HHLB) work well throughout the whole range of the Knudsen number, as checked by comparison to DSMC, LB, DVM and analytical results
- Future work might be considered in order to address challenging microfluidics problems, expecially in complex geometries
- Comparison to experimental results, as well as to analytical results and / or other computer simulation results are needed to achive a better understanding of the physical processes at the micro scale
- Acknowledgments. This work was supported by grants from the Romanian National Authority for Scientific Research and Innovation, CNCS-UEFISCDI, project number PN-II-RU-TE-2014-4-2910