Flows of dense gases confined between two parallel plates

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Outline

1. The Enskog equation
2. The simplified Enskog collision operator
3. The Finite-Difference Lattice Boltzmann algorithm
4. Numerical results:
   - Fourier flow
   - Couette flow
   - Poisseuille flow

The Enskog equation

- The dynamics of the system of particles can be described by the following *exact* kinetic equation:

$$\frac{\partial f}{\partial t} + \boldsymbol{v} \cdot \nabla_{\boldsymbol{r}} f = \sigma^2 \int_{\mathbb{R}^3} d\boldsymbol{v}_* \int_{\mathcal{S}_+} d^2\hat{\boldsymbol{k}} \left\{ f_2(\boldsymbol{r}, \boldsymbol{v}', \boldsymbol{r} + \sigma\hat{\boldsymbol{k}}, \boldsymbol{v}'_*) - f_2(\boldsymbol{r}, \boldsymbol{v}, \boldsymbol{r} - \sigma\hat{\boldsymbol{k}}, \boldsymbol{v}_*) \right\} (\boldsymbol{v}_r \cdot \hat{\boldsymbol{k}}).$$

- Let us now make the following *simplifying* assumption:
  - Short-range correlations are taken into account as in Enskog theory:

$$f_2(\boldsymbol{r}, \boldsymbol{v}, \boldsymbol{r} \pm d\hat{\boldsymbol{k}}, \boldsymbol{v}_*, t) = \chi\left[n\left(\boldsymbol{r} \pm \frac{\sigma}{2}\hat{\boldsymbol{k}}\right)\right] f(\boldsymbol{r}, \boldsymbol{v}, t) f(\boldsymbol{r} \pm \sigma\hat{\boldsymbol{k}}, \boldsymbol{v}_*, t).$$

  where χ is the contact value of the pair correlation function of a hard sphere fluid.

The Enskog equation

The right-hand side is given by the Enskog collision operator J_E which reads[1]:

$$J_E = \sigma^2 \int \left\{ \chi\left(\boldsymbol{x} + \frac{\sigma}{2}\boldsymbol{k}\right) f(\boldsymbol{x}, \boldsymbol{p}^*) f(\boldsymbol{x} + \sigma\boldsymbol{k}, \boldsymbol{p}_1^*) - \chi\left(\boldsymbol{x} - \frac{\sigma}{2}\boldsymbol{k}\right) f(\boldsymbol{x}, \boldsymbol{p}) f(\boldsymbol{x} - \sigma\boldsymbol{k}, \boldsymbol{p}_1) \right\} (\boldsymbol{p}_r \cdot \boldsymbol{k}) d\boldsymbol{k} d\boldsymbol{p}_1 \quad (1)$$

where σ is the molecular diameter. $\boldsymbol{p}_r = \boldsymbol{p}_1 - \boldsymbol{p}$ is the relative momentum and $\boldsymbol{k}$ is the unit vector giving the relative position of the two colliding particles.
The contact value of the pair correlation function:

$$\chi = \chi_{\text{SET}}\left(n\left(\boldsymbol{r} \pm \frac{a}{2}\hat{\boldsymbol{k}}\right)\right) = \frac{1}{nb}\left(\frac{p^{CS}}{nk_B T} - 1\right) = \frac{1}{2}\frac{2-\eta}{(1-\eta)^3}; \; b = \frac{2\pi\sigma^3}{3}; \; \eta = \frac{\pi\sigma^3 n}{6}. \quad (2)$$

where $p^{CS} = nk_B T \frac{1+\eta+\eta^2-\eta^3}{(1-\eta)^3}$.

[1] G. M. Kremer, An introduction to the Boltzmann equation and transport processes in gases (Springer-Verlag, Berlin Heidelberg, 2010).

The Enskog equation

- Revised Enskog Theory (RET): value of the pair correlation function in a fluid in *non-uniform equilibrium* with density at the contact point.

Fischer-Methfessel approximation	$\rightsquigarrow \quad \chi = \chi_{\text{RET-FM}}\left[n\left(\boldsymbol{r} \pm \frac{\sigma}{2}\hat{\boldsymbol{k}}\right)\right] = \chi_{\text{SET}}\left(\overline{n}\left(\boldsymbol{r} \pm \sigma\frac{\hat{\boldsymbol{k}}}{2}\right)\right).$

where

$$\overline{n}\,(\boldsymbol{r}, t) = \frac{3}{4\pi\sigma^3}\int_S n(\boldsymbol{r}_1, t) w(\boldsymbol{r}, \boldsymbol{r}_1)\, d\boldsymbol{r}_1, \qquad w(\boldsymbol{r}, \boldsymbol{r}_1) = \begin{cases} 1, & \|\boldsymbol{r}_1 - \boldsymbol{r}\| < \sigma \\ 0, & \|\boldsymbol{r}_1 - \boldsymbol{r}\| > \sigma \end{cases}.$$

The simplified Enskog collision operator

By assuming that the factor χ and the distribution functions are smooth functions one can approximate these functions in the Enskog collision integral through a Taylor series near the point $\boldsymbol{x}$. The resulting terms up first order gradient are[1]:

$$J_0(f,f) = \chi \int (f^* f_1^* - f f_1) \Omega^2 (\boldsymbol{p_r} \cdot \boldsymbol{k}) d\boldsymbol{k} d\boldsymbol{p_1} \quad (3)$$

$$J_1(f,f) = \chi\sigma \int \boldsymbol{k} (f^* \boldsymbol{\nabla} f_1^* - f \boldsymbol{\nabla} f_1) \Omega^2 (\boldsymbol{p_r} \cdot \boldsymbol{k}) d\boldsymbol{k} d\boldsymbol{p_1} + \frac{\sigma}{2} \int \boldsymbol{k} \boldsymbol{\nabla} \chi (f^* f_1^* - f f_1) \Omega^2 (\boldsymbol{p_r} \cdot \boldsymbol{k}) d\boldsymbol{k} d\boldsymbol{p_1} \quad (4)$$

The collision term $J_0(f,f)$ is the usual collision term of the Boltzmann equation.

[1] G. M. Kremer, An introduction to the Boltzmann equation and transport processes in gases (Springer-Verlag, Berlin Heidelberg, 2010).

The simplified Enskog collision operator

The collision term $J_0(f,f)$ is treated applying the usual relaxation time approximation. In this paper we will employ the Shakhov collision term[1], namely:

$$J_0(f,f) = -\frac{1}{\tau}(f - f^S), \tag{5}$$

where τ is the relaxation time and f_S is the equilibrium Maxwell-Boltzmann distribution times a correction factor[1]:

$$f^S = f_{\text{MB}}\left[1 + \frac{1-\text{Pr}}{P_i k_B T}\left(\frac{\boldsymbol{\xi}^2}{5mk_BT} - 1\right)\boldsymbol{\xi}\cdot\boldsymbol{q}\right], \quad \boldsymbol{q} = \int d^3p f \frac{\boldsymbol{\xi}^2}{2m}\frac{\boldsymbol{\xi}}{m}, \tag{6}$$

where $\boldsymbol{\xi} = \boldsymbol{p} - m\boldsymbol{u}$ is the peculiar momentum, $\text{Pr} = c_P\mu/\lambda$ is the Prandtl number, $c_P = 5k_B/2m$ is the specific heat at constant pressure and $P_i = \rho RT = nk_BT$ is the ideal gas equation of state, with R being the specific gas constant. The Maxwell-Boltzmann distribution f_{MB} is given by:

$$f_{\text{MB}} = \frac{n}{(2m\pi k_BT)^{3/2}}\exp\left(-\frac{\boldsymbol{\xi}^2}{2mk_BT}\right) \tag{7}$$

[1] E. Shakhov, “Approximate kinetic equations in rarefied gas theory”, Fluid Dynamics 3, 95 – 96 (1968).

The simplified Enskog collision operator

The second term of J_E, namely $J_1(f,f)$, can be approximated by replacing the distribution functions (f^*, f_1^*, f, f_1) with the corresponding equilibrium distribution functions. By using $f^*_{\text{MB}} f^*_{\text{MB},1} = f_{\text{MB}} f_{\text{MB},1}$, and integrating over $\boldsymbol{k}$ and $\boldsymbol{p_1}$, one obtains[1]:

$$J_1(f,f) \approx J_1(f_{\text{MB}}, f_{\text{MB}}) = - b\rho\chi f_{\text{MB}} \left\{ \boldsymbol{\xi} \left[\boldsymbol{\nabla} \ln(\rho^2 \chi T) + \frac{3}{5}\left(\zeta^2 - \frac{5}{2}\right) \boldsymbol{\nabla} \ln T \right] + \frac{2}{5}\left[2\boldsymbol{\zeta}\boldsymbol{\zeta} : \boldsymbol{\nabla u} + \left(\zeta^2 - \frac{5}{2}\right) \boldsymbol{\nabla} \cdot \boldsymbol{u} \right] \right\} \quad (8)$$

where $\zeta = \boldsymbol{\xi}/\sqrt{2RT}$.
With the above approximations and considering no external force, the Enskog equation becomes:

$$\frac{\partial f}{\partial t} + \frac{\boldsymbol{p}}{m} \nabla_{\boldsymbol{x}} f = -\frac{1}{\tau}(f - f_S) + J_1(f_{\text{MB}}, f_{\text{MB}}) \quad (9)$$

[1] G. M. Kremer, An introduction to the Boltzmann equation and transport processes in gases (Springer-Verlag, Berlin Heidelberg, 2010).

The simplified Enskog collision operator

Multiplying the Enskog equation with the collision invariants 1, $\boldsymbol{p}$ and $\boldsymbol{p}^2/2m$ and integrating over the momentum space yields the following conservation equations for mass, momentum and energy[1]:

$$\frac{D\rho}{Dt} + \rho\nabla\boldsymbol{u} = 0 \tag{10a}$$

$$\rho\frac{D\boldsymbol{u}}{Dt} + \nabla P = -\nabla\cdot\Pi \tag{10b}$$

$$\rho\frac{De}{Dt} + P\nabla\cdot\boldsymbol{u} = -\nabla\cdot\boldsymbol{q} + \Pi : \nabla\boldsymbol{u} \tag{10c}$$

where $D/Dt = \partial_t + \boldsymbol{u}\cdot\nabla$ is the material derivative and $P = P_i(1 + b\rho\chi)$ is the equation of state of a non-ideal gas. The heat flux $\boldsymbol{q}$ and the viscous part of the stress tensor $\Pi_{\alpha\beta}$ are given by:

$$\boldsymbol{q} = -\lambda\nabla T; \quad \Pi = -\mu_v\mathcal{I}\boldsymbol{\nabla}\cdot\boldsymbol{u} - \mu\left(\nabla u + (\nabla u)^T - \frac{2}{3}\mathcal{I}\boldsymbol{\nabla}\cdot\boldsymbol{u}\right) \tag{11}$$

where $\mathcal{I}$ is the identity matrix.

[1] G. M. Kremer, An introduction to the Boltzmann equation and transport processes in gases (Springer-Verlag, Berlin Heidelberg, 2010).

The simplified Enskog collision operator

The bulk viscosity μ_v, shear viscosity μ and the thermal conductivity λ are given by[1]:

$$\mu_v = \frac{16}{5\pi}\mu_0 b^2\rho^2\chi, \tag{12a}$$

$$\mu = \tau P_i = \mu_0 b\rho\left(\frac{1}{b\rho\chi} + 0.8 + \frac{4}{25}\left(1 + \frac{12}{\pi}\right)b\rho\chi\right), \tag{12b}$$

$$\lambda = \frac{5}{2}\frac{\tau P_i}{\mathrm{Pr}} = \lambda_0 b\rho\left(\frac{1}{b\rho\chi} + 1.2 + \frac{9}{25}\left(1 + \frac{32}{9\pi}\right)b\rho\chi\right), \tag{12c}$$

where $\mu_0 = \mu_{\text{ref}}\sqrt{T/T_0}$ is the viscosity coefficient for hard sphere molecules, with μ_{ref} representing the viscosity coefficient for dilute gases at temperature T_0, and $\lambda_0 \equiv \lambda_{\text{ref}}$ is the reference thermal conductivity at temperature T_0. The reference values are:

$$\mu_{\text{ref}} = \frac{5}{16\sigma^2}\sqrt{\frac{mk_BT_0}{\pi}}, \qquad \lambda_{\text{ref}} = \frac{75k_B}{64m\sigma^2}\sqrt{\frac{mk_BT_0}{\pi}}. \tag{13}$$

[1] G. M. Kremer, An introduction to the Boltzmann equation and transport processes in gases (Springer-Verlag, Berlin Heidelberg, 2010).

The simplified Enskog collision operator

For the dense gas the Prandtl number is:

$$\mathrm{Pr} = \frac{2}{3}\,\frac{1 + \frac{4}{5}b\rho\chi + \frac{4}{25}\left(1 + \frac{12}{\pi}\right)(b\rho\chi)^2}{1 + \frac{6}{5}b\rho\chi + \frac{9}{25}\left(1 + \frac{32}{9\pi}\right)(b\rho\chi)^2}. \tag{14}$$

The Chapman-Enskog expansion of Eq. (9) gives the relations between the relaxation time τ and the transport coefficients. It follows that the relaxation time τ is given by:

$$\tau = \frac{\mu}{P_i} \tag{15}$$

Note that the viscosity of the dense gas of a fixed reduced density η can be changed by varying the molecular diameter σ and the number density n. By using the reference mean free path $l = m/\sqrt{2}\pi\sigma^2 n\chi$, one can define the Knudsen number as:

$$Kn = \frac{1}{\sqrt{2}\pi\sigma^2 n\chi(n)L} \tag{16}$$

Reduced distributions - 1D flows

The y and z degrees of freedom can be integrated out and two reduced distribution functions, ϕ and θ, can be introduced as[2]:

$$\phi_{1\mathrm{D}}(\boldsymbol{x}, p_x, t) = \int dp_y dp_z f(\boldsymbol{x}, \boldsymbol{p}, t), \quad \theta_{1\mathrm{D}}(\boldsymbol{x}, p_x, t) = \int dp_y dp_z \frac{p_y^2 + p_z^2}{m} f(\boldsymbol{x}, \boldsymbol{p}, t) \tag{17}$$

The macroscopic quantities are given by:

$$\begin{pmatrix} n \\ \rho u_x \\ \Pi_{xx} \end{pmatrix} = \int dp_x \begin{pmatrix} 1 \\ p_x \\ \frac{\xi_x^2}{m} \end{pmatrix} \phi_{1\mathrm{D}}, \tag{18}$$

$$\begin{pmatrix} \frac{3}{2} n k_B T \\ q_x \end{pmatrix} = \int dp_x \begin{pmatrix} 1 \\ \frac{\xi_x}{m} \end{pmatrix} \left(\frac{\xi_x^2}{2m} \phi_{1\mathrm{D}} + \frac{1}{2} \theta_{1\mathrm{D}} \right) \tag{19}$$

The evolution equations for the reduced distribution functions are:

$$\frac{\partial}{\partial t} \begin{pmatrix} \phi_{1\mathrm{D}} \\ \theta_{1\mathrm{D}} \end{pmatrix} + \frac{p_x}{m} \frac{\partial}{\partial x} \begin{pmatrix} \phi_{1\mathrm{D}} \\ \theta_{1\mathrm{D}} \end{pmatrix} = -\frac{1}{\tau} \begin{pmatrix} \phi_{1\mathrm{D}} - \phi_{1\mathrm{D}}^S \\ \theta_{1\mathrm{D}} - \theta_{1\mathrm{D}}^S \end{pmatrix} + \begin{pmatrix} J_1^{\phi_{1\mathrm{D}}} \\ J_1^{\theta_{1\mathrm{D}}} \end{pmatrix} \tag{20}$$

[2] V. E. Ambrus and V. Sofonea, "Quadrature-based lattice Boltzmann models, for rarefied gas flow," in Flowing Matter, (Springer International Publishing, Cham, 2019) pp. 271–299.

Reduced distributions - 1D flows

In the above the, ϕ_S and θ_S are given by:

$$\phi_S = f^x_{\text{MB}}\left[1 + \frac{1-\text{Pr}}{5P_i m k_B T}\left(\frac{\xi_x^2}{mk_BT} - 3\right)\xi_x q_x\right],$$

$$\theta_S = 2k_BTf^x_{\text{MB}}\left[1 + \frac{1-\text{Pr}}{5P_i m k_B T}\left(\frac{\xi_x^2}{mk_BT} - 1\right)\xi_x q_x\right]$$

while the first order corrections J_1^ϕ and J_1^θ are:

$$J_1^{\phi_{1\text{D}}} = -\left[\xi_x\partial_x \ln\chi + 2\xi_x\partial_x\ln\rho + \frac{3}{5}\left(\frac{\xi_x^2}{mk_BT} - 1\right)\partial_x u_x \right.$$
$$\left. + \frac{3}{10}\left(\frac{\xi_x^3}{m^2k_BT} + \frac{\xi_x}{3m}\right)\partial_x \ln T\right] f_x^{\text{MB}} b\rho\chi \qquad \text{(21a)}$$

$$J_1^{\theta_{1\text{D}}} = -\left[\xi_x\partial_x \ln\chi + 2\xi_x\partial_x\ln\rho + \frac{3}{5}\left(\frac{\xi_x^2}{mK_BT} - \frac{1}{3}\right)\partial_x u_x \right.$$
$$\left. + \frac{3}{10}\left(\frac{\xi_x^3}{m^2k_BT} + \frac{7\xi_x}{3m}\right)\partial_x \ln T\right] 2mk_BTf_x^{\text{MB}} b\rho\chi \qquad \text{(21b)}$$

Finite difference Lattice Boltzmann

We introduce the notation $\psi \in \{\phi, \theta\}$ to represent the reduced distributions, and the macroscopic quantities are evaluated by replacing the integrals with quadrature sums. The distribution function ψ is projected on a set of Hermite polynomials up to order N[3]:

$$\psi(x,p,t) \equiv \psi^N(x,p,t) = \omega(p_k) \sum_{\ell=0}^{N} \frac{1}{\ell!} a_\ell(x,t) H_\ell(p_k), \quad a_\ell(x,t) = \int dp \psi(x,p,t) H_\ell(p)$$

The momentum set $\{p_k\}$ has $Q \geq Q_{\text{min}}$ elements that belong to the set $\{r_k\}$, $1 \leq k \leq Q$, of the roots of the full-range/half-range Hermite polynomial $H_Q(p)$ and the their associated weights w_k given by

$$w_k = \frac{Q!}{[H_{Q+1}(r_k)]^2}, \quad w_k^{\mathfrak{h}} = \frac{p_k a_Q^2}{\mathfrak{h}_{Q+1}^2(p_k)\left[p_k + \mathfrak{h}_{Q,0}^2/\sqrt{2\pi}\right]}, \tag{22}$$

where $a_Q = \mathfrak{h}_{Q+1,Q+1}/\mathfrak{h}_{Q,Q}$ and $\mathfrak{h}_{\ell,s}$ represents the coefficient of p^s in $\mathfrak{h}_\ell(p)$:

$$\mathfrak{h}_\ell(p) = \sum_{s=0}^{\ell} \mathfrak{h}_{\ell,s} p^s. \tag{23}$$

[3] X. Shan, X.-F. Yuan, and H. Chen, Journal of Fluid Mechanics 550, 413–441 (2006)

$f^{(\mathrm{eq})}$ truncated expansion

The equilibrium functions $f^k_{\mathrm{MB}} \equiv f_{\mathrm{MB}}(x, p_k, t)$ are replaced by[4]:

- Full-range Hermite:

$$g_k = w_k \sum_{\ell=0}^{N} H_\ell(\overline{p}_k) \sum_{s=0}^{\lfloor \ell/2 \rfloor} \frac{1}{2^s s!(\ell-2s)!} \left(\frac{mK_BT}{p_0^2} - 1 \right)^2 \left(\frac{mu}{p_0} \right)^{\ell-2s}. \qquad (24)$$

- Half-range Hermite: by writing $g(p) = \theta(p)g_+(p) + \theta(p-)g_-(p)$, with

$$g_\pm = \frac{\omega(|p|)}{p_0} \sum_{\ell=0}^{N} \mathcal{G}_\ell^\pm \mathfrak{h}_\ell(|p|), \qquad (25)$$

where $\mathcal{G}_\ell^+ = \int_0^\infty dp\, g(p)\mathfrak{h}_\ell(p), \quad \mathcal{G}_\ell^- = \int_{-\infty}^0 dp\, g(p)\mathfrak{h}_\ell(-p).$

[4] V. E. Ambrus, V. Sofonea, J. Comput. Phys. 316 (2016) 1–29.

Lattice Boltzmann

The non-dimensionalized form of the evolution equation of the functions ϕ_k and θ_k is:

$$\frac{\partial}{\partial t}\begin{pmatrix}\phi_k\\ \theta_k\end{pmatrix} + \frac{p_k}{m}\frac{\partial}{\partial x}\begin{pmatrix}\phi_k\\ \theta_k\end{pmatrix} = -\frac{1}{\tau}\begin{pmatrix}\phi_k - \phi_{S;k}\\ \theta_k - \theta_{S;k}\end{pmatrix} + \begin{pmatrix}J^{\phi}_{1;k}\\ J^{\theta}_{1;k}\end{pmatrix}. \tag{26}$$

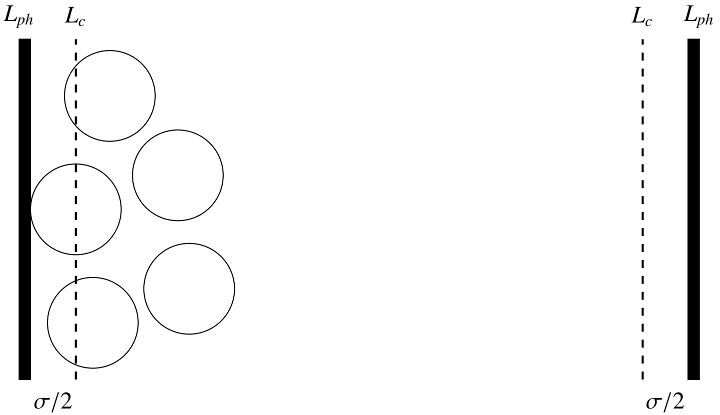
The macroscopic quantities are evaluated as:

$$\begin{pmatrix}n\\ \rho u\\ \Pi\end{pmatrix} = \sum_{k=1}^{Q}\begin{pmatrix}1\\ p_k\\ \frac{\xi_k^2}{m}\end{pmatrix}\phi_k, \tag{27}$$

$$\begin{pmatrix}\frac{3}{2}nk_BT\\ q\end{pmatrix} = \sum_{k=1}^{Q} dp_k\begin{pmatrix}1\\ \frac{\xi_k}{m}\end{pmatrix}\left(\frac{\xi_k^2}{2m}\phi_k + \frac{1}{2}\theta_k\right) \tag{28}$$

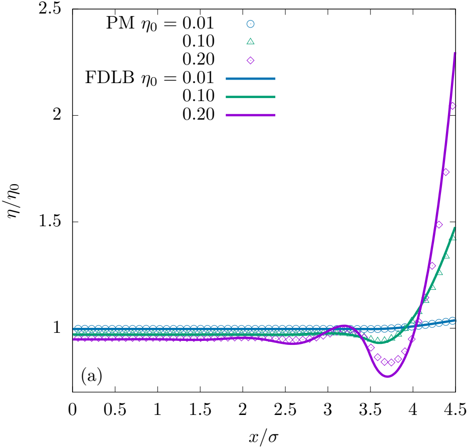
The time evolution is performed using the TVD RK-3 scheme and the advection is performed using 5^{th} order WENO numerical scheme.

Boundary condition

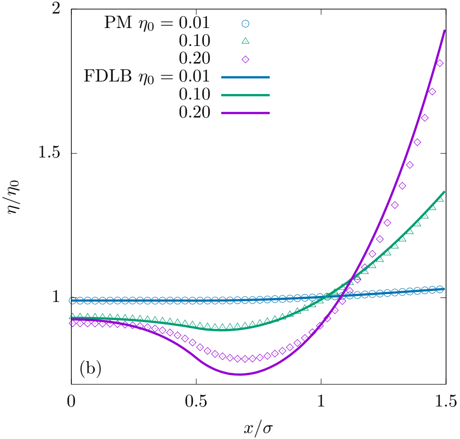


- Diffuse boundary conditions are applied at L_c. Confinement ratio defined as $R = L_{ph}/\sigma$.

Stationary gas

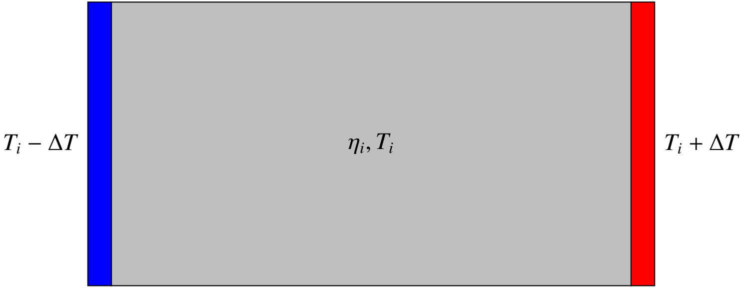


$R = 10$

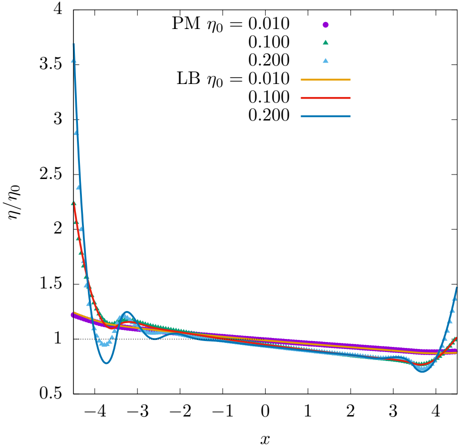


$R = 4$

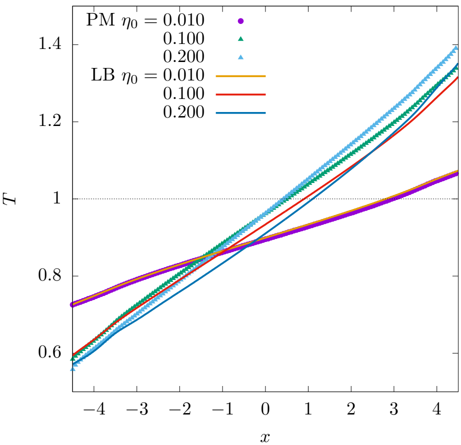
Fourier flow - Setup



Fourier flow - $\Delta T = 0.5; L_c = 9$

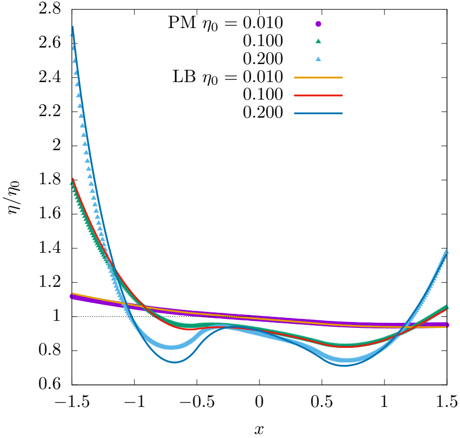


Reduced density

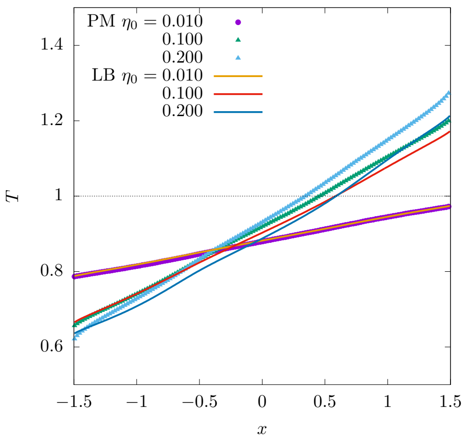


Temperature

Fourier flow - $\Delta T = 0.5; L_c = 3$



Reduced density



Temperature

Fourier flow - heat flux ϕ_q

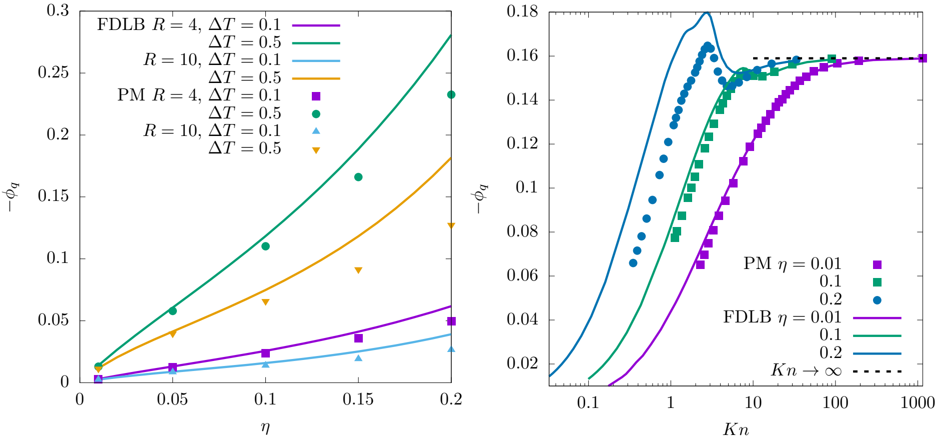
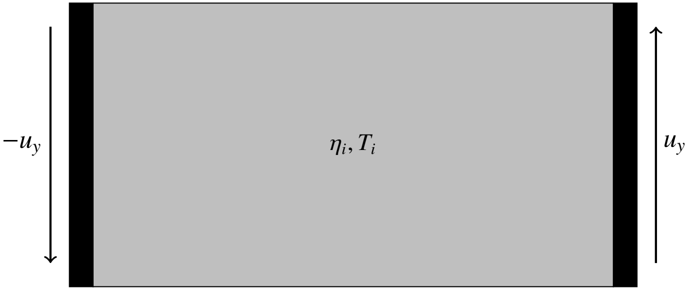
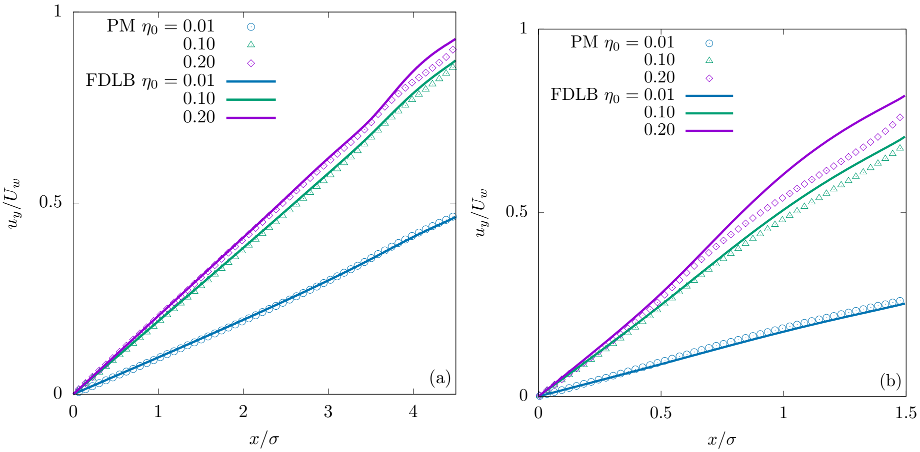


Figure: Heat transfer: (a) Heat flux ϕ_q values at temperature difference of $\Delta T = \{0.1, 0.5\}$, confinement ratios of $R = \{4, 10\}$. (b) Heat flux ϕ_q with respect to the Knudsen number Kn.

Couette flow

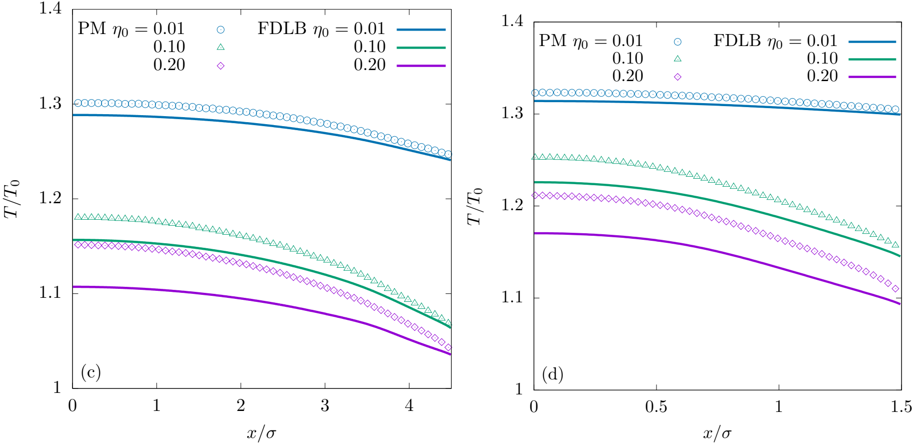


Couette flow - $U_w = 1.0$; Velocity



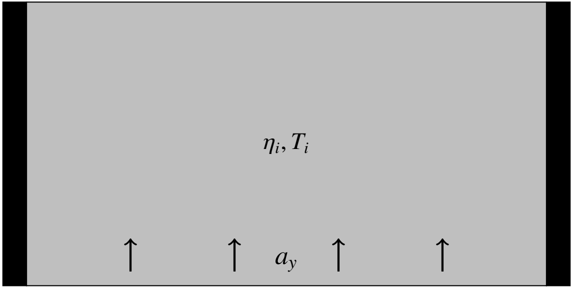
$R = 10$ $R = 4$

Couette flow - $U_w = 1.0$; Temperature

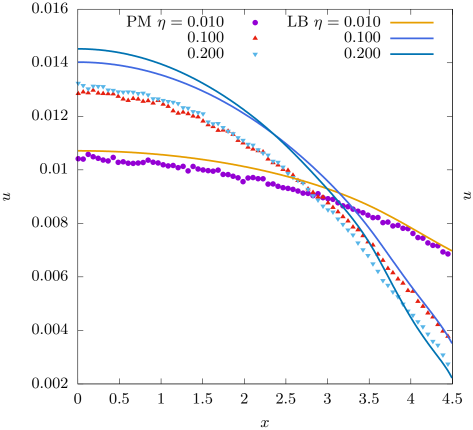


$R = 10$ $R = 4$

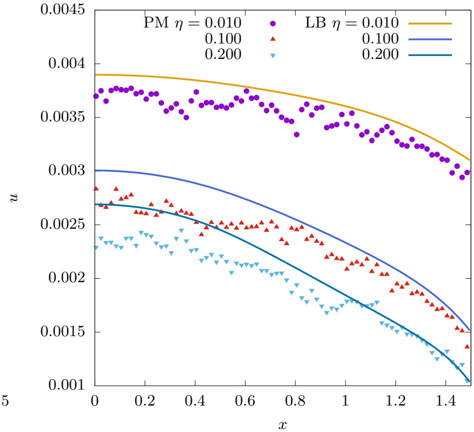
Poisseuille flow



Poisseuille flow - $a_y = 0.001$; Velocity

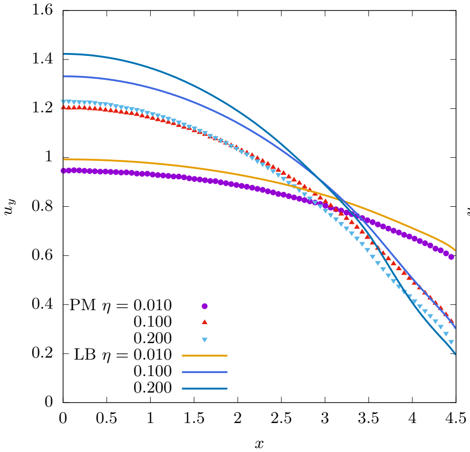


(a) $R = 10$

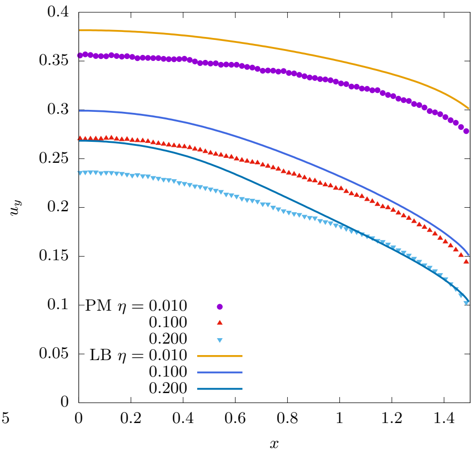


(b) $R = 4$

Poisseuille flow - $a_y = 0.1$; Velocity

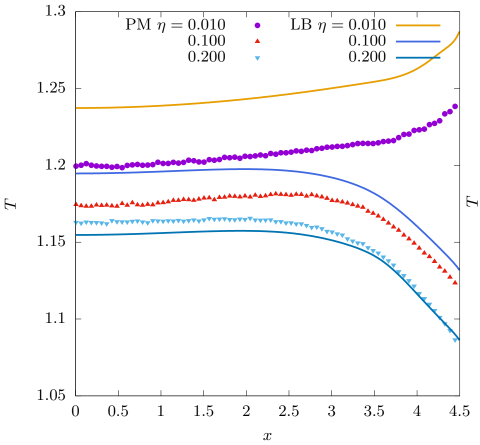


(a) $R = 10$

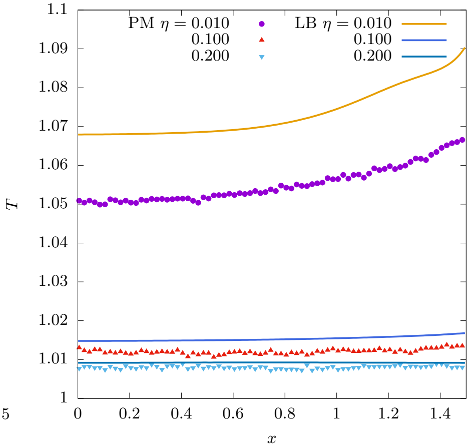


(b) $R = 4$

Poisseuille flow - $a_y = 0.1$; Temperature

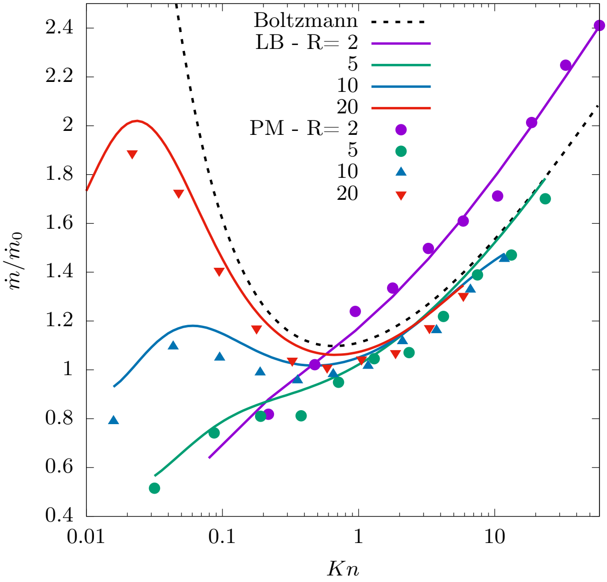


(a) $R = 10$



(b) $R = 4$

Poisseuille flow - Mass flow rate



Conclusions

- The simplified Enskog collision integral can be successfully employed when dealing with moderately dense gases.
- The numerical results obtained for the Couette flow, Fourier flow, and Poiseuille flow exhibit good agreement with the solutions obtained using the Particle method with much smaller computational time.
- Within the range of flow parameters investigated, our kinetic model captures the effects of denseness, density inhomogeneity, and nonequilibrium phenomena.

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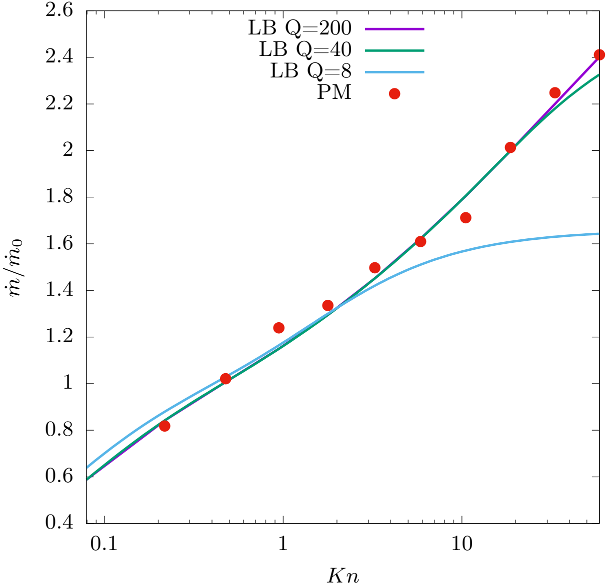
Poisseuille flow - Mass flow rate



Reduced distributions - 2D flows

The y and z degrees of freedom can be integrated out and two reduced distribution functions, ϕ and θ, can be introduced as[5]:

$$\phi_{\text{2D}}(\boldsymbol{x}, p_x, t) = \int dp_z f(\boldsymbol{x}, \boldsymbol{p}, t), \quad \theta_{\text{2D}}(\boldsymbol{x}, p_x, t) = \int dp_z \frac{p_z^2}{m} f(\boldsymbol{x}, \boldsymbol{p}, t) \tag{29}$$

The macroscopic moments can be evaluated as:

$$\begin{pmatrix} n \\ \rho u_i \\ \Pi_{ij} \end{pmatrix} = \int d^2p \begin{pmatrix} 1 \\ p_i \\ \xi_i \xi_j / m \end{pmatrix} \phi_{\text{2D}}, \tag{30}$$

$$\begin{pmatrix} \frac{3}{2} n k_B T \\ q_i \end{pmatrix} = \int d^2p \begin{pmatrix} 1 \\ \xi_i / m \end{pmatrix} \left(\frac{\xi_j \xi_j}{2m} \phi_{\text{2D}} + \frac{1}{2} \theta_{\text{2D}} \right) \tag{31}$$

The evolution equations for the reduced distribution functions are:

$$\frac{\partial}{\partial t} \begin{pmatrix} \phi_{\text{2D}} \\ \theta_{\text{2D}} \end{pmatrix} + \left(\frac{p_x}{m} \frac{\partial}{\partial x} + \frac{p_y}{m} \frac{\partial}{\partial y} \right) \begin{pmatrix} \phi_{\text{2D}} \\ \theta_{\text{2D}} \end{pmatrix} = -\frac{1}{\tau} \begin{pmatrix} \phi_{\text{2D}} - \phi_{\text{2D}}^S \\ \theta_{\text{2D}} - \theta_{\text{2D}}^S \end{pmatrix} + \begin{pmatrix} J_E^{\phi_{\text{2D}}} \\ J_E^{\theta_{\text{2D}}} \end{pmatrix} \tag{32}$$

[5] V. E. Ambrus and V. Sofonea, "Quadrature-based lattice Boltzmann models, for rarefied gas flow," in Flowing Matter, (Springer International Publishing, Cham, 2019) pp. 271–299.

Reduced distributions - 2D flows

In the above the, ϕ^S_{2D} and θ^S_{2D} are given by:

$$\phi^S_{2D} = f^{MB}_{xy}\left[1 + \frac{1-\mathrm{Pr}}{5P_i m k_B T}\left(\frac{\xi_x^2+\xi_y^2}{mk_BT} - 4\right)(\xi_x q_x + \xi_y q_y)\right], \tag{33}$$

$$\theta^S_{2D} = k_B T f^{MB}_{xy}\left[1 + \frac{1-\mathrm{Pr}}{5P_i m k_B T}\left(\frac{\xi_x^2+\xi_y^2}{mk_BT} - 2\right)(\xi_x q_x + \xi_y q_y)\right] \tag{34}$$

while the first order corrections J_1^ϕ and J_1^θ are:

$$J_E^{\phi_{2D}} = -\Bigg[\xi_x \partial_x \ln\chi + 2\xi_x\partial_x \ln\rho + \frac{2}{5}\left(\frac{\xi_x^2}{mk_BT} + \frac{\xi_x^2+\xi_y^2}{2mk_BT} - 2\right)\partial_x u_x + \frac{3\xi_x}{10m}\left(\frac{\xi_x^2+\xi_y^2}{mk_BT} - \frac{2}{3}\right)\partial_x \ln T\Bigg] f^{MB}_{xy} b\rho\chi \tag{35a}$$

$$J_E^{\theta_{2D}} = -\Bigg[\xi_x \partial_x \ln\chi + 2\xi_x\partial_x \ln\rho + \frac{2}{5}\left(\frac{\xi_x^2}{mk_BT} + \frac{\xi_x^2+\xi_y^2}{2mk_BT} - 1\right)\partial_x u_x + \frac{3\xi_x}{10m}\left(\frac{\xi_x^2+\xi_y^2}{mk_BT} + \frac{4}{3}\right)\partial_x \ln T\Bigg] 2mk_BTf^{MB}_{xy} b\rho\chi \tag{35b}$$

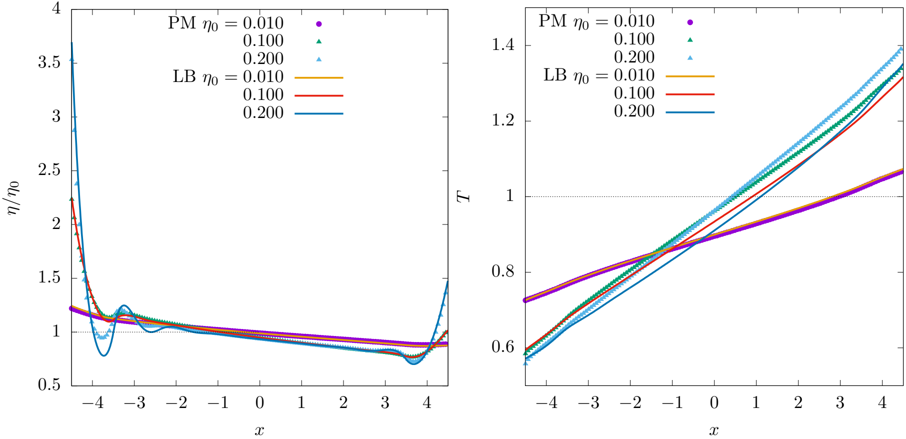


Figure: Heat transfer: Reduced density profiles at temperature difference of $\Delta T = 0.5$, three values of the initial density $\eta_0 = \{0.01, 0.1, 0.2\}$ and $R = 10$.

Fourier flow - $\Delta T = 0.5; L_c = 3$

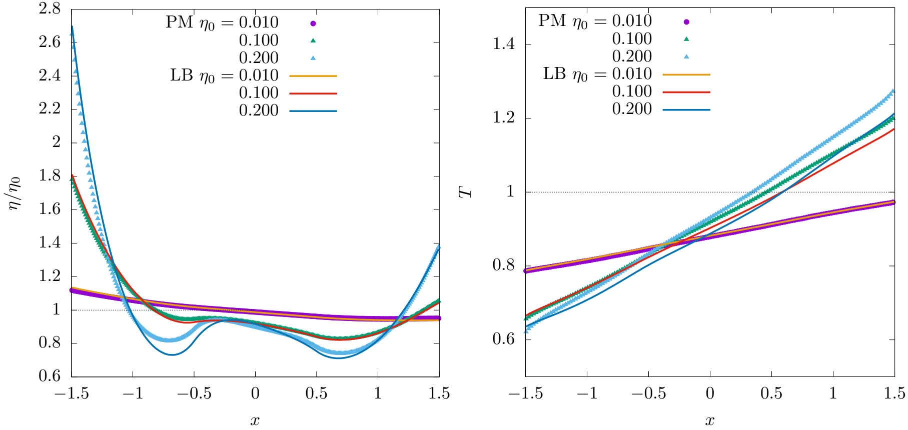
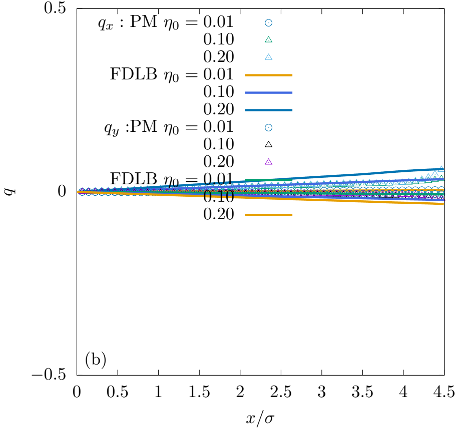


Figure: Heat transfer: Reduced density profiles at temperature difference of $\Delta T = 0.5$, three values of the initial density $\eta_0 = \{0.01, 0.1, 0.2\}$ and $R = 4$.

Couette flow - $U_w = 1.0$; $L_c = 9$; q_x



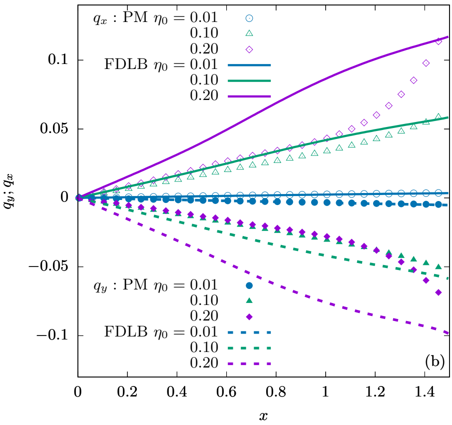


Figure: Couette flow: Transversal and longitudinal heat flux at a wall velocity of $U_w = 1$, three values of the initial density $\eta_0 = \{0.01, 0.1, 0.2\}$ and (a) $R = 10$ and (b) $R = 4$.

Poisseuille flow - $a_y = 0.1$; Transversal heat flux

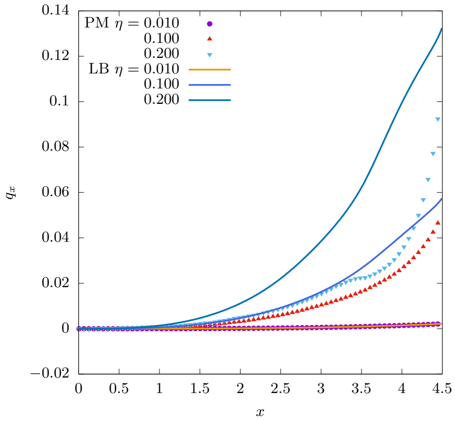
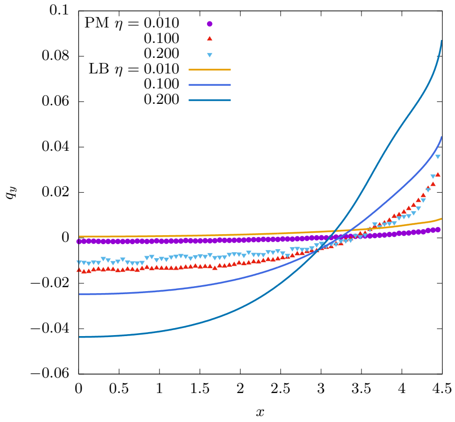


Figure: Poisseuille flow: Transversal heat flux q_x at an external acceleration of $a_y = 0.1$, three values of the initial density $\eta_0 = \{0.01, 0.1, 0.2\}$ and (a) $R = 10$ and (b) $R = 4$.

Poisseuille flow - $a_y = 0.1$;Longitudinal heat flux



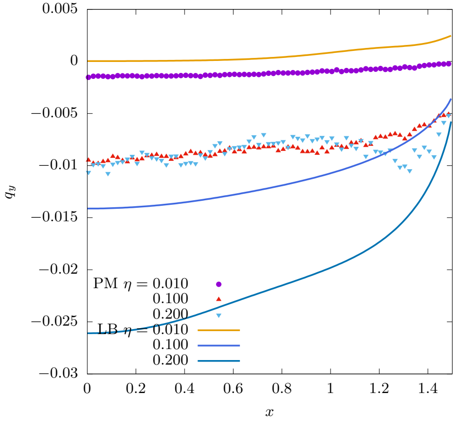


Figure: Poisseuille flow: longitudinal heat flux q_y at an external acceleration of $a_y = 0.1$, three values of the initial density $\eta_0 = \{0.01, 0.1, 0.2\}$ and (a) $R = 10$ and (b) $R = 4$.