Analytical and numerical solutions of the regularized 13 moment equations for rarefied gases

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The task of finding continuum approximations

conservation laws for mass, momentum, energy

$\Longrightarrow$ 5 equations for ρ, v_i, $\theta = RT$

$$\frac{D\rho}{Dt} + \rho\frac{\partial v_k}{\partial x_k} = 0$$

$$\rho\frac{Dv_i}{Dt} + \rho\frac{\partial \theta}{\partial x_i} + \theta\frac{\partial \rho}{\partial x_i} + \left[\frac{\partial \sigma_{ik}}{\partial x_k}\right] = 0$$

$$\frac{3}{2}\rho\frac{D\theta}{Dt} + \rho\theta\frac{\partial v_k}{\partial x_k} + \left[\frac{\partial q_k}{\partial x_k} + \sigma_{kl}\frac{\partial v_k}{\partial x_l}\right] = 0$$

closure problem

find additional equations for pressure deviator σ_{ij} and heat flux q_i

Boltzmann equation and moments

Boltzmann equation

$$\frac{\partial f}{\partial t} + c_k \frac{\partial f}{\partial x_k} = \frac{1}{\mathrm{Kn}} \mathcal{S}\left(f\right)$$ e.g. BGK-model: $\mathcal{S}(f) = -\frac{1}{\tau}(f - f_M)$

some moments

mass density	$\rho = m \int f \, d\mathbf{c}$
momentum density	$\rho v_i = m \int c_i f \, d\mathbf{c}$
energy density	$\rho u = \frac{3}{2}\rho\theta = \frac{m}{2} \int C^2 f \, d\mathbf{c}$
pressure tensor	$p_{ij} = p\delta_{ij} + \sigma_{ij} = m \int C_i C_j f d\mathbf{c}$
heat flux vector	$q_i = \frac{m}{2} \int C^2 C_i f d\mathbf{c}$
general moments	$u^a_{i_1 \cdots i_n} = m \int C^{2a} C_{\langle i_1} \cdots C_{i_n \rangle} f d\mathbf{c}$

ideal gas law: $p = \rho\theta$

peculiar velocity: $C_i = c_i - v_i$

equilibrium phase density (Maxwell): $f_{|E} = \frac{\rho}{m} \sqrt{\frac{1}{2\pi\theta}}^3 \exp\left[-\frac{C^2}{2\theta}\right]$

$\mathrm{Kn} = \frac{\text{mean free path } l_0}{\text{macroscopic length scale } L}$: Knudsen number $\hat{=}$ smallness parameter

Bulk reduction methods

$$\mathrm{Kn} = \frac{\text{mean free path}}{\text{macroscopic length scale}}$$

goal: Replace Boltzmann eq with simplified models for Knudsen number $\mathrm{Kn} < 1$

- **Chapman-Enskog expansion** in powers of Kn
  - $\Longrightarrow$ Euler, Navier-Stokes-Fourier [Enskog 1917, Chapman 1916/17]
  - $\Longrightarrow$ Burnett, super-Burnett (*unstable*) [Burnett 1935, Bobylev 1981]
  - $\Longrightarrow$ augmented Burnett (*stable*) [Zhong et al. 1993]
  - $\Longrightarrow$ hyperbolic Burnett (*stable*) [Bobylev 2007/08]
- **Grad's moment method** (choice of moments not related to Kn) [Grad 1949]
  - $\Longrightarrow$ Euler, 13 moments, 26 moments, etc. (*discontinuous shocks*)
- **Regularization of 13 moment equations** (based on Kn orders)
  - $\Longrightarrow$ linear **R13 eqs** [Karlin et al. 1998]
  - $\Longrightarrow$ Regularized Burnett [Jin & Slemrod 2001]
  - $\Longrightarrow$ Consistent order ET [Müller et al. 2003]
  - $\Longrightarrow$ **Combined Grad/CE** $\Longrightarrow$ **R13 eqs** [HS & M. Torrilhon 2003/04]
  - $\Longrightarrow$ **Order of magnitude method** $\Longrightarrow$ **R13 eqs** [HS 2004]

R13 equations (non-linear) [HS & MT 2003, HS 2004]

(Euler / NSF / Grad13 / R13)

$$\frac{D\rho}{Dt} + \rho\frac{\partial v_k}{\partial x_k} = 0$$

$$\rho\frac{Dv_i}{Dt} + \rho\frac{\partial \theta}{\partial x_i} + \theta\frac{\partial \rho}{\partial x_i} + \left[\frac{\partial \sigma_{ik}}{\partial x_k}\right] = \rho G_i$$

$$\frac{3}{2}\rho\frac{D\theta}{Dt} + \rho\theta\frac{\partial v_k}{\partial x_k} + \left[\frac{\partial q_k}{\partial x_k} + \sigma_{kl}\frac{\partial v_k}{\partial x_l}\right] = 0$$

$$\left[\frac{D\sigma_{ij}}{Dt} + \frac{4}{5}\frac{\partial q_{\langle i}}{\partial x_{j\rangle}} + 2\sigma_{k\langle i}\frac{\partial v_{j\rangle}}{\partial x_k} + \sigma_{ij}\frac{\partial v_k}{\partial x_k}\right] + \left[\frac{\partial u^0_{ijk}}{\partial x_k}\right] = -\rho\theta\left[\frac{\sigma_{ij}}{\mu} + 2\frac{\partial v_{\langle i}}{\partial x_{j\rangle}}\right]$$

$$\left[\frac{Dq_i}{Dt} + \frac{5}{2}\sigma_{ik}\frac{\partial \theta}{\partial x_k} - \sigma_{ik}\theta\frac{\partial \ln \rho}{\partial x_k} + \theta\frac{\partial \sigma_{ik}}{\partial x_k} + \frac{7}{5}q_i\frac{\partial v_k}{\partial x_k} + \frac{7}{5}q_k\frac{\partial v_i}{\partial x_k} + \frac{2}{5}q_k\frac{\partial v_k}{\partial x_i}\right] + \left[-\frac{\sigma_{ij}}{\varrho}\frac{\partial \sigma_{jk}}{\partial x_k} + \frac{1}{2}\frac{\partial w^1_{ik}}{\partial x_k} + \frac{1}{6}\frac{\partial w^2}{\partial x_i} + u^0_{ijk}\frac{\partial v_j}{\partial x_k}\right] = -\frac{5}{2}\rho\theta\left[\frac{q_i}{\kappa} + \frac{\partial \theta}{\partial x_i}\right]$$

$$w^2 = -\frac{\sigma_{ij}\sigma_{ij}}{\rho} - 12\frac{\mu}{p}\left[\theta\frac{\partial q_k}{\partial x_k} + \frac{5}{2}q_k\frac{\partial \theta}{\partial x_k} - \theta q_k\frac{\partial \ln \rho}{\partial x_k} + \theta\sigma_{ij}\frac{\partial v_i}{\partial x_k}\right]$$

$$u^0_{ijk} = -2\,\frac{\mu}{p}\left[\theta\frac{\partial \sigma_{\langle ij}}{\partial x_{k\rangle}} - \sigma_{\langle ij}\frac{\partial \ln \rho}{\partial x_{k\rangle}} + \frac{4}{5}q_{\langle i}\frac{\partial v_j}{\partial x_{k\rangle}}\right]$$

$$w^1_{ij} = -\frac{4}{7}\frac{\sigma_{k\langle i}\sigma_{j\rangle k}}{\rho} - \frac{24}{5}\frac{\mu}{p}\left[\theta\frac{\partial q_{\langle i}}{\partial x_{j\rangle}} + q_{\langle i}\frac{\partial \theta}{\partial x_{j\rangle}} - \theta q_{\langle i}\frac{\partial \ln \rho}{\partial x_{j\rangle}} + \frac{5}{7}\theta\left(\sigma_{k\langle i}\frac{\partial v_{j\rangle}}{\partial x_k} + \sigma_{k\langle i}\frac{\partial v_k}{\partial x_{j\rangle}} - \frac{2}{3}\sigma_{ij}\frac{\partial v_k}{\partial x_k}\right)\right]$$

Chapman-Enskog expansion of R13 ⇒ Euler / NSF / Burnett / super-Burnett

R13 equations (linear, dimensionless) [HS & MT 2003]

(Euler / NSF / Grad13 / R13)

$$\frac{\partial \rho}{\partial t} + \frac{\partial v_k}{\partial x_k} = 0$$

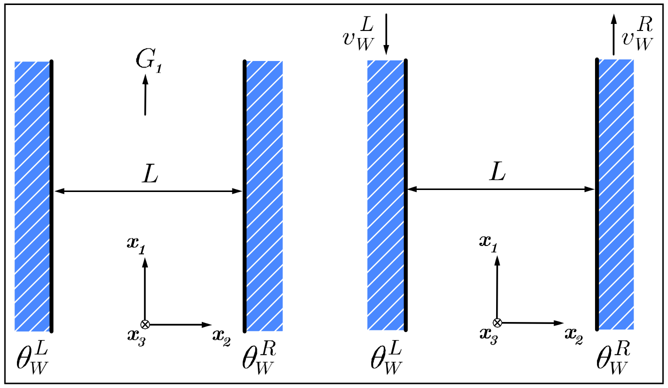
$$\frac{\partial v_i}{\partial t} + \frac{\partial \rho}{\partial x_i} + \frac{\partial \theta}{\partial x_i} + \frac{\partial \sigma_{ik}}{\partial x_k} = G_i$$

$$\frac{3}{2}\frac{\partial \theta}{\partial t} + \frac{\partial v_k}{\partial x_k} + \frac{\partial q_k}{\partial x_k} = 0$$

$$\frac{\partial \sigma_{ij}}{\partial t} + \frac{4}{5}\frac{\partial q_{\langle i}}{\partial x_{j\rangle}} - 2\mathrm{Kn}\frac{\partial}{\partial x_k}\frac{\partial \sigma_{\langle ij}}{\partial x_{k\rangle}} + 2\frac{\partial v_{\langle i}}{\partial x_{j\rangle}} = -\frac{\sigma_{ij}}{\mathrm{Kn}}$$

$$\frac{\partial q_i}{\partial t} + \frac{\partial \sigma_{ik}}{\partial x_k} - \frac{12}{5}\mathrm{Kn}\frac{\partial}{\partial x_k}\frac{\partial q_{\langle i}}{\partial x_{k\rangle}} - 2\mathrm{Kn}\frac{\partial}{\partial x_i}\frac{\partial q_k}{\partial x_k} + \frac{5}{2}\frac{\partial \theta}{\partial x_i} = -\frac{2}{3}\frac{q_i}{\mathrm{Kn}}$$

Semi-linearized R13 for shear flow (dimless) [PT, MT & HS 2009]



include quadratic contributions in σ_{12}, $\dfrac{dv_1}{dx_2}$

velocity problem

$$\frac{d\sigma_{12}}{dx_2} = G_1$$

$$\frac{2}{5}\frac{dq_1}{dx_2} - \frac{16}{15}\mathrm{Kn}\frac{d^2\sigma_{12}}{dx_2^2} + \frac{dv_1}{dx_2} = -\frac{1}{\mathrm{Kn}}\sigma_{12}$$

$$\frac{d\sigma_{12}}{d\tilde{x}_2} - \frac{6}{5}\mathrm{Kn}\frac{d^2 q_1}{dx_2^2} = -\frac{2}{3}\frac{1}{\mathrm{Kn}}q_1$$

temperature problem

$$\frac{dq_2}{dx_2} = -\sigma_{12}\frac{dv_1}{dx_2}$$

$$\frac{d\sigma_{22}}{dx_2} - \frac{13}{7}\sigma_{12}\frac{d\sigma_{12}}{dx_2} - \frac{67}{105}\mathrm{Kn}\frac{d\sigma_{12}}{dx_2}\frac{dv_1}{dx_2} + \frac{36}{35}\mathrm{Kn}\sigma_{12}\frac{d^2 v_1}{dx_2^2} + \frac{5}{2}\frac{d\theta}{dx_2} = -\frac{2}{3}\frac{1}{\mathrm{Kn}}q_2$$

$$-\frac{6}{5}\sigma_{12}\frac{dv_1}{dx_2} - \frac{6}{5}\mathrm{Kn}\frac{d^2\sigma_{22}}{dx_2^2} - \frac{12}{25}\mathrm{Kn}^2\frac{d}{dx_2}\left(\frac{d\sigma_{12}}{dx_2}\frac{dv_1}{dx_2}\right) = -\frac{1}{\mathrm{Kn}}\sigma_{22}$$

the rest

$$\frac{d(\rho + \theta + \sigma_{22})}{dx_2} = 0$$

$$\frac{8}{5}\sigma_{12}\frac{dv_1}{dx_2} - \frac{2}{3}\mathrm{Kn}\frac{d^2\sigma_{11}}{dx_2^2} + \frac{4}{15}\mathrm{Kn}\frac{d^2\sigma_{22}}{dx_2^2} + \frac{16}{25}\mathrm{Kn}^2\frac{d}{dx_2}\left(\frac{d\sigma_{12}}{dx_2}\frac{dv_1}{dx_2}\right) = -\frac{1}{\mathrm{Kn}}\sigma_{11}$$

Boundary conditions for moments [MT & HS 2008]

kinetic BC for odd fluxes (at left and right boundary)

$$\textbf{slip} \quad \sigma_{nt} = -\frac{\chi}{2-\chi}\sqrt{\frac{2}{\pi\theta}}\left[PV_t + \frac{1}{5}q_t + \frac{1}{2}u^0_{tnn}\right]$$

$$\textbf{jump} \quad q_n = -\frac{\chi}{2-\chi}\sqrt{\frac{2}{\pi\theta}}\left[2P\left(\theta-\theta_W\right) + \frac{5}{28}w_{nn} + \frac{1}{15}w_{kk} + \frac{1}{2}\theta\sigma_{nn} - \frac{1}{2}PV_t^2\right]$$

$$w_{tn} = \frac{\chi}{2-\chi}\sqrt{\frac{2}{\pi\theta}}\left[P\theta V_t - \frac{1}{2}\theta u^0_{tnn} - \frac{11}{5}\theta q_t - PV_t^3 + 6P\left(\theta-\theta_W\right)V_t\right]$$

$$u^0_{nnn} = \frac{\chi}{2-\chi}\sqrt{\frac{2}{\pi\theta}}\left[\frac{2}{5}P\left(\theta-\theta_W\right) - \frac{1}{14}w_{nn} + \frac{1}{75}w_{kk} - \frac{7}{5}\sigma_{nn} - \frac{3}{5}PV_t^2\right]$$

$$u^0_{ttn} + \frac{1}{2}u^0_{nnn} = -\frac{\chi}{2-\chi}\sqrt{\frac{2}{\pi\theta}}\left[\theta\left(\sigma_{tt} + \frac{1}{2}\sigma_{nn}\right) + \frac{1}{14}\left(w_{tt} + \frac{1}{2}w_{nn}\right) - \frac{1}{2}PV_t^2\right]$$

with $V_t = v_t - v_t^W$, $P = \left(\rho\theta + \frac{1}{2}\sigma_{nn} - \frac{1}{28}\frac{w_{nn}}{\theta} - \frac{1}{120}\frac{w_{kk}}{\theta}\right)$

indices n, t indicate normal/tangential components

mass conservation

$$M = \int_{-L/2}^{L/2} \rho dx$$

Semi-linear channel flow $\Longrightarrow$ well-posed problem!

kinetic BC for R13 pioneered by [Gu&Emerson 2007], **but too many BC lead to spurious wall layers**

H-Theorem at wall in linear case [HS & MT 2007]

Analytical solution for Couette flow [PT, MT & HS 2008]

velocity problem

$$v_1 = -\frac{\mathsf{C}_1}{\mathrm{Kn}} x_2 - \frac{2}{5} q_1$$

$$\sigma_{12} = \mathsf{C}_1$$

$$q_1 = \mathsf{C}_2 \sinh\left[\frac{\sqrt{5}}{3\mathrm{Kn}} x_2\right]$$

temperature problem

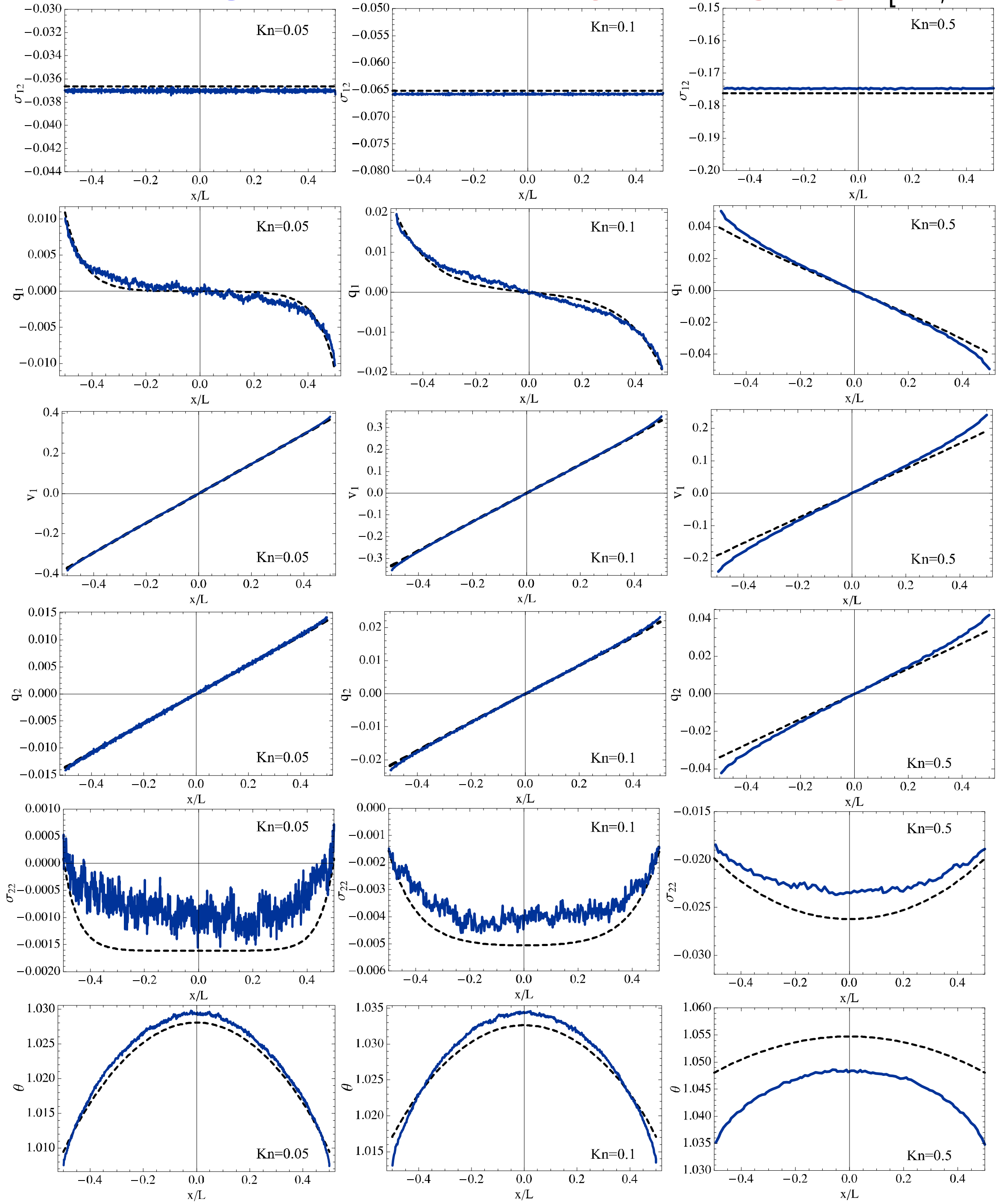
$$\theta = \mathsf{C}_3 - \frac{2\mathsf{C}_1^2}{15\mathrm{Kn}^2} x_2^2 - \frac{2\mathsf{C}_4}{5} \cosh\left[\frac{\sqrt{5}x_2}{\sqrt{6}\mathrm{Kn}}\right] + \frac{32\mathsf{C}_2}{35\sqrt{5}} \sigma_{12} \cosh\left[\frac{\sqrt{5}x_2}{3\mathrm{Kn}}\right]$$

$$\sigma_{22} = \mathsf{C}_4 \cosh\left[\frac{\sqrt{5}x_2}{\sqrt{6}\mathrm{Kn}}\right] - \frac{6\mathsf{C}_1^2}{5} - \frac{12\mathsf{C}_2}{5\sqrt{5}} \sigma_{12} \cosh\left[\frac{\sqrt{5}x_2}{3\mathrm{Kn}_0}\right]$$

$$q_2 = \frac{\mathsf{C}_1^2}{\mathrm{Kn}} x_2 + \frac{2\mathsf{C}_2}{5} \sigma_{12} \sinh\left[\frac{\sqrt{5}x_2}{3\mathrm{Kn}}\right]$$

superpositions of bulk and Knudsen layer contributions

Analytical solution for Couette flow: R13 vs. DSMC [PT, MT & HS 2008]



Analytical solution for Poiseuille flow [PT, MT & HS 2008]

velocity problem

$$v_1 = \mathsf{C}_1 - \frac{G_1}{2\mathrm{Kn}_0} x_2^2 - \frac{2}{5} q_1$$

$$\sigma_{12} = G_1 x_2$$

$$q_1 = -\frac{3 G_1 \mathrm{Kn}}{2} + \mathsf{C}_2 \cosh\left[\frac{\sqrt{5} x_2}{3\mathrm{Kn}}\right]$$

temperature problem

$$\theta = \mathsf{C}_4 - \frac{G_1^2 x_2^4}{45\mathrm{Kn}^2} + \frac{488 G_1^2 x_2^2}{525} - \frac{2\mathsf{C}_3}{5} \cosh\left[\frac{\sqrt{5} x_2}{\sqrt{6}\mathrm{Kn}}\right] + \frac{956 G_1 \mathrm{Kn} \mathsf{C}_2}{375} \cosh\left[\frac{\sqrt{5} x_2}{3\mathrm{Kn}}\right] + \frac{32\mathsf{C}_2}{35\sqrt{5}} \sigma_{12} \sinh\left[\frac{\sqrt{5} x_2}{3\mathrm{Kn}}\right]$$

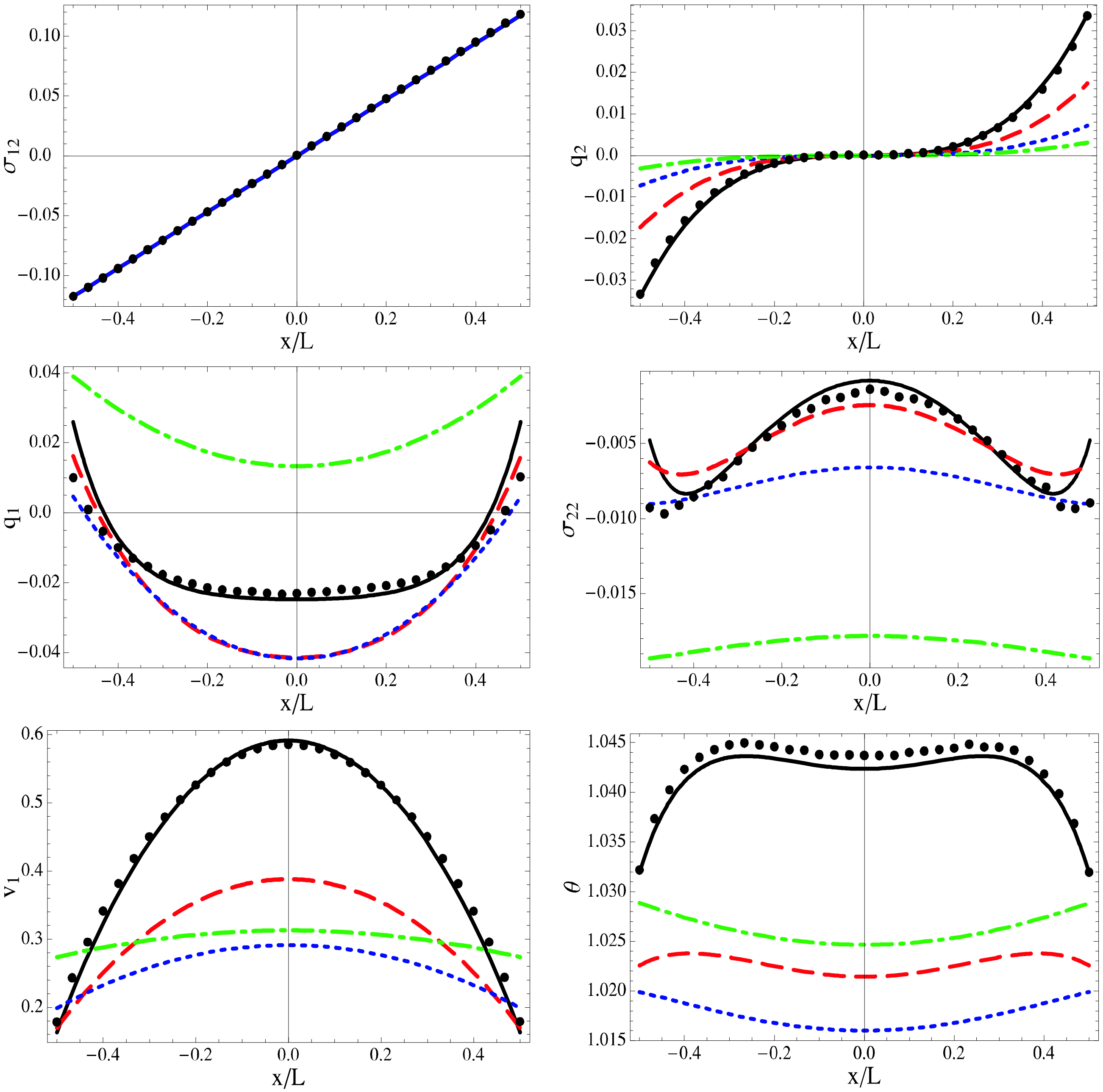
$$q_2 = \frac{G_1^2 x_2^3}{3\mathrm{Kn}} - \frac{6 G_1 \mathrm{Kn} \mathsf{C}_2}{5\sqrt{5}} \sinh\left[\frac{\sqrt{5} x_2}{3\mathrm{Kn}}\right] + \frac{2\mathsf{C}_2}{5} \sigma_{12} \cosh\left[\frac{\sqrt{5} x_2}{3\mathrm{Kn}}\right]$$

$$\sigma_{22} = -\frac{6 G_1^2}{5} x_2^2 - \frac{84 G_1^2 \mathrm{Kn}^2}{25} - \frac{152 G_1 \mathrm{Kn} \mathsf{C}_2}{25} \cosh\left[\frac{\sqrt{5} x_2}{3\mathrm{Kn}}\right] + \mathsf{C}_3 \cosh\left[\frac{\sqrt{5} x_2}{\sqrt{6}\mathrm{Kn}}\right] - \frac{12\mathsf{C}_2}{5\sqrt{5}} \sigma_{12} \sinh\left[\frac{\sqrt{5} x_2}{3\mathrm{Kn}}\right]$$

superpositions of bulk and Knudsen layer contributions

Force driven Poiseuille flow [PT, MT & HS 2008]

R13 equations exhibit temperature dip [Tij & Santos 1994/98, Xu 2003]



$$\theta = \mathsf{C}_4 - \frac{G_1^2}{\mathrm{Kn}^2}\left[\frac{y^4}{45} - \frac{488}{525}\,\mathrm{Kn}^2\,y^2\right]$$

$$- \mathsf{C}_3\,\frac{2}{5}\,\cosh\left[\frac{\sqrt{5}y}{\sqrt{6}\mathrm{Kn}}\right]$$

$$+ \mathsf{C}_2\,\frac{956}{375}\,G_1\,\mathrm{Kn}\,\cosh\left[\frac{\sqrt{5}y}{3\mathrm{Kn}}\right]$$

$$+ \mathsf{C}_2\,\frac{32}{35\sqrt{5}}\,\sigma_{12}\,\sinh\left[\frac{\sqrt{5}y}{3\mathrm{Kn}}\right]$$

superposition of

bulk solution

Knudsen layers

$\mathrm{Kn} = 0.072, 0.15, 0.4, 1.0$

R13 to 2nd order in the bulk (shear flow geometry) [HS & MT 2008]

conservation laws + Navier-Stokes-Fourier

$$\frac{\partial\tilde{\sigma}_{12}}{\partial y}=\rho\tilde{G}_1\ ,\quad \frac{\partial\left(p+\mathrm{Kn}^2\tilde{\sigma}_{22}\right)}{\partial y}=0\ ,\quad \frac{\partial\tilde{q}_2}{\partial y}=-\tilde{\sigma}_{12}\frac{\partial v}{\partial y}\ ,\quad \tilde{\sigma}_{12}=-\mu\frac{\partial v_1}{\partial y}\ ,\quad \tilde{q}_2=-\frac{15}{4}\mu\frac{\partial\theta}{\partial y}$$

second order contributions

$$\tilde{\sigma}_{11}=\frac{8}{5}\frac{\tilde{\sigma}_{12}\tilde{\sigma}_{12}}{p}\ ,\quad \tilde{\sigma}_{22}=-\frac{6}{5}\frac{\tilde{\sigma}_{12}\tilde{\sigma}_{12}}{p}\ ,\quad \tilde{q}_1=-\frac{3}{2}\frac{\mu\theta}{p}\frac{\partial\tilde{\sigma}_{12}}{\partial y}+\frac{7}{2}\frac{\tilde{\sigma}_{12}\tilde{q}_2}{p}$$

$$\tilde{\Delta}=-12\frac{\mu\theta}{p}\frac{\partial\tilde{q}_2}{\partial y}+\frac{56}{5}\frac{\tilde{q}_2\tilde{q}_2}{p}+10\frac{\theta}{p}\tilde{\sigma}_{12}\tilde{\sigma}_{12}\ ,\quad \tilde{R}_{22}=-\frac{16}{5}\frac{\mu\theta}{p}\frac{\partial\tilde{q}_2}{\partial y}+\frac{128}{75}\frac{\tilde{q}_2\tilde{q}_2}{p}+\frac{20}{21}\frac{\theta}{p}\tilde{\sigma}_{12}\tilde{\sigma}_{12}\ ,\quad \tilde{m}_{122}=-\frac{16}{15}\frac{\mu\theta}{p}\frac{\partial\tilde{\sigma}_{12}}{\partial y}+\frac{32}{45}\frac{\tilde{\sigma}_{12}\tilde{q}_2}{p}$$

jump and slip BC

$$\mathcal{V}=\frac{v_i-v_i^W}{\mathrm{Kn}}=-\frac{2-\chi_1}{\chi_1}\sqrt{\frac{\pi\theta}{2}}\frac{\tilde{\sigma}_{12}}{p}n_2-\frac{1}{5}\mathrm{Kn}\frac{\tilde{q}_1}{p}-\frac{1}{2}\mathrm{Kn}\frac{\tilde{m}_{122}}{p}$$

$$\mathcal{T}=\frac{\theta-\theta_W}{\mathrm{Kn}}=-\frac{2-\chi_2}{\chi_2}\sqrt{\frac{\pi\theta}{2}}\frac{\tilde{q}_2}{2p}n_2+\frac{1}{4}\mathrm{Kn}\mathcal{V}^2-\frac{1}{4}\theta\mathrm{Kn}\frac{\tilde{\sigma}_{22}}{p}-\frac{1}{60}\mathrm{Kn}\frac{\tilde{\Delta}}{p}-\frac{5}{56}\mathrm{Kn}\frac{\tilde{R}_{22}}{p}$$

second order jump and slip BC combine the above

$$v_i-v_i^W=-\frac{2-\chi_1}{\chi_1}\mathrm{Kn}\sqrt{\frac{\pi\theta}{2}}\frac{\tilde{\sigma}_{12}}{p}n_2+\frac{5}{6}\mathrm{Kn}^2\frac{\mu\theta}{p^2}\frac{\partial\tilde{\sigma}_{12}}{\partial y}-\frac{19}{18}\mathrm{Kn}^2\frac{\tilde{\sigma}_{12}\tilde{q}_2}{p^2}$$

$$\theta-\theta_W=-\frac{2-\chi_2}{\chi_2}\mathrm{Kn}\sqrt{\frac{\pi\theta}{2}}\frac{\tilde{q}_2}{2p}n_2+\frac{17}{35}\mathrm{Kn}^2\frac{\mu\theta}{p^2}\frac{\partial\tilde{q}_2}{\partial y}+\mathrm{Kn}^2\left[\frac{\pi}{8}\left(\frac{2-\chi_1}{\chi_1}\right)^2+\frac{71}{1470}\right]\theta\frac{\tilde{\sigma}_{12}\tilde{\sigma}_{12}}{p^2}-\mathrm{Kn}^2\frac{178}{525}\frac{\tilde{q}_2\tilde{q}_2}{p^2}$$

Force driven Poiseuille flow — Knudsen minimum [HS & MT 2008]

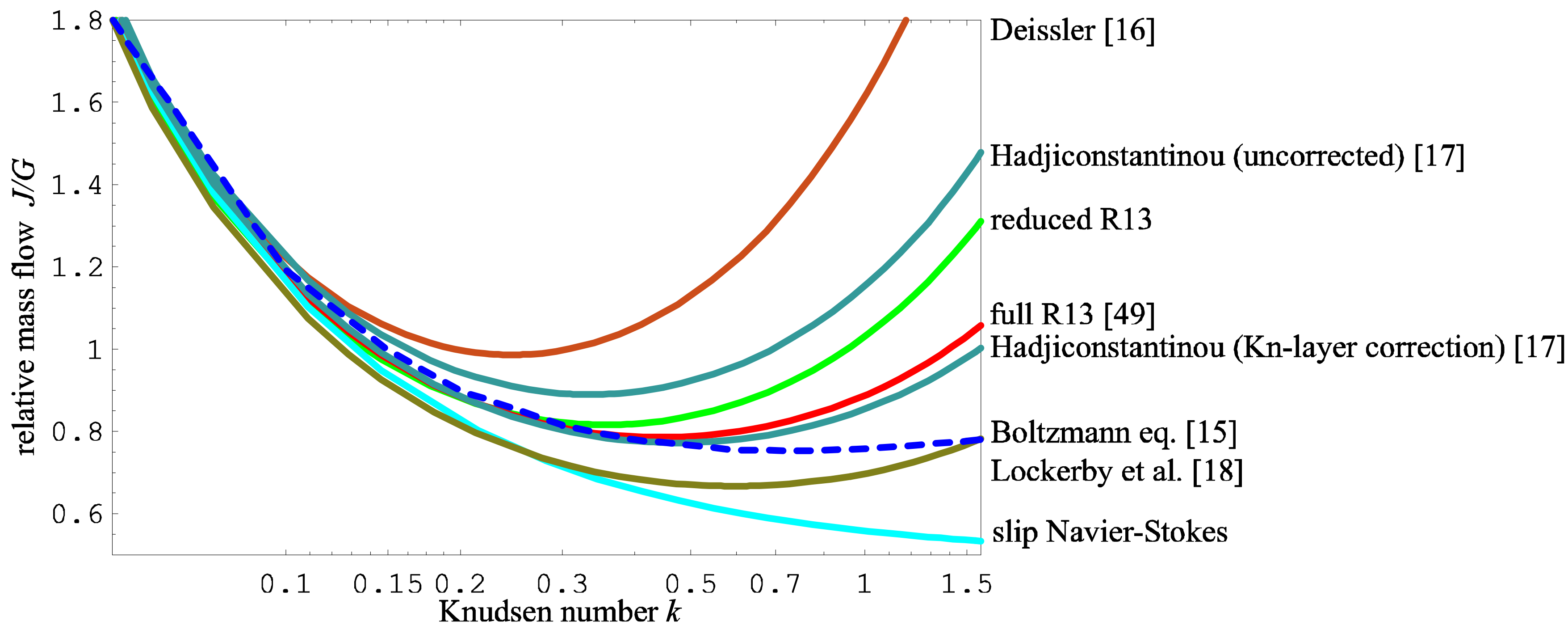
linearized Navier-Stokes with 2nd order slip (values for α and β vary between authors)

$$\frac{\partial \sigma_{12}}{\partial y} = G_1 \quad , \quad \sigma_{12} = -\frac{\partial v}{\partial y} \quad , \quad v - v_W = \alpha \mathrm{Kn} \sqrt{\frac{\pi}{2}} \frac{\partial v}{\partial y} n_2 - \beta \mathrm{Kn}^2 \frac{\partial^2 v}{\partial y^2}$$

average mass flux $J = \int v dy$

$$J_{NS} = \frac{G_1}{12\mathrm{Kn}} \left[1 + 6\sqrt{\tfrac{\pi}{2}} \ \alpha \ \mathrm{Kn} + 12 \ \beta \ \mathrm{Kn}^2 \right]$$

$$J_{R13} = \frac{G_1}{12\mathrm{Kn}} \left[1 + 6\sqrt{\tfrac{\pi}{2}} \left(1 + \frac{\frac{1}{4}\sqrt{\frac{2}{5\pi}}}{1+\frac{5\sqrt{5}}{12}} \right) \mathrm{Kn} + 12 \ \frac{\frac{8}{15}+\frac{17\sqrt{5}}{36}}{1+\frac{5\sqrt{5}}{12}} \ \mathrm{Kn}^2 - \frac{18}{25}\mathrm{Kn} \left(\frac{(1+5\mathrm{Kn})^2}{1+\frac{5\sqrt{5}}{12} \coth \frac{\sqrt{5}}{6\mathrm{Kn}})} - \frac{1+10\mathrm{Kn}}{1+\frac{5\sqrt{5}}{12})} \right) \right]$$



comparison suggests $\alpha = 1.046 \quad , \quad \beta = 0.823$

Absorption heating (similar to Knudsen minimum) [HS & MT 2008]

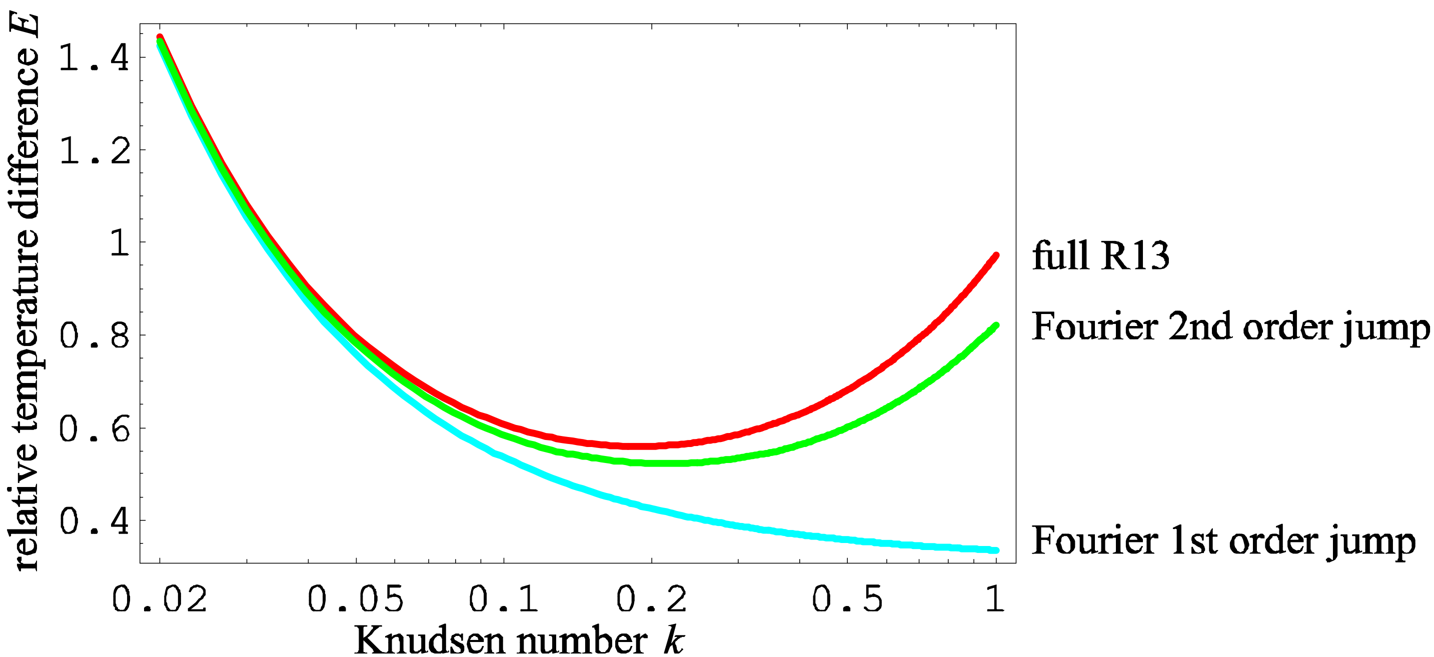
gas heated by radiation: gas at rest, walls at θ_W, energy absorbed S

average relative temperature $E = \int \frac{\theta - \theta_W}{S} dy$

Fourier and R13 (second order jump condition)

$$E_F = \frac{1}{45}\frac{1}{\mathrm{Kn}} + \frac{1}{4}\sqrt{\frac{\pi}{2}} + \frac{17}{35}\mathrm{Kn}$$

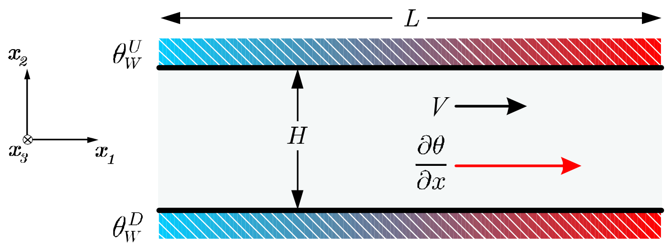
$$E_{R13} = \frac{1}{45}\frac{1}{\mathrm{Kn}} + \frac{13}{50}\sqrt{\frac{\pi}{2}} + \frac{18}{25}\mathrm{Kn} + \frac{\sqrt{\frac{6}{5}}\left(7\pi + 160\mathrm{Kn}\sqrt{\frac{\pi}{2}} + 384\mathrm{Kn}^2\right)}{140\left(15\coth\left[\sqrt{\frac{5}{6}}\frac{1}{2\mathrm{Kn}}\right] + 2\sqrt{15\pi}\right)}$$

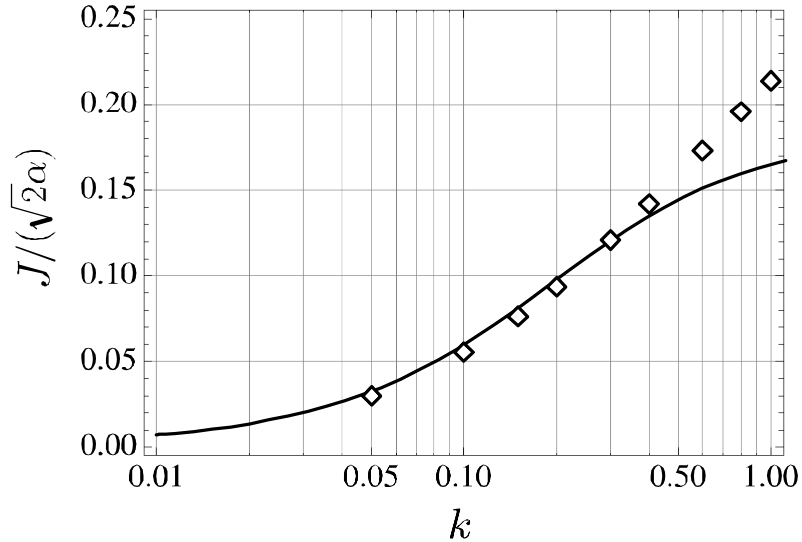


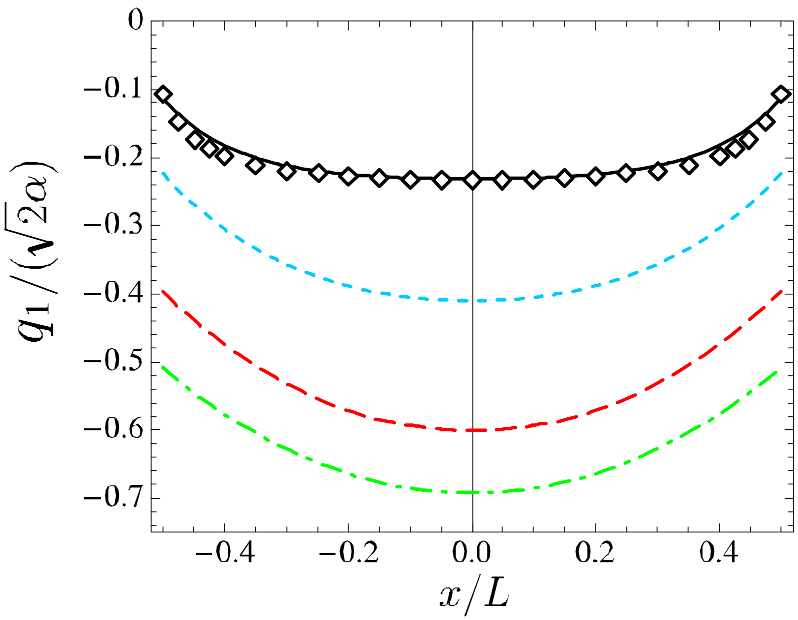
Thermal transpiration flow [PT & HS 2009]

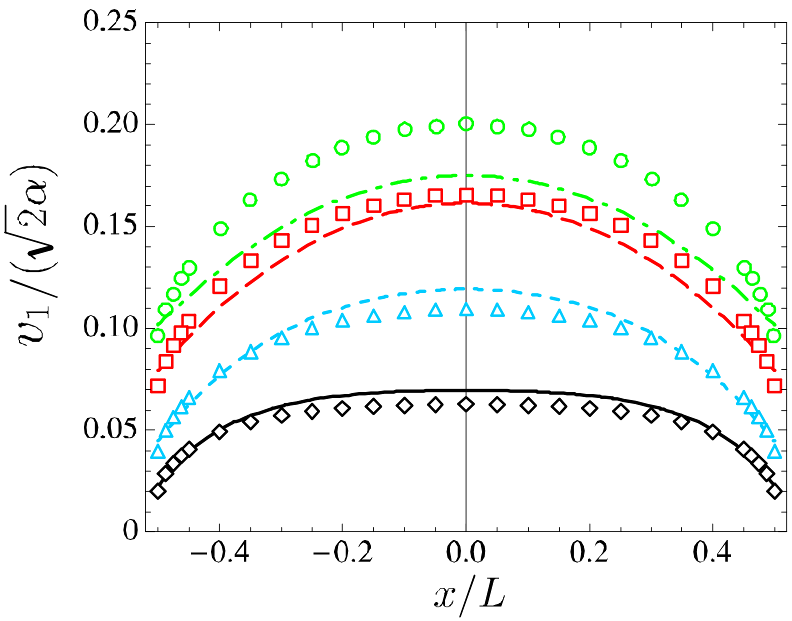
flow driven by T-gradient in wall $\mathrm{Kn} = 0.09, 0.18, 0.35, 0.53$

mass flow, heat flux, velocity : R13, linear Boltzmann [Ohwada, Aoki]



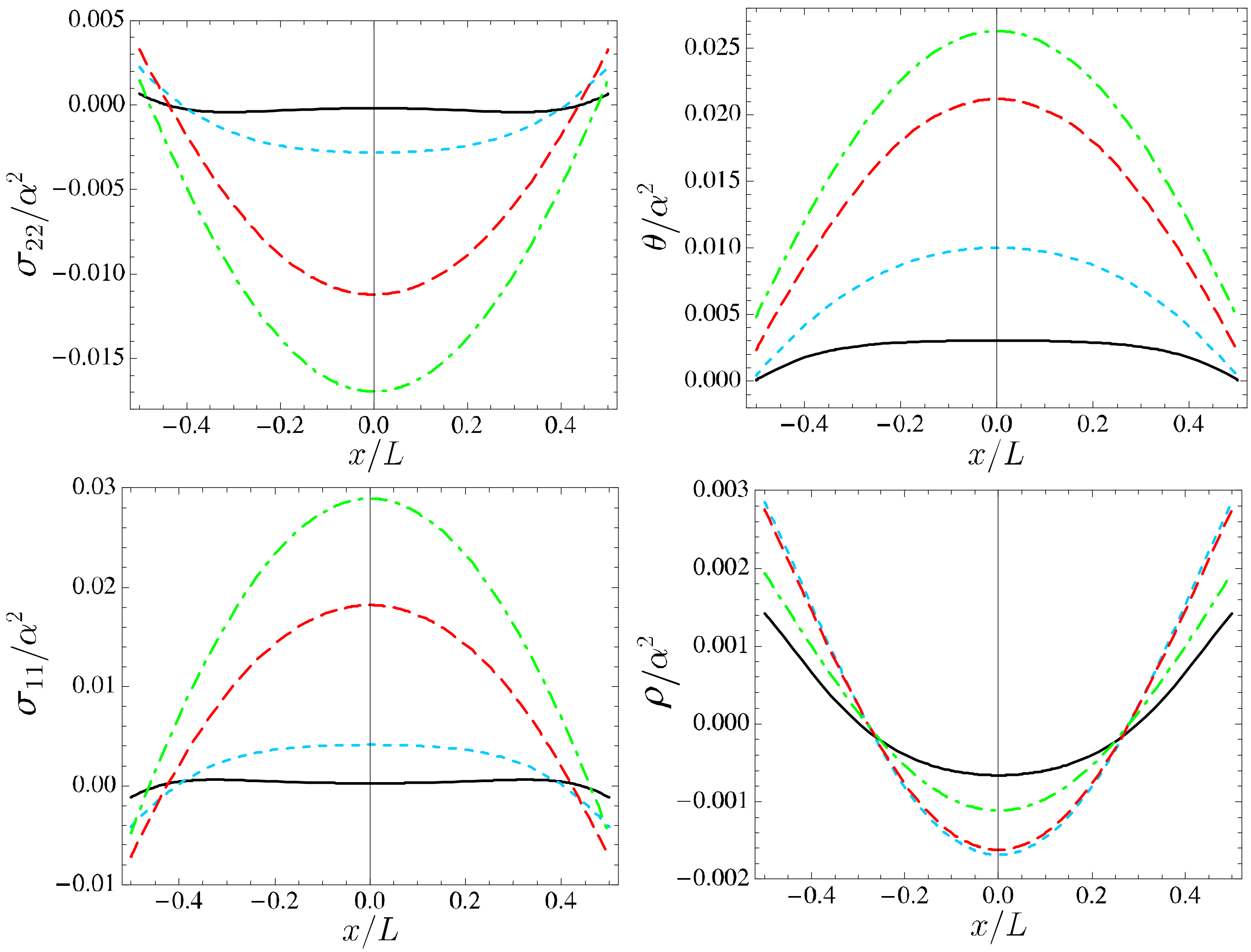






Thermal transpiration flow [PT & HS 2009]

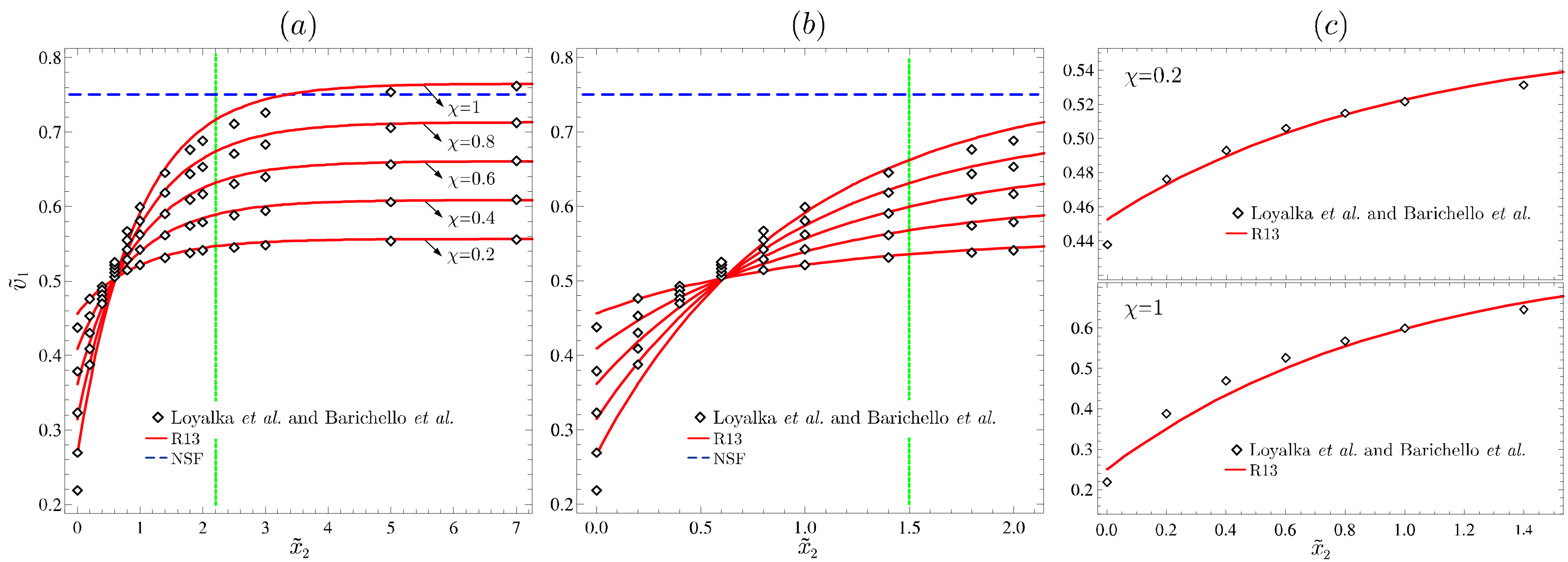
temperature profile and other non-linear effects: R13 prediction

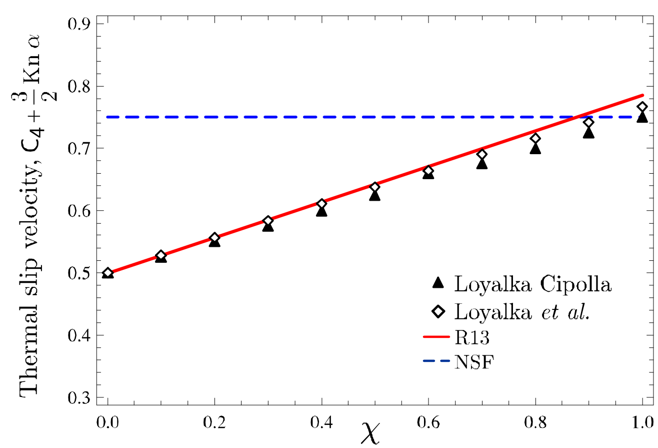


Thermal transpiration flow [PT & HS 2009]

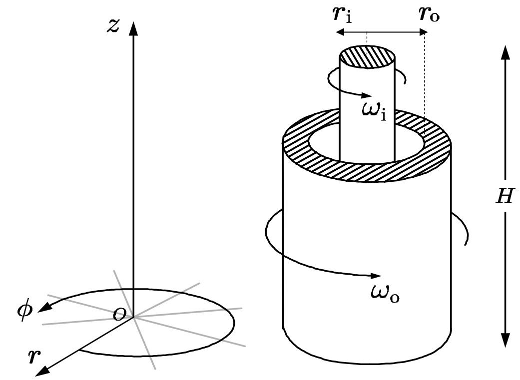
half space problem influence of accommodation coefficient χ

NSF / linearized Boltzmann / R13





Cylindrical flows [PT & HS 2009]



velocity problem (linear)

$$
\begin{aligned}
\frac{\partial \sigma_{r\phi}}{\partial r} + 2\frac{\sigma_{r\phi}}{r} &= 0 \\
\frac{\partial}{\partial r}\left[\frac{2}{5}\frac{q_\phi}{r} + \frac{v_\phi}{r}\right] &= -\frac{1}{\mathrm{Kn}}\frac{\sigma_{r\phi}}{r} \\
\frac{\partial}{\partial r}\left[\frac{\partial q_\phi}{\partial r} + \frac{q_\phi}{r}\right] &= \frac{5}{9\,\mathrm{Kn}^2} q_\phi
\end{aligned}
$$

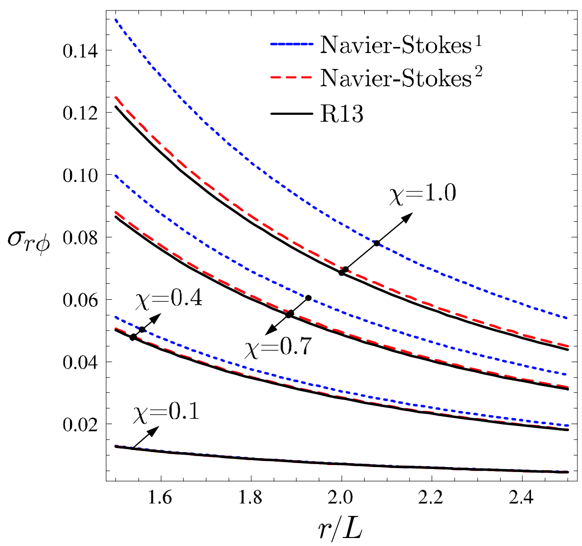
analytical solution

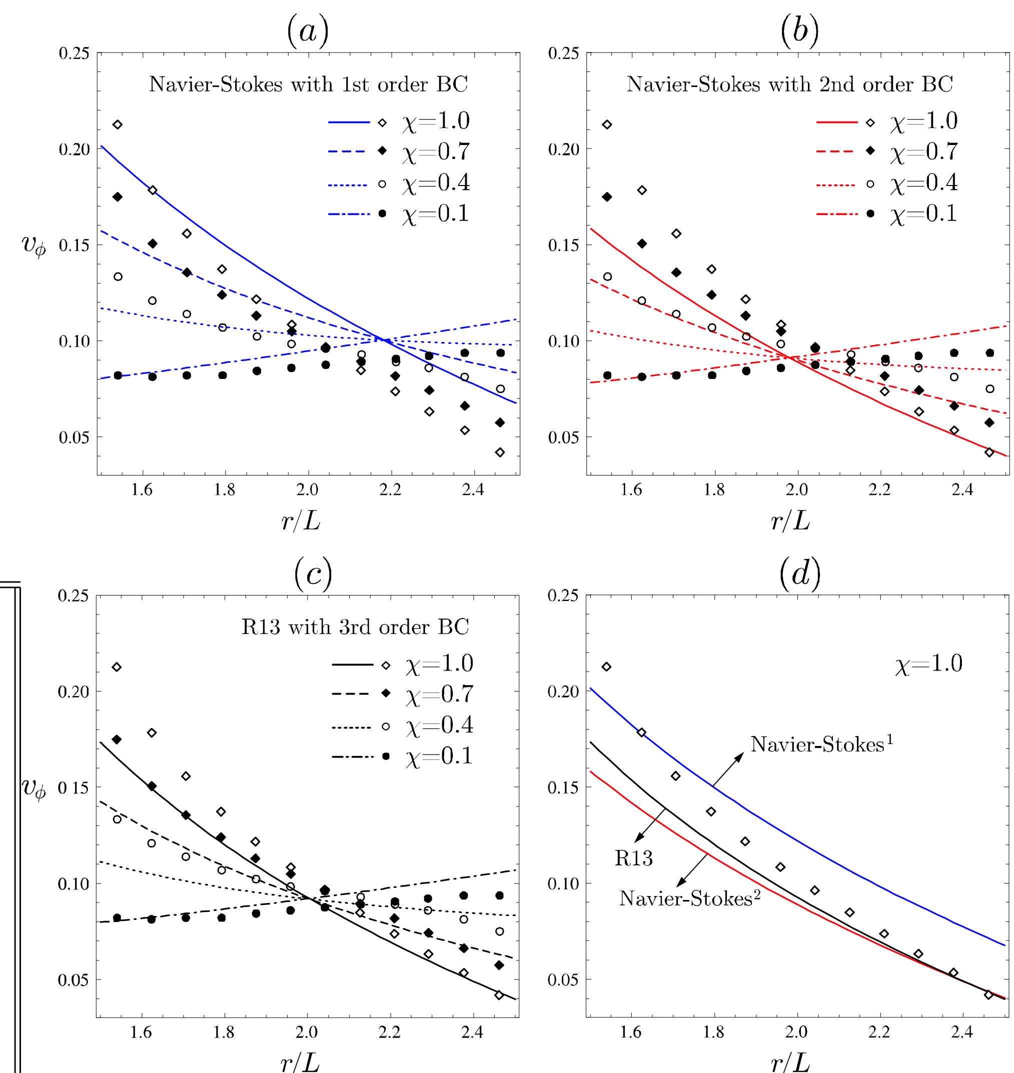
$$
\begin{aligned}
v_\phi &= \frac{\mathsf{C}_1}{2\,\mathrm{Kn}}\frac{1}{r} + \mathsf{C}_4 r - \frac{2}{5} q_\phi \\
\sigma_{r\phi} &= \frac{\mathsf{C}_1}{r^2} \\
q_\phi &= \mathsf{C}_2\,\mathcal{I}_1\left[\frac{\sqrt{5}r}{3\,\mathrm{Kn}}\right] + \mathsf{C}_3\,\mathcal{K}_1\left[\frac{\sqrt{5}r}{3\,\mathrm{Kn}}\right]
\end{aligned}
$$

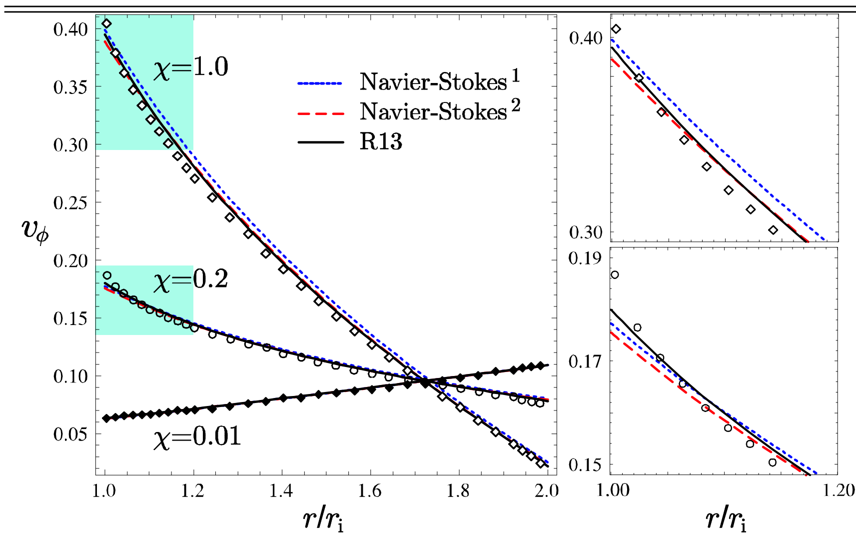
Knudsen layers are Bessel functions

Cylindrical flows [PT & HS 2009]

velocity problem $\mathrm{Kn} = 0.08$, $\mathrm{Kn} = 0.447$, accommodation coefficients χ [Aoki, Garcia]

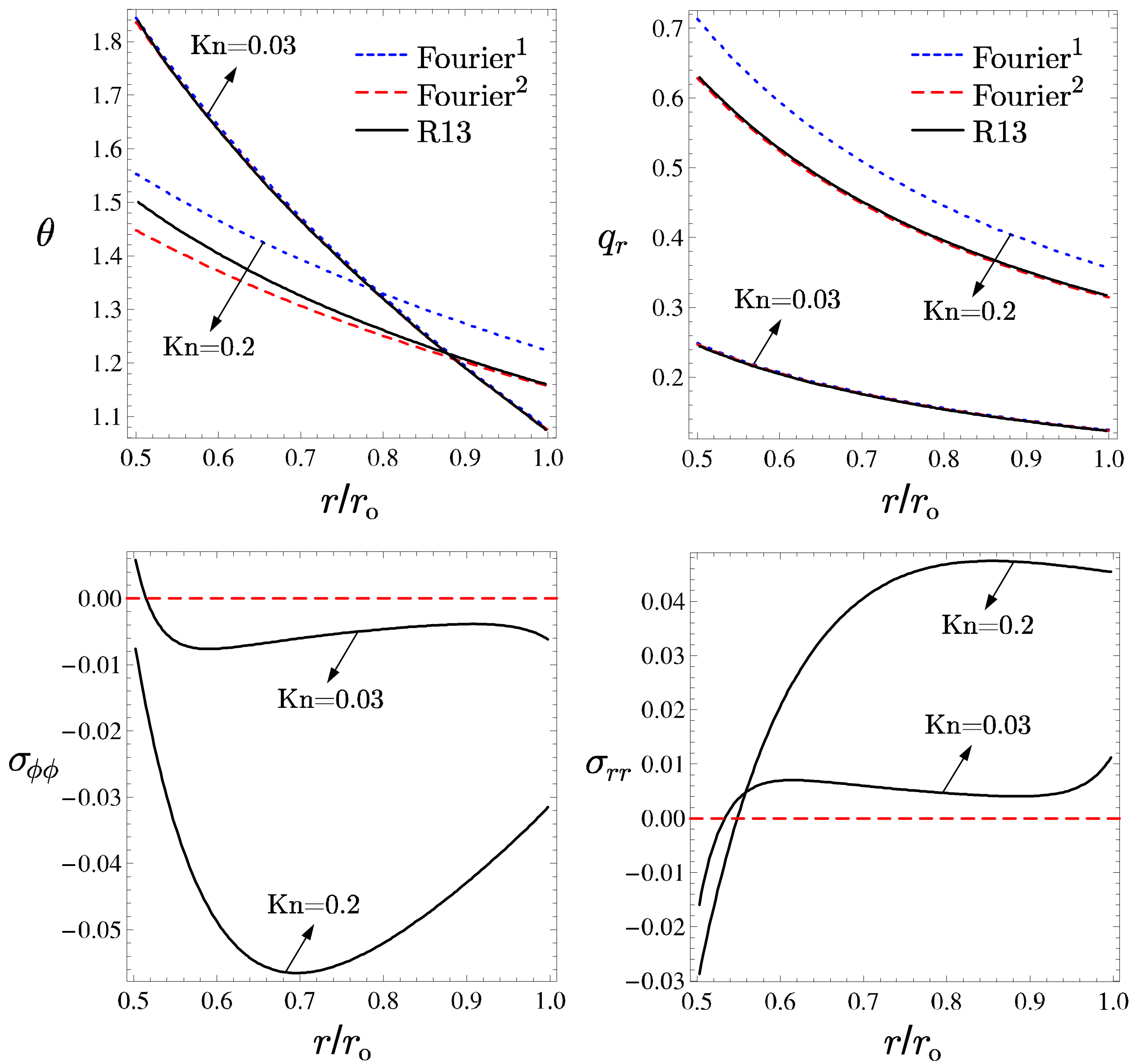






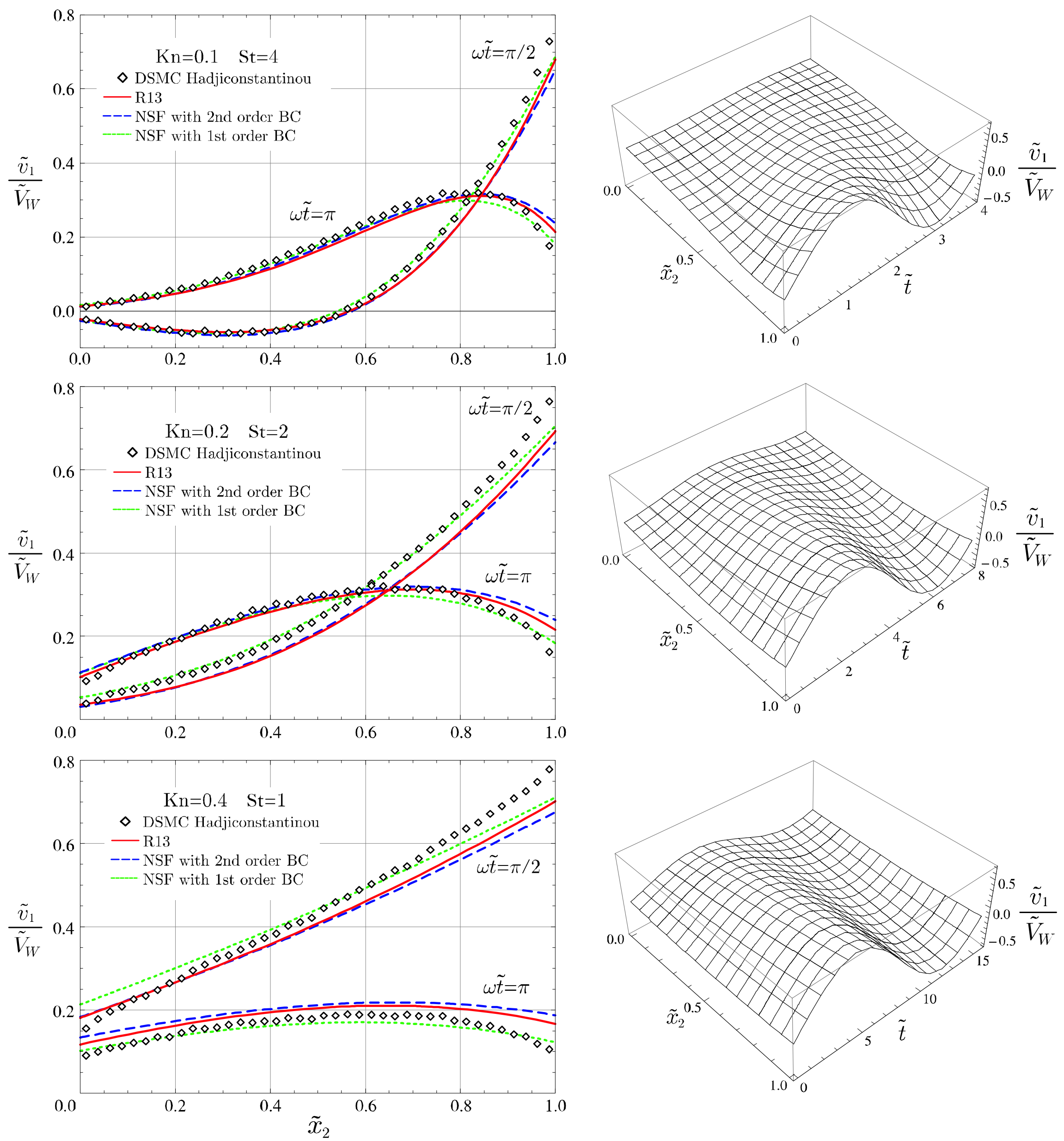
Cylindrical flows [PT & HS 2009]

temperature problem $\mathrm{Kn} = 0.03$, $\mathrm{Kn} = 0.2$ (numerical solution)



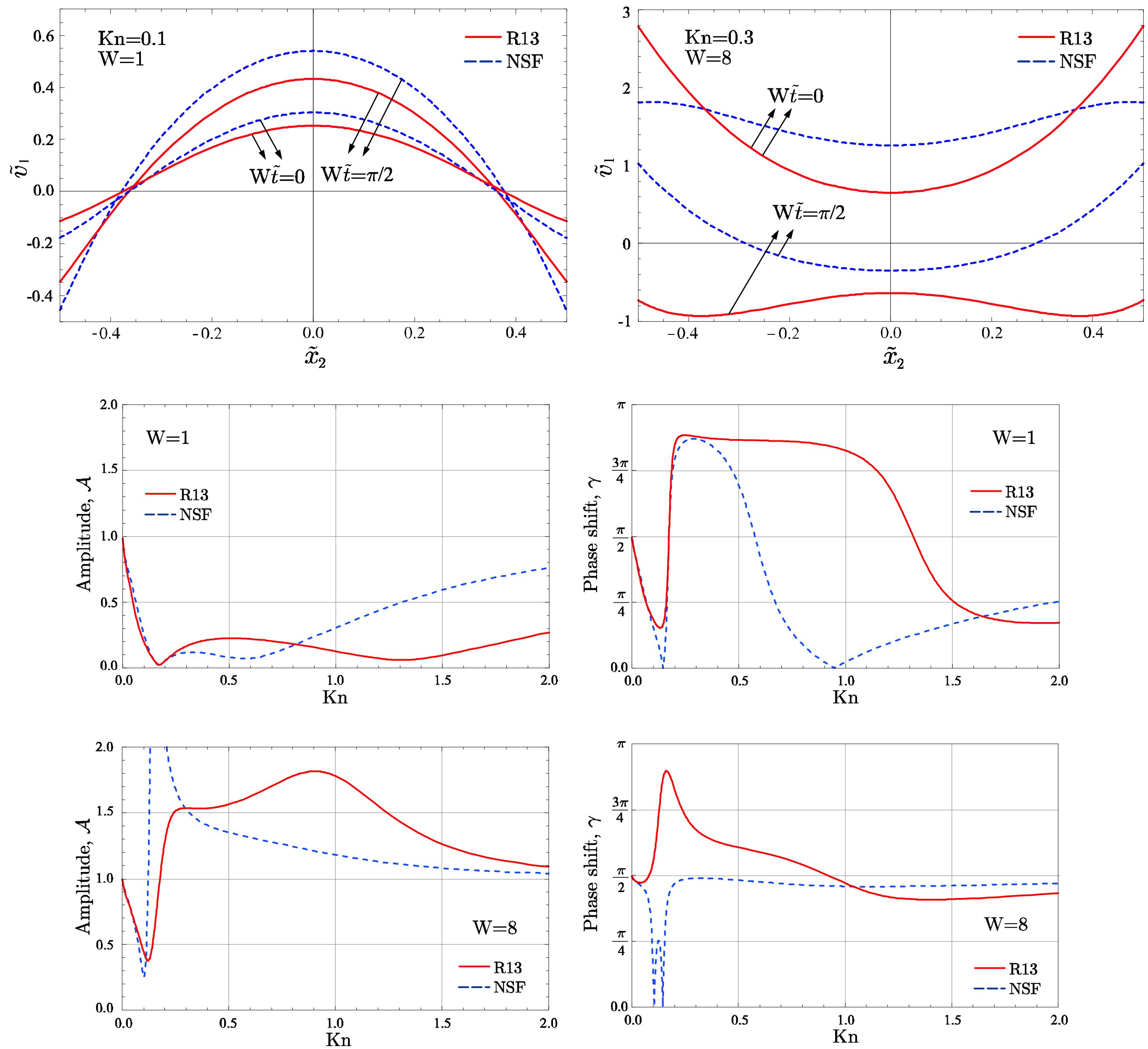
Oscillating Couette flow [PT, AR, MT & HS 2009]

$$v^w = v_0^w \sin \omega t \,, \quad \mathrm{Kn} = \frac{\mu_0}{\rho_0 \sqrt{\theta_0} H} \,, \quad \textbf{Stokes number } \mathrm{St} = H \sqrt{\frac{\rho_0 \, \omega}{\mu_0}}$$



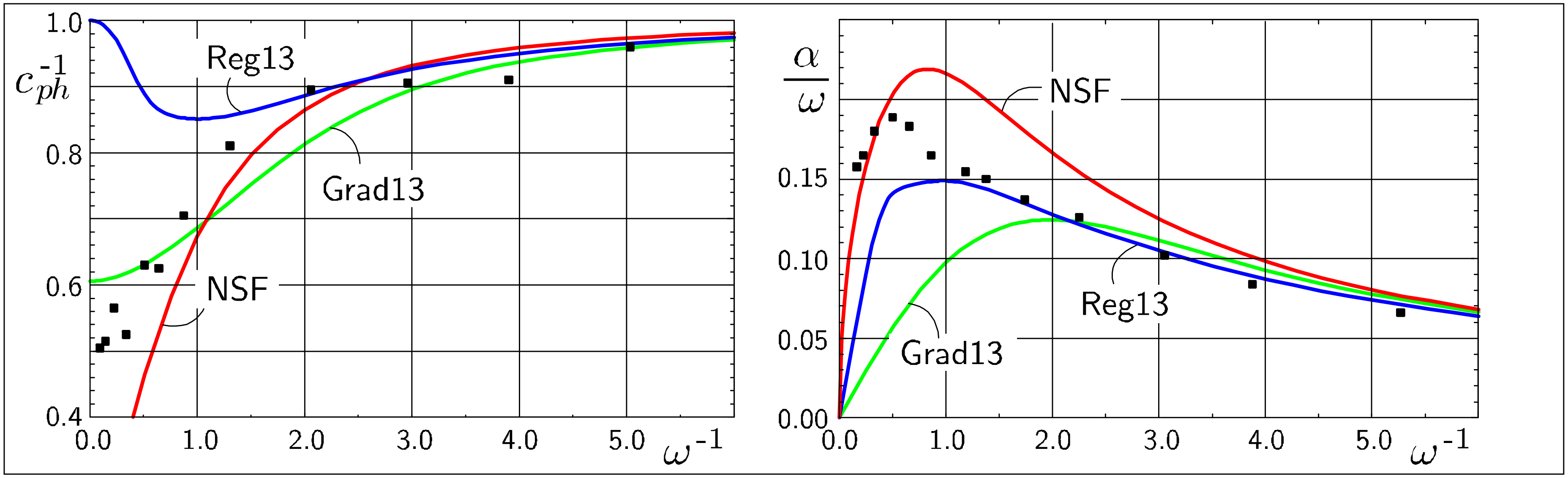
Oscillating Poiseuille flow [PT, AR, MT & HS 2009]

$G = G_0 \sin \omega t$, $\quad \mathrm{Kn} = \dfrac{\mu_0}{\rho_0 \sqrt{\theta_0} H}$ **dimensionless frequency** $\mathrm{W} = \dfrac{\omega H}{\sqrt{\theta_0}}$



Dispersion and Damping [HS & MT 2003]

phase speed and damping measured by Meyer and Sessler



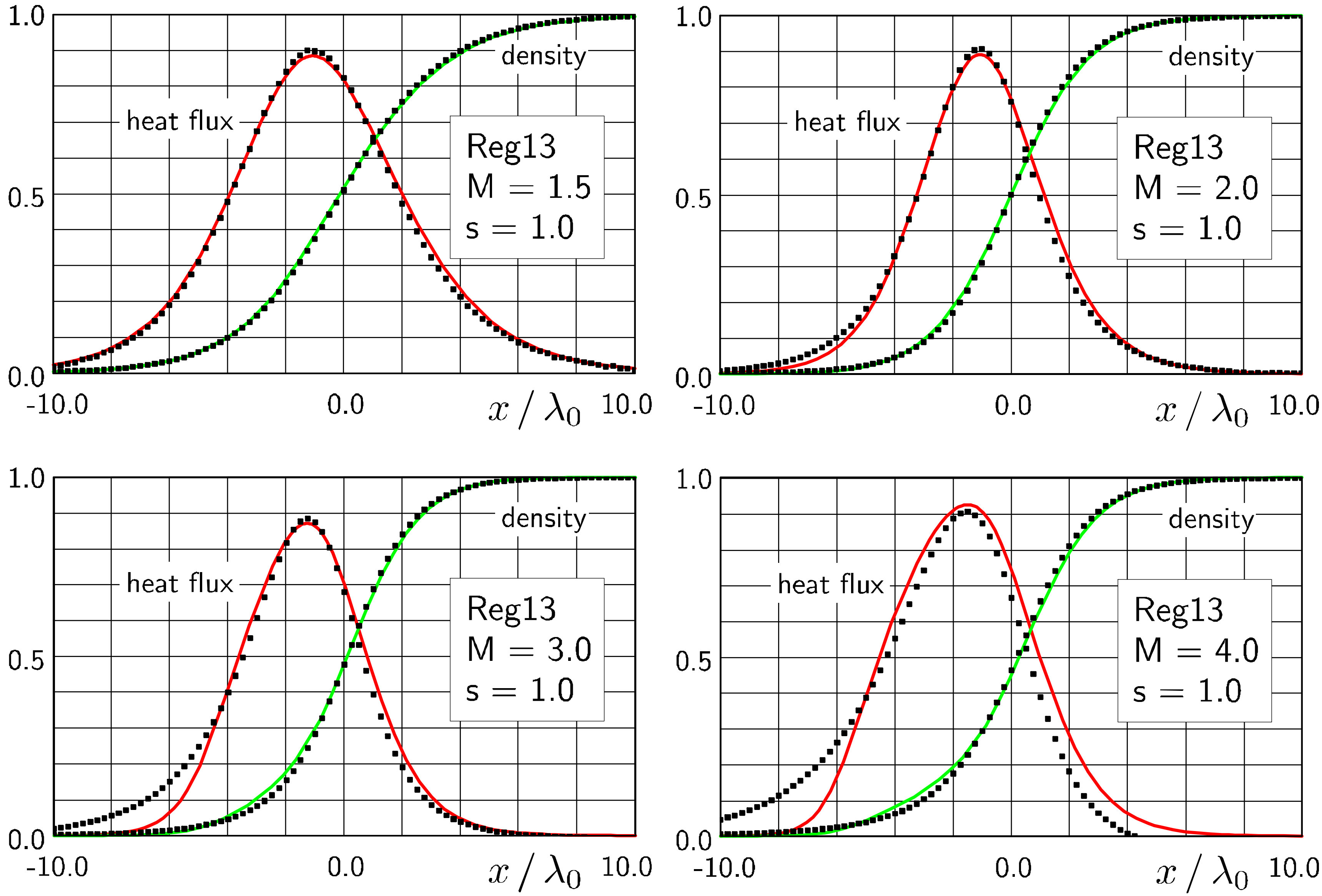
proper Knudsen number for oscillation

$$\mathrm{Kn}_{\Omega} = \omega$$

$\Rightarrow$ **R13 allows proper description close to natural limit** $\mathrm{Kn}_{\Omega} = 1$

Shocks: Comparison with DSMC results [MT & HS 2004]

Success of R13



Switching criteria for hybrid codes [D.Lockerby, J.Reese, HS 2009]

hybrid Boltzmann/NSF solvers:

use NSF for “small” Kn, **Boltzmann for “large”** Kn

requires local Knudsen number to distinguish domains

usual choice: gradient Knudsen number (mean free path λ)

$$\mathrm{Kn}_G = \frac{\lambda}{\rho}\left|\frac{d\rho}{dx}\right|$$

not too bad: for strongly non-linear flow (steep gradients, shocks etc.)

problem: $\mathrm{Kn}_G \to 0$ **for linear flow** (microflows, ultrasound)

goal: local Knudsen number for linear and non-linear regime

Switching criteria for hybrid codes [D.Lockerby, J.Reese, HS 2009]

Switch Boltzmann/R13 $\Longrightarrow$ NSF

Step 1:

compute ρ, v_i, θ, σ_{ij} , q_i **from Boltzmann/R13**

Step 2:

compute $\sigma_{ij}^{(NSF)} = -\mu \frac{\partial v_{\langle i}}{\partial x_{j\rangle}}$, $q_i^{(NSF)} = -\kappa \frac{\partial \theta}{\partial x_i}$ **from Boltzmann/R13**

Step 3:

local Knudsen number as deviation from NSF

$$\mathrm{Kn}_\sigma = \frac{\left\| \sigma_{ij} - \sigma_{ij}^{(NSF)} \right\|}{\left\| \sigma_{ij}^{(NSF)} \right\|} \quad , \quad \mathrm{Kn}_q = \frac{\left\| q_i - q_i^{(NSF)} \right\|}{\left\| q_i^{(NSF)} \right\|}$$

with

$$\|q_i\| = \sqrt{q_i q_i} = \sqrt{q_1^2 + q_2^2 + q_3^2}$$

$$\|\sigma_{ij}\| = \sqrt{\frac{1}{2} \left| \sigma_{ii}\sigma_{jj} - \sigma_{ij}\sigma_{ij} \right|} = \sqrt{\frac{1}{2} \left| \sigma_{ij}\sigma_{ij} \right|} = \sqrt{\left| \sigma_{11}^2 + \sigma_{11}\sigma_{22} + \sigma_{22}^2 + \sigma_{12}^2 + \sigma_{13}^2 + \sigma_{23}^2 \right|}$$

Switching criteria for hybrid codes [D.Lockerby, J.Reese, HS 2009]

Switch Boltzmann/R13 $\Longrightarrow$ NSF

Example I: Shock structure with Burnett/R13

NSF and Burnett/R13 in shock (leading term)

$$\sigma_{11}^{(NSF)} = -\frac{4}{3}\mu\frac{dv}{dx}\,, \qquad \sigma_{11}^{(B)} = \frac{A\mu^2}{p}\left(\frac{dv}{dx}\right)^2$$

local Knudsen number

$$\mathrm{Kn}_{\sigma}^{(\mathsf{shock})} = \frac{\sqrt{\frac{3}{4}\sigma_{11}^{(B)}}}{\sqrt{\frac{3}{4}\sigma_{11}^{(NSF)}}} = \left|\frac{\frac{A\mu^2}{p}\left(\frac{dv}{dx}\right)^2}{\frac{4}{3}\mu\left(\frac{dv}{dx}\right)}\right| = \left|\frac{3}{4}\frac{A}{p}\mu\frac{dv}{dx}\right| = \alpha\mathrm{Ma}\frac{\lambda}{\rho}\left|\frac{d\rho}{dx}\right|\ .$$

similar to gradient Knudsen number

Switching criteria for hybrid codes [Lockerby, Reese, HS 2009]

Switch Boltzmann/R13 $\Longrightarrow$ NSF

Example II: Nonlinear shear flow with second order hydrodynamics

R13/Burnett (to second order in Kn)

$$\sigma_{12} = -\mu \frac{dv}{dy} \ , \quad \sigma_{11} = \frac{8}{5} \frac{\sigma_{12}\sigma_{12}}{p} \ , \quad \sigma_{22} = -\frac{6}{5} \frac{\sigma_{12}\sigma_{12}}{p} \ , \quad q_1 = \frac{7}{2} \frac{\sigma_{12} q_2}{p} \ , \quad q_2 = -\frac{15}{4} \mu \frac{d\theta}{dy}$$

local Knudsen numbers

$$\mathrm{Kn}_\sigma^{(\text{shear})} = \sqrt{\frac{52}{25}} \left| \frac{\sigma_{12}}{p} \right| = \hat{\alpha} \mathrm{Ma} \frac{\lambda}{v} \left| \frac{dv}{dy} \right|$$

$$\mathrm{Kn}_q^{(\text{shear})} = \frac{7}{2} \left| \frac{\sigma_{12}}{p} \right| = \check{\alpha} \mathrm{Ma} \frac{\lambda}{v} \left| \frac{dv}{dy} \right|$$

similar to gradient Knudsen number

Switching criteria for hybrid codes [Lockerby, Reese, HS 2009]

Switch Boltzmann/R13 $\Longrightarrow$ NSF

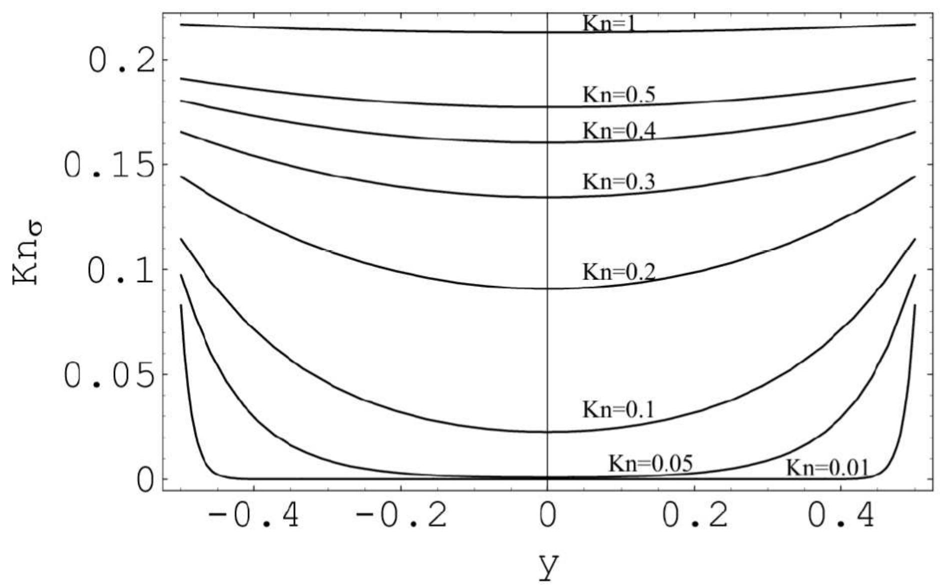
Example III: Linear Poiseuille flow with R13 equations

R13 (driving force F, global Knudsen number Kn)

$$\sigma_{12} = Fy \quad , \quad v = F\left[\frac{1}{2\mathrm{Kn}}\left(\frac{1}{4}-y^2\right)+\frac{1}{2}\sqrt{\frac{\pi}{2}}+\frac{5}{6}\mathrm{Kn}+\frac{\frac{3}{25}\left(1+5\mathrm{Kn}\right)\left(\frac{1}{2}-\frac{\cosh\left[\sqrt{\frac{5}{9}}\frac{y}{\mathrm{Kn}}\right]}{\cosh\left[\frac{\sqrt{5}}{6\mathrm{Kn}}\right]}\right)}{1+\frac{12}{5\sqrt{5}}\tanh\left[\frac{\sqrt{5}}{6\mathrm{Kn}}\right]}\right]$$

local Knudsen number

$$\mathrm{Kn}_\sigma = \frac{\left\|\sigma_{ij}-\sigma_{ij}^{(NS)}\right\|}{\left\|\sigma_{ij}^{(NS)}\right\|} \quad \text{with} \quad \sigma_{12}^{(NSF)} = -\mathrm{Kn}\frac{\partial v}{\partial y} = Fy + F\frac{\frac{1}{5\sqrt{5}}\left(1+5\mathrm{Kn}\right)}{1+\frac{12}{5\sqrt{5}}\tanh\left[\frac{\sqrt{5}}{6\mathrm{Kn}}\right]}\frac{\sinh\left[\sqrt{\frac{5}{9}}\frac{y}{\mathrm{Kn}}\right]}{\cosh\left[\frac{\sqrt{5}}{6\mathrm{Kn}}\right]}$$



Switching criteria for hybrid codes [D.Lockerby, J.Reese, HS 2009]

Switch NSF $\Longrightarrow$ Boltzmann/R13

Step 1:

compute $\rho^{(NSF)},\ v_i^{(NSF)},\ \theta^{(NSF)}$, and $\sigma_{ij}^{(NSF)}$, $q_i^{(NSF)}$ **from NSF**

Step 2:

insert NSF result into R13 to compute mismatch

$$\sigma_{ij}^{(R13)} = -\frac{\mu}{p}\left[2p\frac{\partial v_{\langle i}}{\partial x_{j\rangle}} + \frac{D\sigma_{ij}}{Dt} + \sigma_{ij}\frac{\partial v_k}{\partial x_k} + \frac{4}{5}\frac{\partial q_{\langle i}}{\partial x_{j\rangle}} + 2\sigma_{k\langle i}\frac{\partial v_{j\rangle}}{\partial x_k} + \frac{\partial m_{ijk}}{\partial x_k}\right]^{(NSF)}$$

$$q_i^{(R13)} = -\frac{3}{2}\frac{\mu}{p}\left[\frac{5}{2}p\frac{\partial \theta}{\partial x_i} + \frac{Dq_i}{Dt} + \frac{5}{2}\sigma_{ik}\frac{\partial \theta}{\partial x_k} + \theta\frac{\partial \sigma_{ik}}{\partial x_k} - \theta\sigma_{ik}\frac{\partial \ln \rho}{\partial x_k} + \frac{7}{5}q_k\frac{\partial v_i}{\partial x_k} + \cdots\right]^{(NSF)}$$

Step 3:

local Knudsen number as deviation from NSF

$$\mathrm{Kn}_\sigma = \frac{\left\|\sigma_{ij}^{(R13)} - \sigma_{ij}^{(NS)}\right\|}{\left\|\sigma_{ij}^{(NS)}\right\|} \quad , \quad \mathrm{Kn}_q = \frac{\left\|q_i^{(R13)} - q_i^{(F)}\right\|}{\left\|q_i^{(F)}\right\|}$$

identifies non-linear rarefaction effects

identifies linear bulk effects, can't identify Knudsen layers,

Switching criteria for hybrid codes [Lockerby, Reese, HS 2009]

Switch NSF $\Longrightarrow$ Boltzmann/R13

Example: linear shear flow with driving force F

NSF reduce to

$$\frac{d\sigma_{12}^{(NS)}}{dy} = F \quad , \quad \sigma_{12}^{(NS)} = -\mathrm{Kn}\frac{dv}{dy}$$

R13 reduce to

$$\frac{d\sigma_{12}^{(R13)}}{dy} = F \quad , \quad \sigma_{12}^{(R13)} = -\mathrm{Kn}\frac{dv}{dy} + \frac{52}{15}\mathrm{Kn}^2\frac{d^2\sigma_{12}}{dy^2} + \frac{9}{5}\mathrm{Kn}^3\frac{d^3v}{dy^3} - \frac{48}{25}\mathrm{Kn}^4\frac{d^4\sigma_{12}}{dy^4}$$

feed NSF into R13

$$\sigma_{12}^{(R13)} = -\mathrm{Kn}\frac{dv}{dy} - \frac{5}{3}\mathrm{Kn}^3\frac{d^3v}{dy^3} + \frac{48}{25}\mathrm{Kn}^5\frac{d^5v}{dy^5} = \sigma_{12}^{(NS)} + \frac{5}{3}\mathrm{Kn}^2\frac{dF}{dy} - \frac{48}{25}\mathrm{Kn}^4\frac{d^3F}{dy^3}$$

local Knudsen number

$$\mathrm{Kn}_\sigma = \mathrm{Kn}^2\frac{\left|\frac{5}{3}\frac{dF}{dy} - \frac{48}{25}\mathrm{Kn}^2\frac{d^3F}{dy^3}\right|}{\int F dy}$$

Regularized 13 moment equations

- rational derivation from Boltzmann equation
- third order in Knudsen number ($\equiv$ super-Burnett)
- linearly stable
- phase speeds and damping of ultrasound waves agree to experiments
- smooth shock structures for all Ma, agree to DSMC for $\mathrm{Ma} < 3$
- H-theorem for linear case, including boundary conditions
- theory of boundary conditions
- Knudsen boundary layers in good agreement to DSMC
- accurate Poiseuille flow, second order slip conditions
- accurate thermal transpiration flow
- define local Knudsen number

Future work

- 2-D/3-D/transient simulations
- increased understanding of BC for non-linear case
- RXY equations for polyatomic gases and mixtures