Lattice Boltzmann study of flows in non-Cartesian geometries using the vielbein formalism

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Outline

- Boltzmann equation with respect to orthonormal vielbein fields in conservative formalism
- Shear flows between coaxial cylinders
- Heat transfer in cylindrical and spherical symmetric geometries

Boltzmann Equation

- Evolution equation of the one-particle distribution function f with respect to the Cartesian coordinates:

$$\frac{\partial f}{\partial t} + \frac{p^i}{m}\frac{\partial f}{\partial x^i} + F^i \frac{\partial f}{\partial p^i} = J[f]. \tag{1}$$

- Hydrodynamic moments of order N give macroscopic quantities:

$N = 0$: number density: $n = \int d^3p\, f,$

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

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

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

Boltzmann equation - arbitrary coordinates

Consider a coordinate transformation $x^i \to x^{\widetilde{i}}$ such that:

$$p^{\widetilde{\imath}} = p^i \frac{\partial x^{\widetilde{\imath}}}{\partial x^i}, \qquad F^{\widetilde{\imath}} = F^i \frac{\partial x^{\widetilde{\imath}}}{\partial x^i}. \tag{2}$$

This coordinate transformation induces induces a metric $g_{\widetilde{\imath}\widetilde{\jmath}}$, as follows:

$$ds^2 = \delta_{ij} dx^i dx^j = g_{\widetilde{\imath}\widetilde{\jmath}} dx^{\widetilde{\imath}} dx^{\widetilde{\jmath}}, \tag{3}$$

$$g_{\widetilde{\imath}\widetilde{\jmath}} = \delta_{ij} \frac{\partial x^i}{\partial x^{\widetilde{\imath}}} \frac{\partial x^j}{\partial x^{\widetilde{\jmath}}}. \tag{4}$$

The Boltzmann equation with respect to the new coordinates reads:

$$\frac{\partial f}{\partial t} + \frac{p^{\widetilde{\imath}}}{m} \frac{\partial f}{\partial x^{\widetilde{\imath}}} + \left(F^{\widetilde{\imath}} - \frac{1}{m} \Gamma^{\widetilde{\imath}}{}_{\widetilde{\jmath}\widetilde{k}} p^{\widetilde{\jmath}} p^{\widetilde{k}} \right) \frac{\partial f}{\partial p^{\widetilde{\imath}}} = J[f]. \tag{5}$$

Triads (vielbein)

- Consider the triad vector frame and its associated one-form co-frame:

$$e_{\hat{a}} = e_{\hat{a}}^{\widetilde{\imath}} \partial_{\widetilde{\imath}}, \qquad \omega^{\hat{a}} = \omega_{\widetilde{\imath}}^{\hat{a}} dx^{\widetilde{\imath}}, \qquad e_{\hat{a}}^{\widetilde{\imath}} \omega_{\widetilde{\imath}}^{\hat{b}} = \delta^{\hat{b}}{}_{\hat{a}}, \qquad e_{\hat{a}}^{\widetilde{\imath}} \omega_{\widetilde{\jmath}}^{\hat{a}} = \delta^{\widetilde{\imath}}{}_{\widetilde{\jmath}}. \tag{6}$$

- The metric with respect to the triad becomes diagonal:

$$g_{\widetilde{\imath}\widetilde{\jmath}} dx^{\widetilde{\imath}} dx^{\widetilde{\jmath}} = \delta_{\hat{a}\hat{b}} \omega^{\hat{a}} \omega^{\hat{b}}, \qquad g_{\widetilde{\imath}\widetilde{\jmath}} e_{\hat{a}}^{\widetilde{\imath}} e_{\hat{a}}^{\widetilde{\jmath}} = \delta_{\hat{a}\hat{b}}. \tag{7}$$

- The inner product $\mathbf{p} \cdot \mathbf{u}$ is decoupled from the metric:

$$\mathbf{p} \cdot \mathbf{u} = g_{\widetilde{\imath}\widetilde{\jmath}} p^{\widetilde{\imath}} u^{\widetilde{\jmath}} = \delta_{\hat{a}\hat{b}} p^{\hat{a}} u^{\hat{b}}, \tag{8}$$

where $p^{\hat{a}} = \omega_{\widetilde{\imath}}^{\hat{a}} p^{\widetilde{\imath}}$.

Boltzmann equation with respect to triads

- The Boltzmann equation becomes:

$$\frac{\partial f}{\partial t} + \frac{p^{\hat{a}}}{m} e^{\widetilde{\imath}}_{\hat{a}} \frac{\partial f}{\partial x^{\widetilde{\imath}}} + \left(F^{\hat{a}} - \frac{1}{m} \Gamma^{\hat{a}}{}_{\hat{b}\hat{c}} p^{\hat{b}} p^{\hat{c}} \right) \frac{\partial f}{\partial p^{\hat{a}}} = J[f], \tag{9}$$

- Macroscopic quantities are now calculated using:

$$n = \int d^3\hat{p}\, f, \qquad \mathbf{u} = \frac{1}{\rho} \int d^3\hat{p}\, f\, \mathbf{p},$$
$$T^{\hat{a}\hat{b}} = \int d^3\hat{p}\, f\, \frac{\xi^{\hat{a}}\xi^{\hat{b}}}{m}, \qquad \mathbf{q} = \int d\hat{p}\, f\, \frac{\boldsymbol{\xi}^2}{2m} \frac{\boldsymbol{\xi}}{m}. \tag{10}$$

- In general, a moment of f of order s reads:

$$M^{\hat{a}_1 \dots \hat{a}_s} = \int d^3\hat{p}\, f\, p^{\hat{a}_1} \cdots p^{\hat{a}_s}. \tag{11}$$

Boltzmann equation - Conservative form

- Following Cardall et al.[1], the Boltzmann equation can be written in conservative form as follows:

$$\frac{\partial \widetilde{f}}{\partial t} + \frac{\partial}{\partial x^{\widetilde{\imath}}} \left(\frac{p^{\hat{a}}}{m} e_{\hat{a}}^{\widetilde{\imath}} \widetilde{f} \right) + \frac{\partial}{\partial p^{\hat{a}}} \left[\left(F^{\hat{a}} - \frac{1}{m} \Gamma^{\hat{a}}{}_{\hat{b}\hat{c}} p^{\hat{b}} p^{\hat{c}} \right) \widetilde{f} \right] = J[f]\sqrt{g}, \qquad (12)$$

where $\widetilde{f} = f\sqrt{g}$ and we have assumed that $F^{\hat{a}}$ does not depend on $p^{\hat{b}}$.

- Introducing $D/Dt = \partial_t + u^{\hat{a}} \nabla_{\hat{a}}$ and $e = \frac{3}{2} K_B T$, the macroscopic equations can be obtained:

$$\frac{Dn}{Dt} + n\nabla_{\hat{a}} u^{\hat{a}} = 0, \qquad \rho \frac{Du^{\hat{a}}}{Dt} = nF^{\hat{a}} - \nabla_b T^{\hat{a}\hat{b}},$$
$$n\frac{De}{Dt} + \nabla_{\hat{a}} q^{\hat{a}} + T^{\hat{a}\hat{b}} \nabla_{\hat{a}} u_{\hat{b}} = 0. \qquad (13)$$

- In the hydrodynamic regime, the constitutive equations read:

$$T^{\hat{a}\hat{b}} = P\delta^{\hat{a}\hat{b}} - \eta \left(\nabla^{\hat{a}} u^{\hat{b}} + \nabla^{\hat{b}} u^{\hat{a}} - \frac{2}{3} \delta^{\hat{a}\hat{b}} \nabla_{\hat{c}} u^{\hat{c}} \right), \qquad q^{\hat{a}} = -\kappa \nabla^{\hat{a}} T. \qquad (14)$$

[1] C. Y. Cardall, E. Endeve, and A. Mezzacappa, Phys. Rev. D **88**, 023011 (2013).

Cylindrical coordinates

- The line element in cylindrical coordinates and the associated triad are:

$$ds^2 = dR^2 + R^2 d\varphi^2 + dz^2, \qquad e_{\hat{R}} = \partial_R, \qquad e_{\hat{\varphi}} = R^{-1}\partial_\varphi, \qquad e_{\hat{z}} = \partial_z. \tag{15}$$

- The Boltzmann equation when the flow is homogeneous w.r.t. φ and z reads:

$$\frac{\partial f}{\partial t} + \frac{2p^{\hat{R}}}{m}\frac{\partial(fR)}{\partial R^2} + \frac{1}{mR}\left[(p^{\hat{\varphi}})^2 \frac{\partial f}{\partial p^{\hat{R}}} - p^{\hat{R}} \frac{\partial(f p^{\hat{\varphi}})}{\partial p^{\hat{\varphi}}}\right] = -\frac{1}{\tau}(f - f^{(\mathrm{eq})}). \tag{16}$$

- The advection term is implemented following Falle et al.[2]

[2] S. A. E. G. Falle and S. S. Komissarov, Mon. Not. R. Astron. Soc. **278**, 586-602 (1996).

Spherical coordinates

- The line element in spherical coordinates and its associated triad are:

$$ds^2 = dr^2 + r^2(d\theta^2 + \sin^2\theta d\varphi^2), \quad e_{\hat{r}} = \partial_r, \qquad e_{\hat{\theta}} = \frac{\partial_\theta}{r}, \quad e_{\hat{\varphi}} = \frac{r^{-1}}{\sin\theta}\partial_\varphi. \tag{17}$$

- Assuming that the flow is homogeneous w.r.t. θ and φ, the Boltzmann equation reads:

$$\frac{\partial f}{\partial t} + \frac{3p^{\hat{r}}}{m}\frac{\partial(fr^2)}{\partial r^3} + \frac{1}{mR}\left[\left((p^{\hat{\theta}})^2 + (p^{\hat{\varphi}})^2\right)\frac{\partial f}{\partial p^{\hat{r}}} - p^{\hat{r}}\left(\frac{\partial(fp^{\hat{\theta}})}{\partial p^{\hat{\theta}}} + \frac{\partial(fp^{\hat{\varphi}})}{\partial p^{\hat{\varphi}}}\right)\right] = -\frac{1}{\tau}(f - f^{(\mathrm{eq})}). \tag{18}$$

- The advection term is implemented following Falle et al.[3]

[3] S. A. E. G. Falle and S. S. Komissarov, Mon. Not. R. Astron. Soc. **278**, 586-602 (1996).

Lattice Boltzmann - Gauss-Hermite quadratures

The numerical models employed are mixed quadrature lattice Boltzmann[4].
Replace integrals by quadrature sums:

$$\int d^3p\, f\, P(\mathbf{p}) = \sum_k f_k P(\mathbf{p}_k)$$

The one-particle distribution functions f and $f^{(\mathrm{eq})}$ are expanded with respect to a mixture of Hermite(HLB) and Half-Range Hermite(HHLB) polynomials, depending on the flow regime considered. We wil denote such models by:

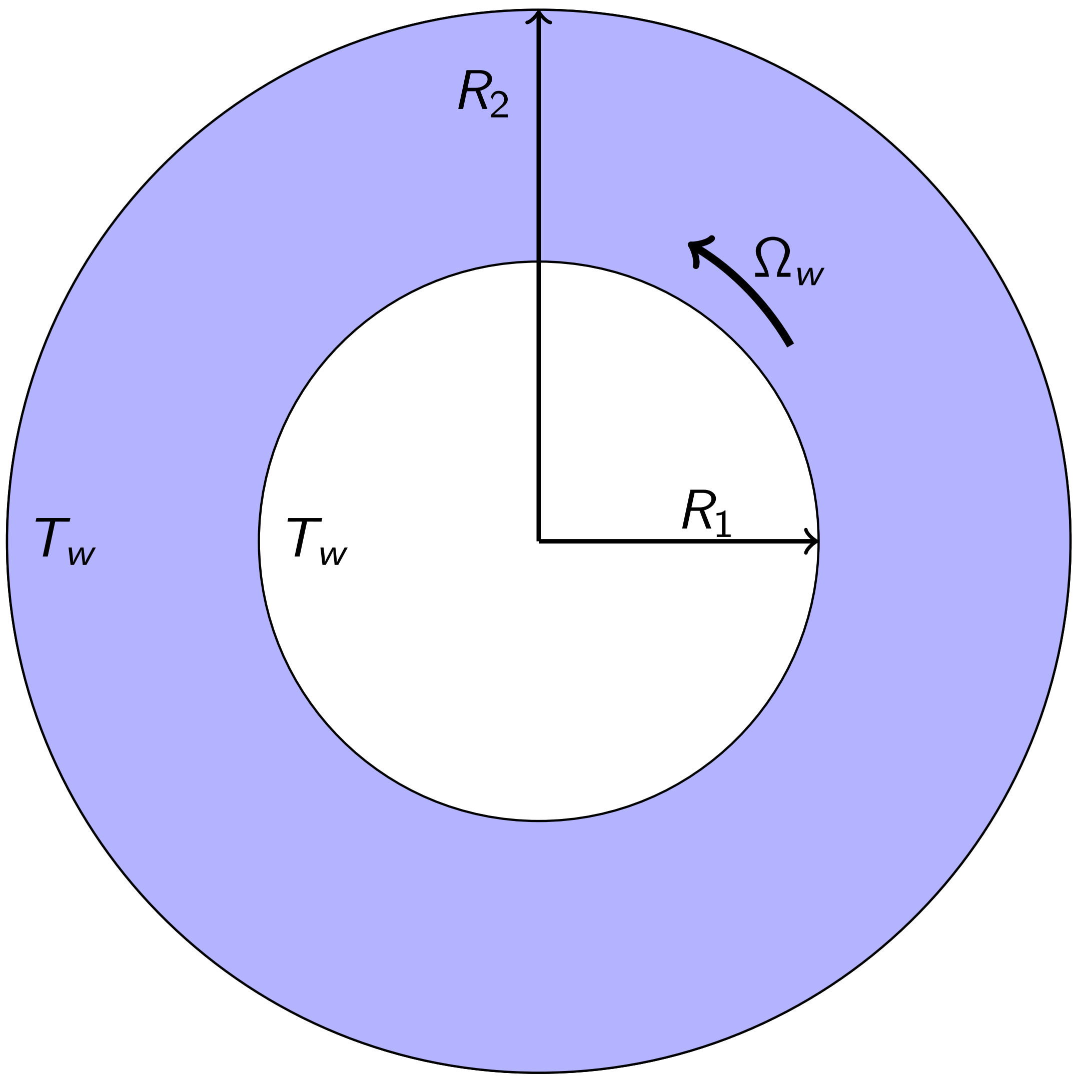
$$\begin{aligned}\text{cylindrical coordinates: } & \mathrm{HHLB}(Q_R) \times \mathrm{HLB}(\mathrm{Q}_\varphi) \times \mathrm{HLB}(Q_z),\\ \text{spherical coordinates: } & \mathrm{HHLB}(Q_R) \times \mathrm{HLB}(\mathrm{Q}_\theta) \times \mathrm{HLB}(Q_\varphi).\end{aligned}$$

The moments of the distribution function are evaluated as:

$$\int d^3\hat{p}\, f\, p^{\hat{a}_1} \cdots p^{\hat{a}_s} = \sum_{i=1}^{\mathcal{Q}_R} \sum_{j=1}^{\mathcal{Q}_\varphi} \sum_{k=1}^{\mathcal{Q}_z} f_{ijk} \prod_{\ell=1}^{s} p_{ijk}^{\hat{a}_\ell}. \tag{19}$$

[4] V.E. Ambruș and V.Sofonea, J. Comput. Phys. **316**, 760-788 (2016)

Circular Couette flow



To describe the flowing regimes we will use the Knudsen number $Kn = \lambda/L$, where λ represents the mean free path and L is the caracteristic system length.

Hydrodynamic flow regime - $Kn \to 0$

By solving the macroscopic equations (13) we obtain the following solutions:

- Number density is evaluated by numerically solving:

$$\partial_R \ln P = \frac{(u^{\hat{\varphi}})^2}{RT}. \tag{20}$$

  where $n = P/T$ and by using the constraint $2\pi \int_{R_{\rm in}}^{R_{\rm out}} nRdR = N_{\rm tot}$.

- Azimuthal velocity:

$$u^{\hat{\varphi}} = R^{-1} \frac{\Omega_{\rm in}}{R_{\rm in}^{-2} - R_{\rm out}^{-2}} - R \frac{\Omega_{\rm in} R_{\rm in}^2}{R_{\rm out}^2 - R_{\rm in}^2}, \tag{21}$$

- Temperature:

$$T = T_w + \frac{\eta}{\kappa} \frac{\Omega_{\rm in}^2}{R_{\rm in}^{-2} - R_{\rm out}^{-2}} \times \left(\frac{R_{\rm in}^{-2} - R^{-2}}{R_{\rm in}^{-2} - R_{\rm out}^{-2}} - \frac{\ln(R/R_{\rm in})}{\ln(R_{\rm out}/R_{\rm in})} \right) \tag{22}$$

- Radial heat flux:

$$q^{\hat{R}} = -\frac{\eta}{R} \frac{\Omega_{\rm in}^2}{R_{\rm in}^{-2} - R_{\rm out}^{-2}} \times \left[\frac{2R^{-2}}{R_{\rm in}^{-2} - R_{\rm out}^{-2}} - \frac{1}{\ln(R_{\rm out}/R_{\rm in})} \right]. \tag{23}$$

Hydrodynamic flow regime - $Kn \to 0$

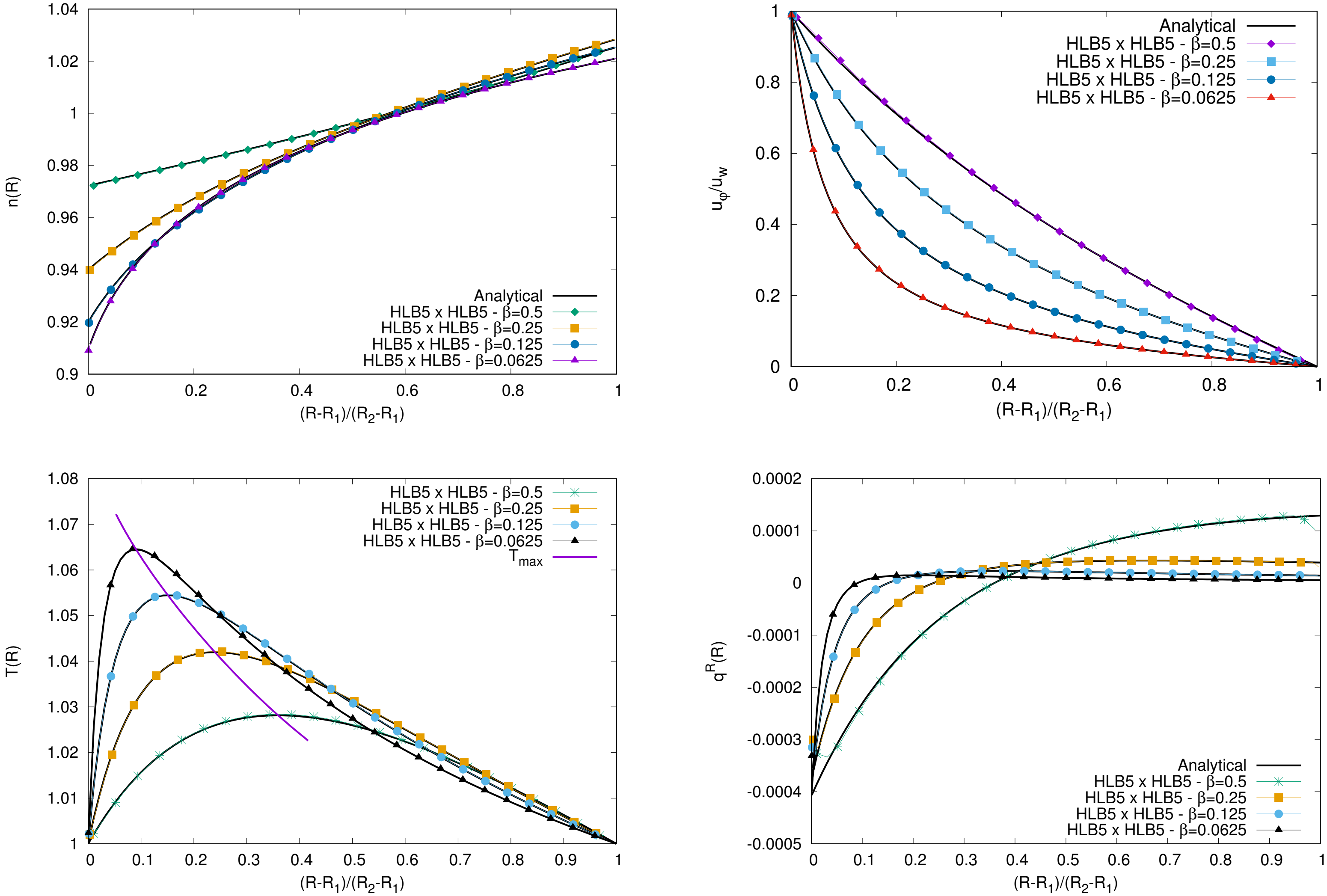
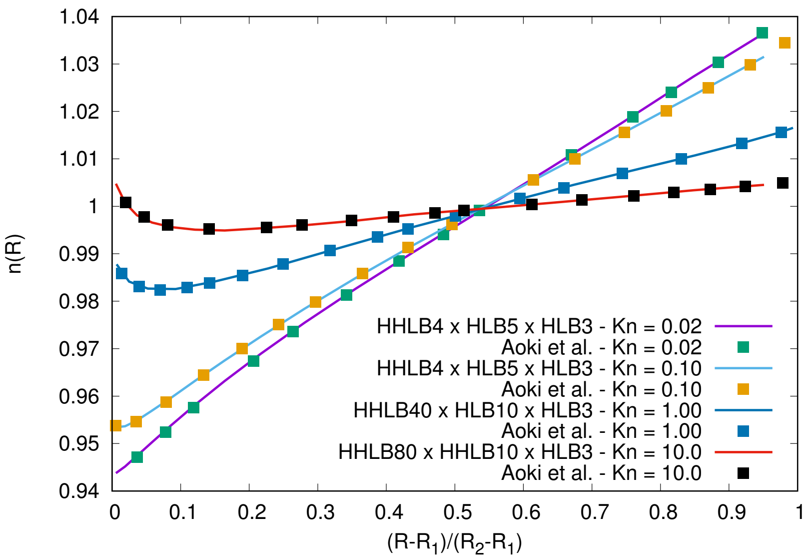
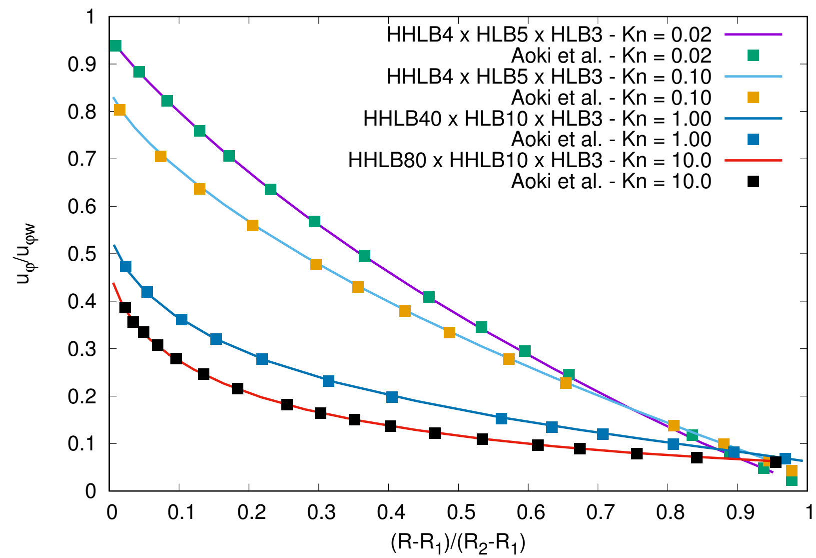
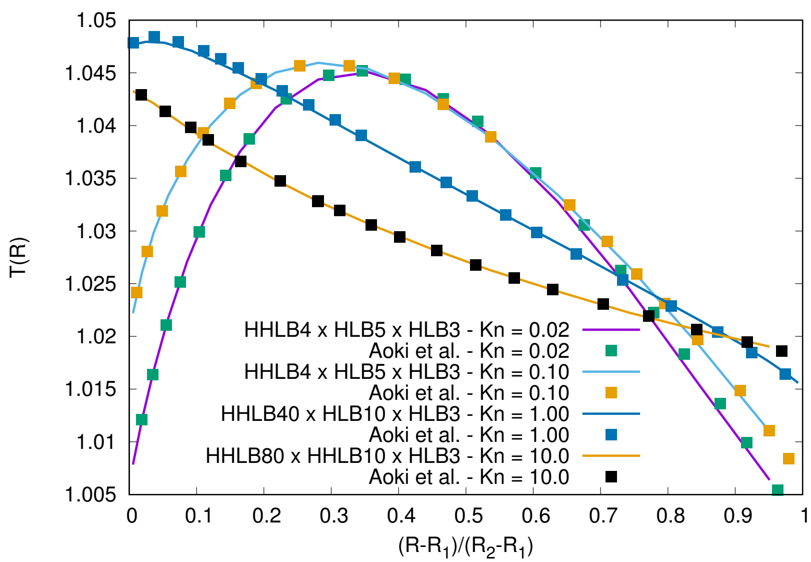


Figure: Profiles of number density, velocity, temperature and radial heat flux for a wall azimuthal velocity of $u_w = 0.5$ and wall temperature $T_w = 1.0$.

Transition flow regime







Profiles of number density, velocity, temperature for a wall azimuthal velocity of $u_w = 1/\sqrt{2}$ and wall temperature $T_w = 1.0$.

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

- Number density:

$$n = n_{\rm out}\left(1 - \frac{\theta_{\rm max}}{\pi}\right) + n_{\rm in} e^{-\widetilde{R}_{\rm in}^2}\left[\frac{\theta_{\rm max}}{\pi} + \frac{I_0(\widetilde{R})}{\widetilde{R}\sqrt{\pi}}\right], \tag{24}$$

- Azimuthal velocity:

$$u^{\hat{\varphi}} = \frac{n_{\rm in} e^{-\widetilde{R}_{\rm in}^2}}{2n\pi}\Omega_{\rm in} R\left\{\arcsin\frac{R_{\rm in}}{R} - \frac{R_{\rm in}}{R}\sqrt{1 - \frac{R_{\rm in}^2}{R^2}} + \frac{\sqrt{\pi}}{\widetilde{R}^3}[I_0(\widetilde{R}) + 2I_1(\widetilde{R})]\right\}. \tag{25}$$

- Temperature:

$$T = \frac{n_{\rm in} T_{\rm in} e^{-\widetilde{R}_{\rm in}^2}}{d\pi n}\left\{(d + \widetilde{R}^2)\theta_{\rm max} - \widetilde{R}_{\rm in}\widetilde{R}\sqrt{1 - \frac{R_{\rm in}^2}{R^2}} + \frac{\sqrt{\pi}}{\widetilde{R}}[(d+1)I_0 + 2I_1]\right\} + \frac{n_{\rm out} T_{\rm out}}{\pi n}(\pi - \theta_{\rm max}) - \frac{m}{d}(u^{\hat{\varphi}})^2. \tag{26}$$

The following notations were used: $I_n(\widetilde{R}) = \int_0^{\widetilde{R}_{\rm in}} \frac{\zeta^{2n+1} d\zeta}{\sqrt{1-\zeta^2/\widetilde{R}^2}} e^{\zeta^2} {\rm erf}\,\zeta$, $\zeta = \widetilde{R}\sin\theta$, $\widetilde{R} = \Omega_{\rm in} R\sqrt{m/2T_{\rm in}}$, $\theta_{\rm max} = \arcsin(R_{\rm in}/R)$.

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

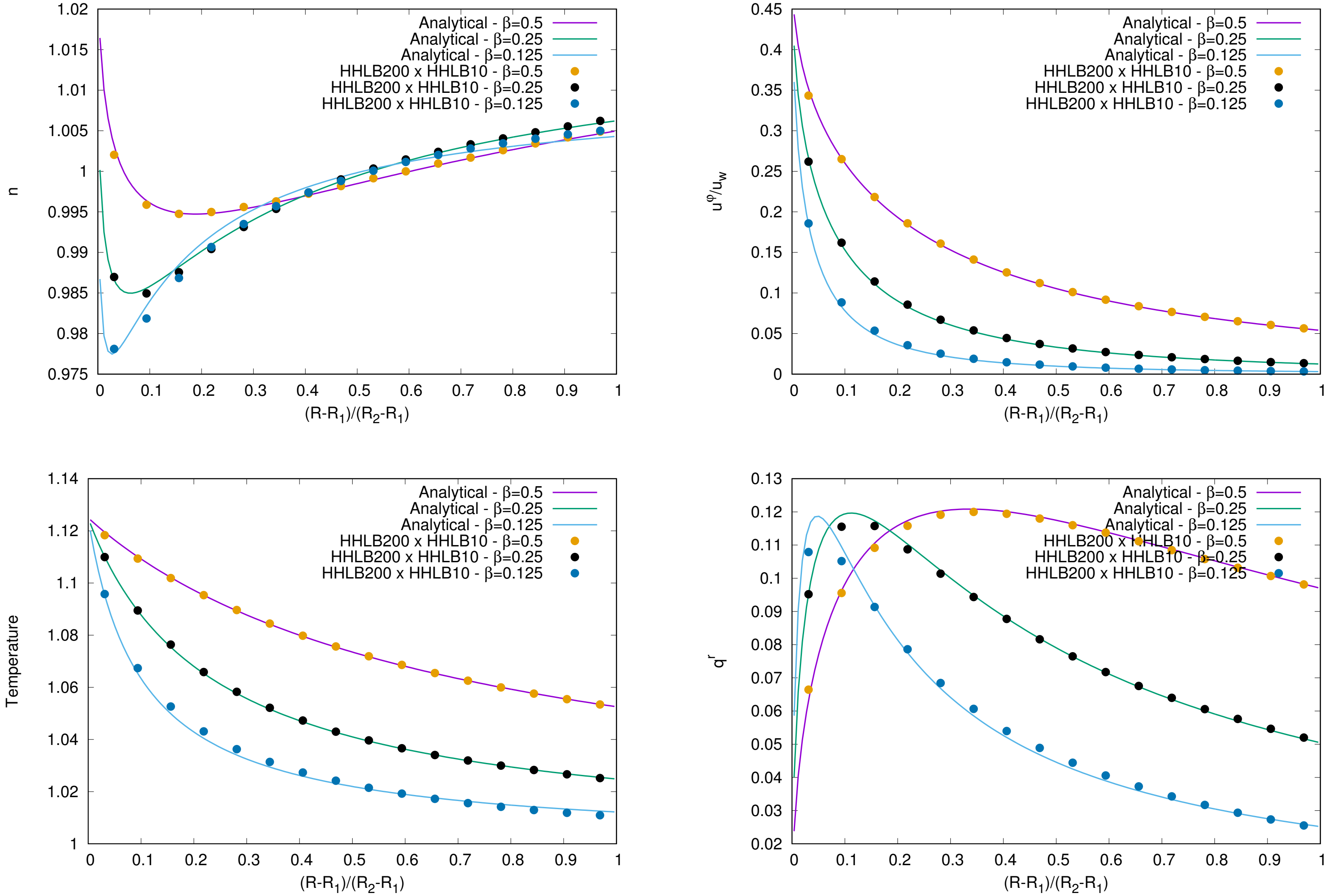


Figure: Profiles of number density, velocity, temperature and radial heat flux for a wall azimuthal velocity of $u_w = 1.0$ and wall temperature $T_w = 1.0$.

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

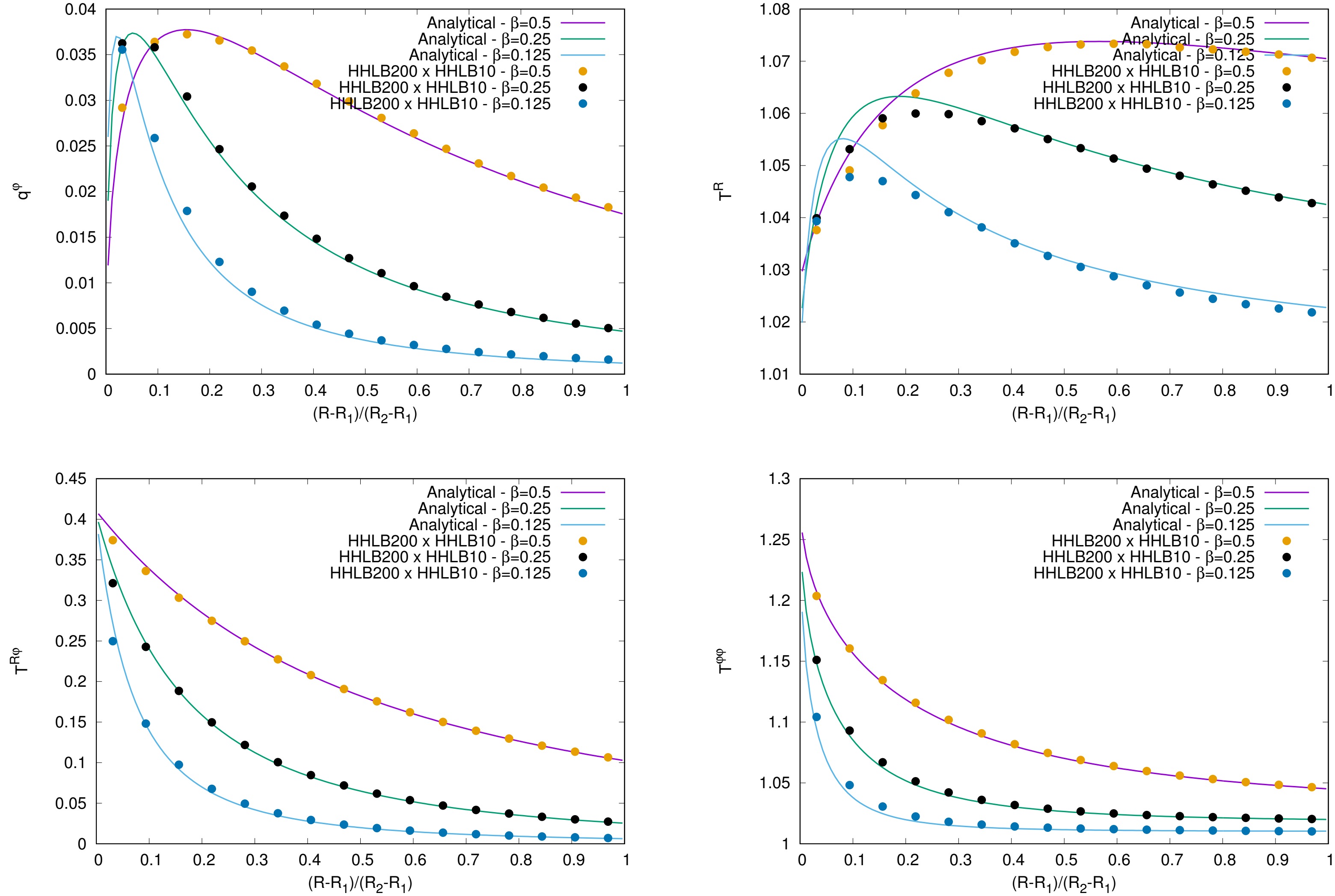
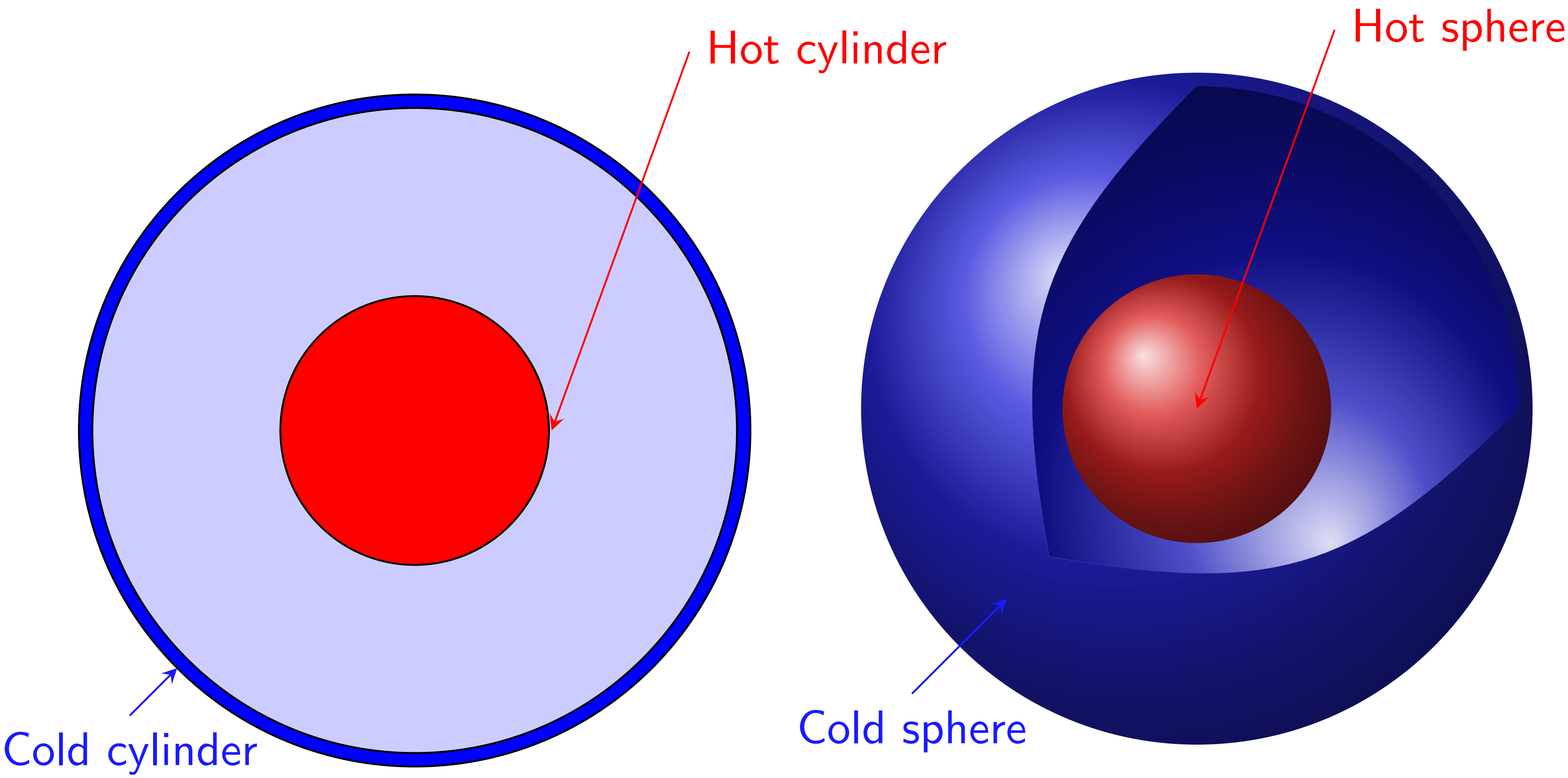


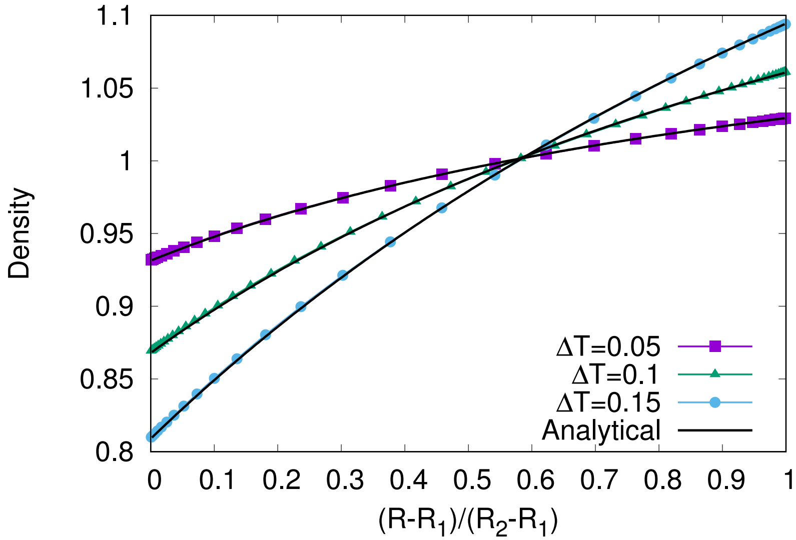
Figure: Profiles of azimuthal heat flux and the stress tensor components $T^{\hat{R}\hat{R}}$, $T^{\hat{R}\hat{\varphi}}$ and $T^{\hat{\varphi}\hat{\varphi}}$ for a wall azimuthal velocity of $u_w = 1.0$ and wall temperature $T_w = 1.0$.

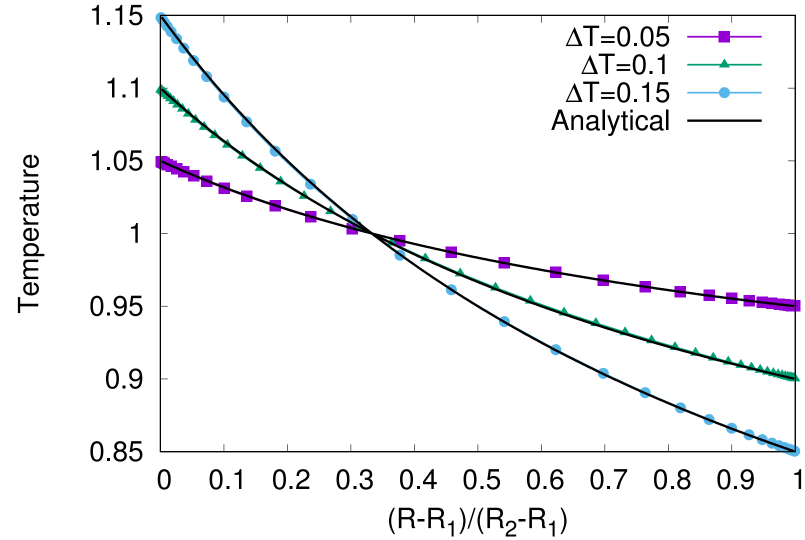
Heat transfer - cylindrical and spherical symmetry

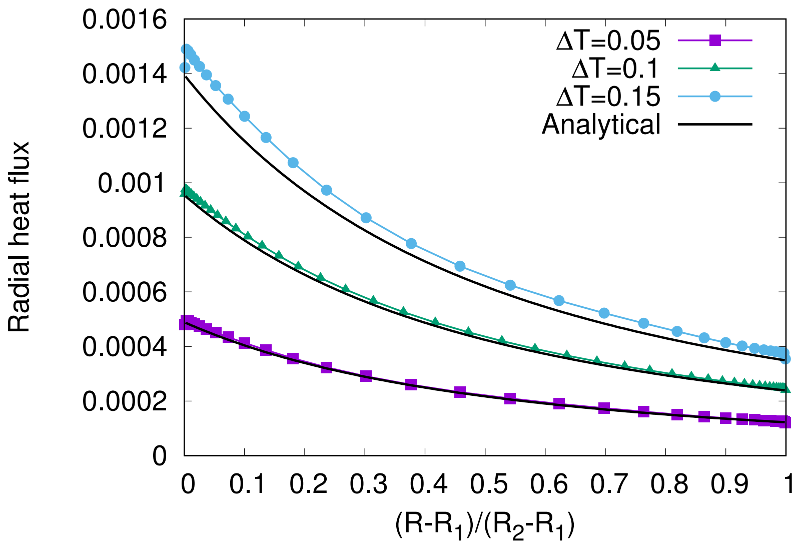


$$T_{hot/cold} = T \pm \Delta T$$

Heat transfer - spherical symmetry $Kn \to 0$

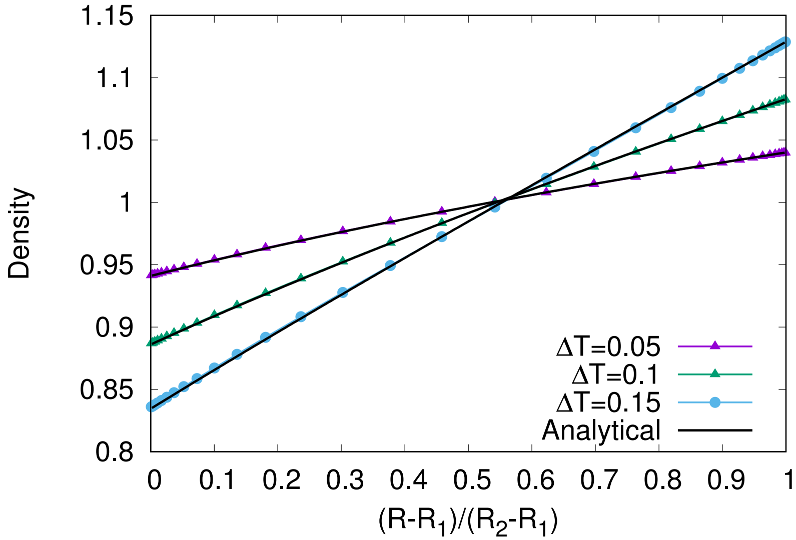


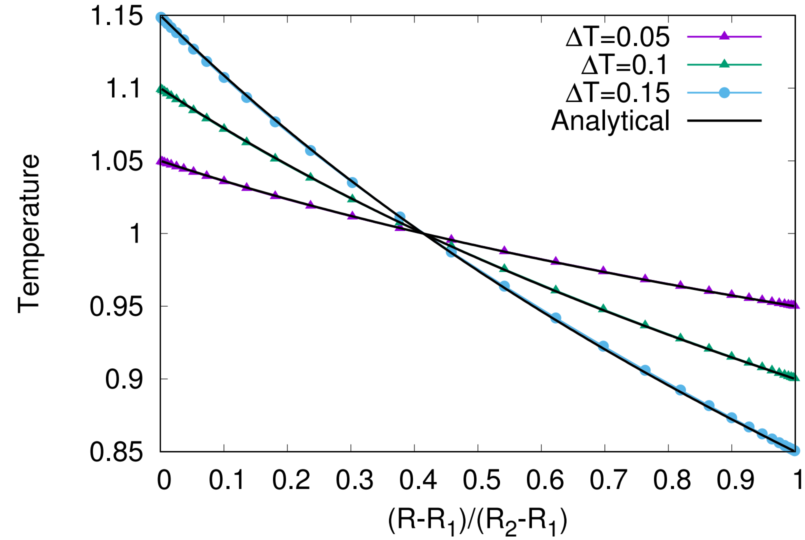


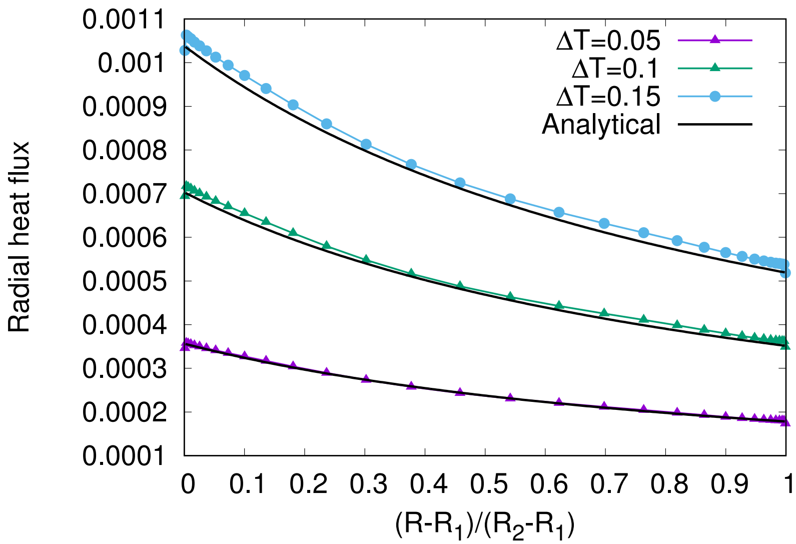


Profiles of number density, temperature for a wall temperature spread $\Delta T = 0.05, 0.1, 0.15$.

Heat transfer - cylindrical symmetry $Kn \to 0$

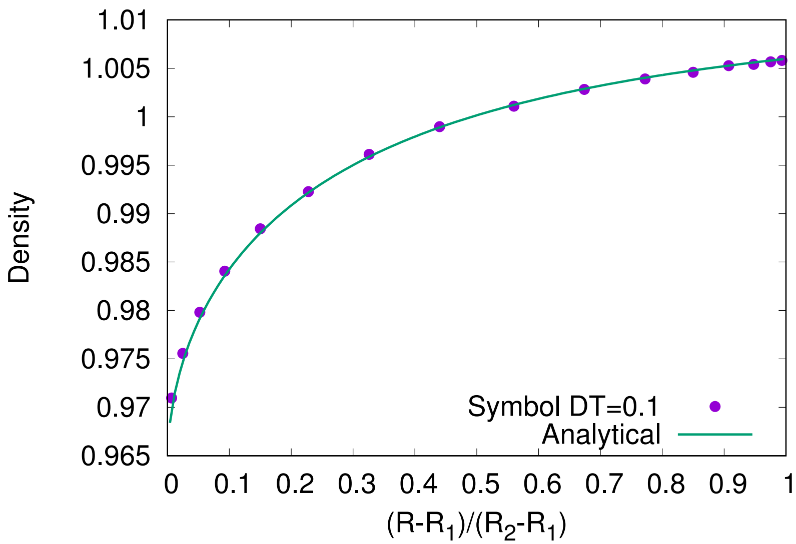


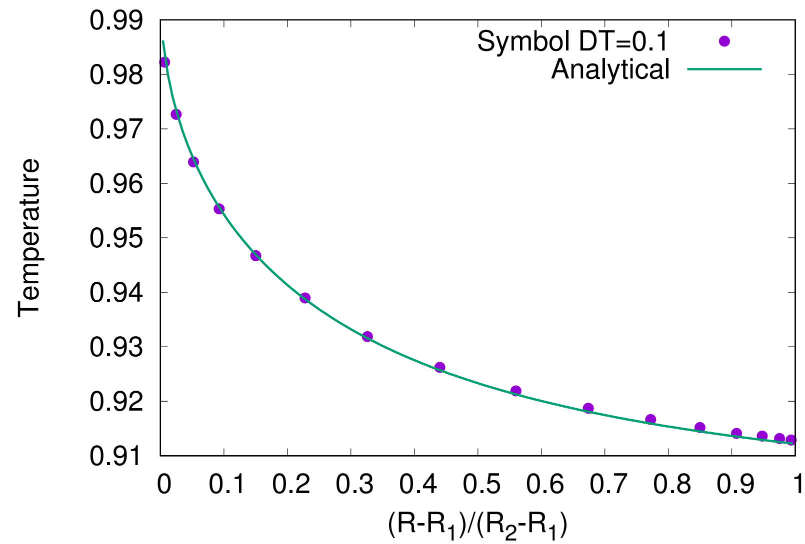


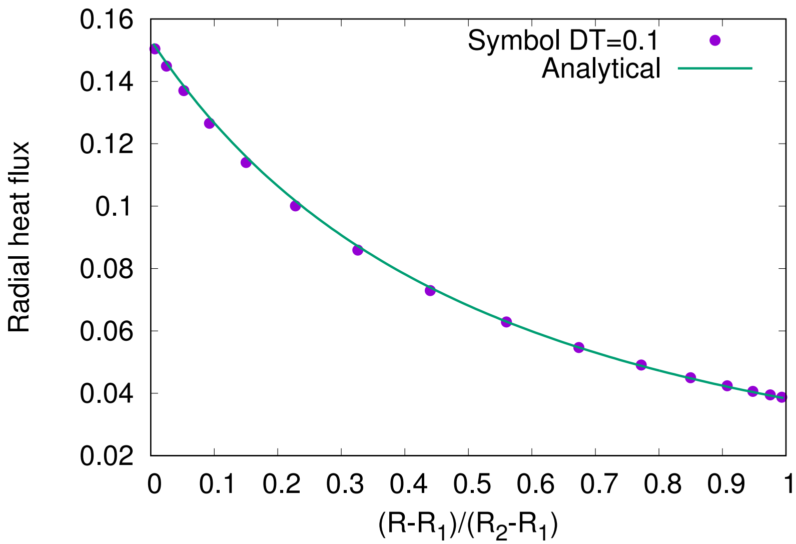


Profiles of number density, temperature for a wall temperature spread $\Delta T = 0.05, 0.1, 0.15$.

Heat transfer - spherical symmetry $Kn \to \infty$

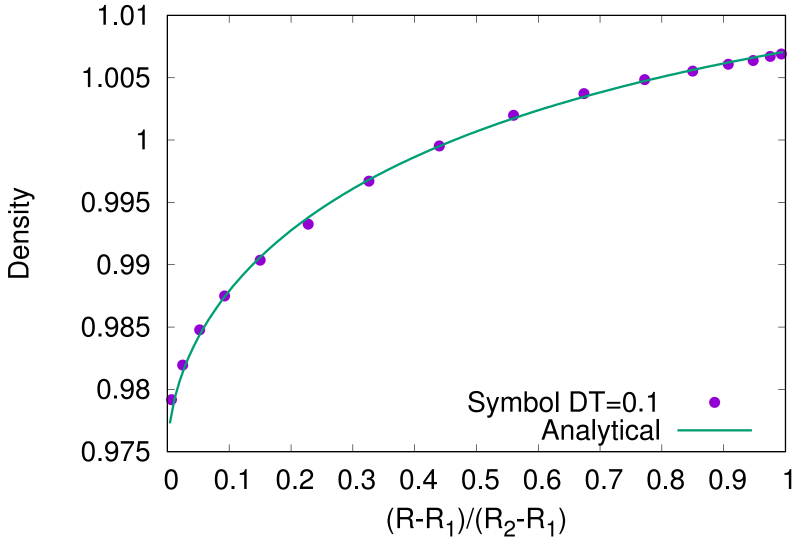


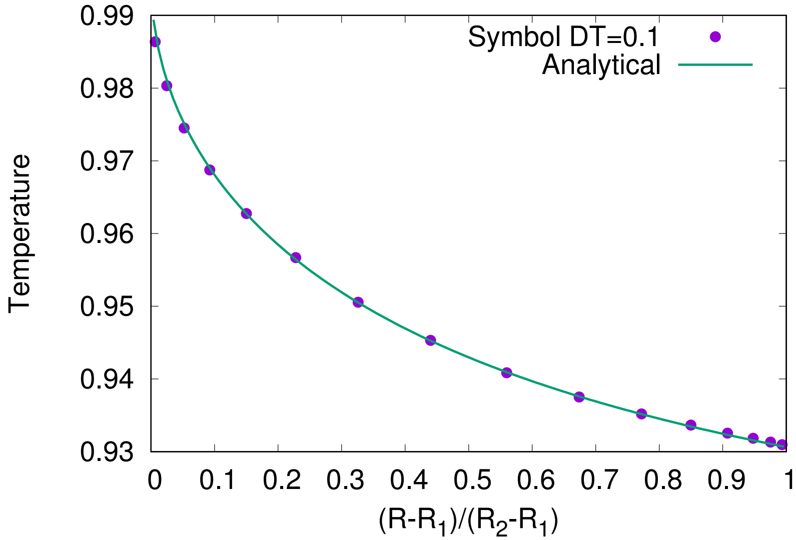


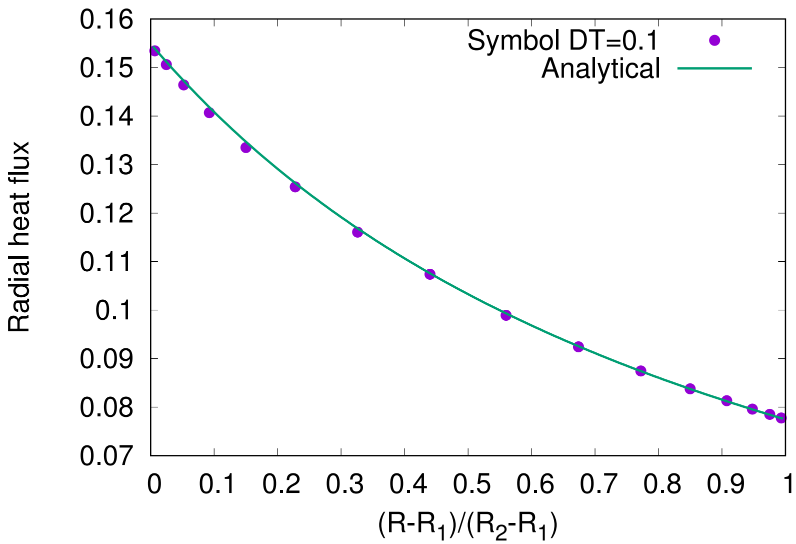


Profiles of number density, temperature for a wall temperature spread $\Delta T = 0.1$.

Heat transfer - cylindrical symmetry $Kn \to \infty$







Profiles of number density, temperature for a wall temperature spread $\Delta T = 0.1$.

Conclusion

- We introduced the Boltzmann equation written with respect to orthogonal vielbeins.
- The vielbeins allow the coupling between the momentum space and the coordinate space, i.e. $\mathbf{p}^2$ is coordinate-independent.
- The vielbein permits the momentum space degrees of freedom to be aligned according to the symmetries of the flow.
- We considered the shear flow between two coaxial cylinders and heat transfer in cylindrical and spherical geometries: problems which become one-dimensional in space since the vielbein allows the symmetry of the geometry to be transferred to the momentum space.
- Our models give accurate results throughout the whole range of Knudsen number.

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- Everybody who contributed to this work is an author or has been formaly acknowledged.

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