Beyond Hydrodynamics:
Macroscopic transport equations for rarefied gas flows

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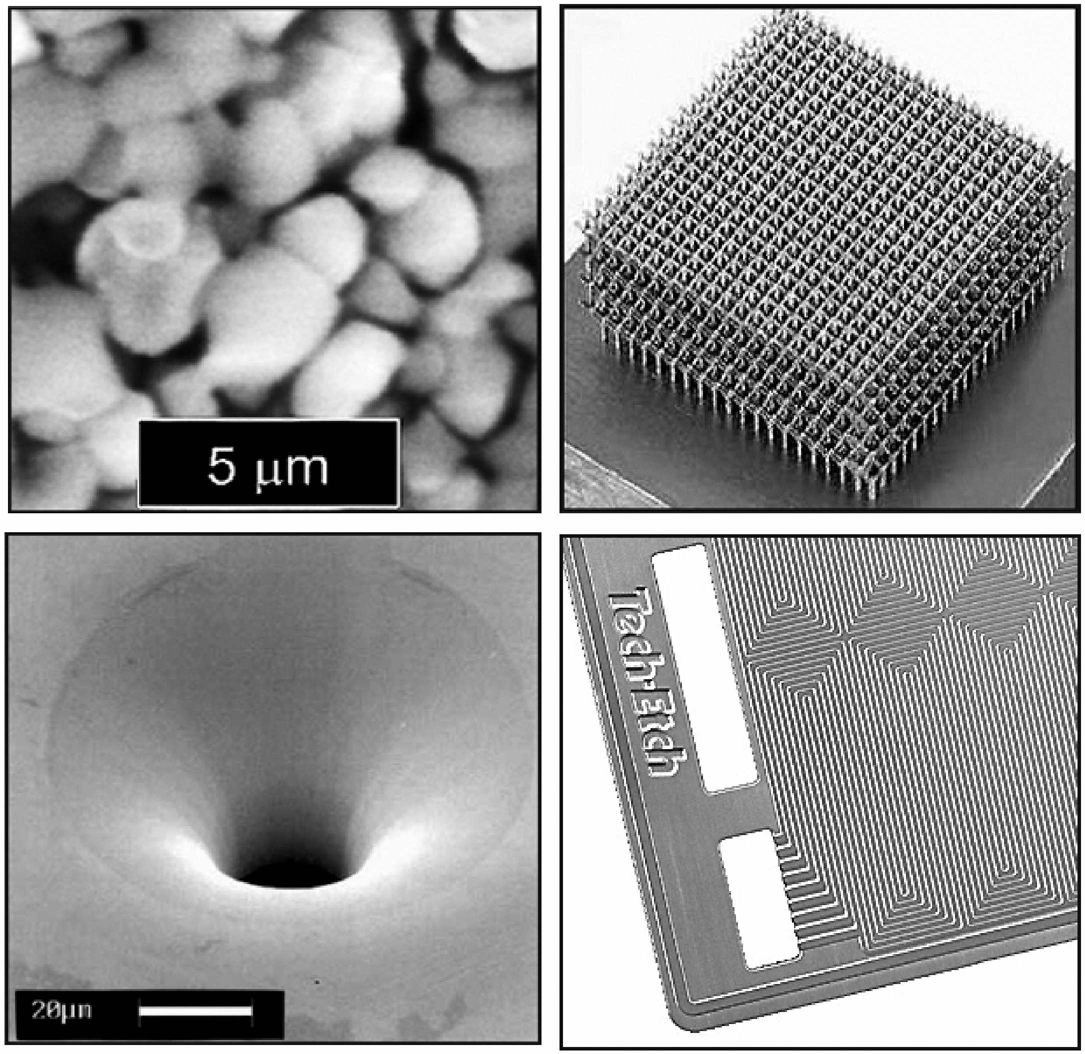
Gas-Microflows



porous material   micro heat exchanger

micro nozzle   micro fuel cell

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

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

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

Generic moment equation

multiply Boltzmann equation with $mC^{2a}C_{\langle i_1}\cdots C_{i_n\rangle}$, integrate over velocity

$$\frac{Du^a_{i_1\cdots i_n}}{Dt}+2au^{a-1}_{i_1\cdots i_nk}\left[\frac{Dv_k}{Dt}-G_k\right]+\frac{n\left(2a+2n+1\right)}{2n+1}u^a_{\langle i_1\cdots i_{n-1}}\left[\frac{Dv_{i_n\rangle}}{Dt}-G_{i_n\rangle}\right]$$

$$+\frac{\partial u^a_{i_1\cdots i_nk}}{\partial x_k}+\frac{n}{2n+1}\frac{\partial u^{a+1}_{\langle i_1\cdots i_{n-1}}}{\partial x_{i_n\rangle}}+2au^{a-1}_{i_1\cdots i_nkl}\frac{\partial v_k}{\partial x_l}+2a\frac{n+1}{2n+3}u^a_{\langle i_1\cdots i_n}\frac{\partial v_{k\rangle}}{\partial x_k}$$

$$+2a\frac{n}{2n+1}u^a_{k\langle i_1\cdots i_{n-1}}\frac{\partial v_k}{\partial x_{i_n\rangle}}+nu^a_{k\langle i_1\cdots i_{n-1}}\frac{\partial v_{i_n\rangle}}{\partial x_k}+u^a_{i_1\cdots i_n}\frac{\partial v_k}{\partial x_k}$$

$$+\frac{n\left(n-1\right)}{4n^2-1}\left(2a+2n+1\right)u^{a+1}_{\langle i_1\cdots i_{n-2}}\frac{\partial v_{i_{n-1}}}{\partial x_{i_n\rangle}}=\mathcal{P}^a_{i_1\cdots i_n}$$

infinte coupled system for central moments $u^a_{i_1\cdots i_n}$ (includes conservation laws)

Generic moment equation

multiply Boltzmann equation with $mC^{2a}C_{\langle i_1} \cdots C_{i_n\rangle}$, integrate over velocity

$$\frac{Du^a_{i_1\cdots i_n}}{Dt} + 2au^{a-1}_{i_1\cdots i_n k}\left[\frac{Dv_k}{Dt} - G_k\right] + \frac{n(2a+2n+1)}{2n+1}u^a_{\langle i_1\cdots i_{n-1}}\left[\frac{Dv_{i_n\rangle}}{Dt} - G_{i_n\rangle}\right]$$

$$+ \frac{\partial u^a_{i_1\cdots i_n k}}{\partial x_k} + \frac{n}{2n+1}\frac{\partial u^{a+1}_{\langle i_1\cdots i_{n-1}}}{\partial x_{i_n\rangle}} + 2au^{a-1}_{i_1\cdots i_n kl}\frac{\partial v_k}{\partial x_l} + 2a\frac{n+1}{2n+3}u^a_{\langle i_1\cdots i_n}\frac{\partial v_{k\rangle}}{\partial x_k}$$

$$+ 2a\frac{n}{2n+1}u^a_{k\langle i_1\cdots i_{n-1}}\frac{\partial v_k}{\partial x_{i_n\rangle}} + nu^a_{k\langle i_1\cdots i_{n-1}}\frac{\partial v_{i_n\rangle}}{\partial x_k} + u^a_{i_1\cdots i_n}\frac{\partial v_k}{\partial x_k}$$

$$+ \frac{n(n-1)}{4n^2-1}(2a+2n+1)\,u^{a+1}_{\langle i_1\cdots i_{n-2}}\frac{\partial v_{i_{n-1}}}{\partial x_{i_n\rangle}} = \mathcal{P}^a_{i_1\cdots i_n}$$

infinte coupled system for central moments $u^a_{i_1\cdots i_n}$ (includes conservation laws)

Moment methods

- **use finite moment number N (but which???)**
- **find constitutive equations for higher moments (but how??)**

The R13 equations

Cercignani, 1970:

. . . on the other hand, if we consider higher-order approximations of the Chapman–Enskog method, we obtain differential equations of higher order (the so-called Burnett and super-Burnett equations), about which nothing is known, not even the proper boundary conditions. These **higher-order equations have never achieved any noticeable success** *in describing departures from continuum fluid mechanics . . .*

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 & MT 2003/04]
  - $\Longrightarrow$ **Order of magnitude method** $\Longrightarrow$ **R13 eqs** [HS 2004]

Regularized 13 moment equations [HS & MT 2003 - 2008]

- rational derivation from Boltzmann equation
- contain Burnett and super-Burnett equations in CE expanison
- 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
- furnished with complete theory of boundary conditions
- Knudsen boundary layers in good agreement to DSMC
- accurate Poiseuille flow, second order slip conditions
- accurate thermal transpiration flow

Order of magnitude method [HS 2004]

Base: **expand infinite set of moment equations, not Boltzmann**

Step 1:

Determine order of magnitude λ of all moments (in powers of Kn)

Step 2:

Construct moment set with minimum number of moments at order λ

Step 3:

For order of accuracy λ_0 delete all terms that lead to contributions of orders $\lambda > \lambda_0$ in energy and momentum eqs.

$\Longrightarrow$

- **stable equations at any order**
  - $\mathcal{O}\left(\mathrm{Kn}^0\right)$: **Euler**
  - $\mathcal{O}\left(\mathrm{Kn}^1\right)$: **Navier-Stokes-Fourier**
  - $\mathcal{O}\left(\mathrm{Kn}^2\right)$: **Grad 13**
  - $\mathcal{O}\left(\mathrm{Kn}^3\right)$: **regularized 13 moment equations (R13)**
- **applicable to any molecular model**

Zeroth order: Euler

delete all terms of order

$$\mathcal{O}\left(\mathrm{Kn}^1\right) \text{ and higher}$$

conservation laws

$$\begin{aligned}
\frac{D\rho}{Dt} + \rho\frac{\partial v_k}{\partial x_k} &= 0 \\
\rho\frac{Dv_i}{Dt} + \rho\frac{\partial \theta}{\partial x_i} + \theta\frac{\partial \rho}{\partial x_i} &= 0 \\
\frac{3}{2}\rho\frac{D\theta}{Dt} + \rho\theta\frac{\partial v_k}{\partial x_k} &= 0
\end{aligned}$$

equations for pressure deviator and heat flux

First order: Navier-Stokes-Fourier

delete all terms of order

$$\mathcal{O}\left(\mathrm{Kn}^2\right) \text{ and higher}$$

conservation laws

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

$$\rho\frac{Dv_i}{Dt} + \rho\frac{\partial \theta}{\partial x_i} + \theta\frac{\partial \rho}{\partial x_i} + \mathrm{Kn}^1\left[\frac{\partial \sigma_{ik}}{\partial x_k}\right] = 0$$

$$\frac{3}{2}\rho\frac{D\theta}{Dt} + \rho\theta\frac{\partial v_k}{\partial x_k} + \mathrm{Kn}^1\left[\frac{\partial q_k}{\partial x_k} + \sigma_{kl}\frac{\partial v_k}{\partial x_l}\right] = 0$$

equations for pressure deviator and heat flux

$$0 = -\rho\theta\mathrm{Kn}^1\left[\sigma_{ij} + 2\mu\frac{\partial v_{\langle i}}{\partial x_{j\rangle}}\right]$$

$$0 = -\frac{5}{2}\rho\theta\mathrm{Kn}^1\left[q_i + \kappa\frac{\partial \theta}{\partial x_i}\right]$$

2nd order: Grad 13 moments

delete all terms of order

$$\mathcal{O}\left(\mathrm{Kn}^3\right) \text{ and higher}$$

conservation laws

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

$$\rho\frac{Dv_i}{Dt} + \rho\frac{\partial \theta}{\partial x_i} + \theta\frac{\partial \rho}{\partial x_i} + \mathrm{Kn}^1\left[\frac{\partial \sigma_{ik}}{\partial x_k}\right] = 0$$

$$\frac{3}{2}\rho\frac{D\theta}{Dt} + \rho\theta\frac{\partial v_k}{\partial x_k} + \mathrm{Kn}^1\left[\frac{\partial q_k}{\partial x_k} + \sigma_{kl}\frac{\partial v_k}{\partial x_l}\right] = 0$$

equations for pressure deviator and heat flux

$$\mathrm{Kn}^2\mu\left[\frac{D\sigma_{ij}}{Dt} + \frac{4}{5}\frac{\partial q_{\langle i}}{\partial x_{j\rangle}} + 2\sigma_{k\langle i}\frac{\partial v_{j\rangle}}{\partial x_k} + \sigma_{ij}\frac{\partial v_k}{\partial x_k}\right] + \qquad = -\rho\theta\mathrm{Kn}^1\left[\sigma_{ij} + 2\mu\frac{\partial v_{\langle i}}{\partial x_{j\rangle}}\right]$$

$$\mathrm{Kn}^2\kappa\left[\frac{Dq_i}{Dt} + \frac{5}{2}\sigma_{ik}\frac{\partial \theta}{\partial x_k} - \sigma_{ik}\theta\frac{\partial \ln\rho}{\partial x_k} + \theta\frac{\partial \sigma_{ik}}{\partial x_k} + \frac{7}{5}q_i\frac{\partial v_k}{\partial x_k} + \frac{7}{5}q_k\frac{\partial v_i}{\partial x_k} + \frac{2}{5}q_k\frac{\partial v_k}{\partial x_i}\right]$$

$$= -\frac{5}{2}\rho\theta\mathrm{Kn}^1\left[q_i + \kappa\frac{\partial \theta}{\partial x_i}\right]$$

3rd order: R13 equations

delete all terms of order

$$\mathcal{O}\left(\mathrm{Kn}^4\right) \text{ and higher}$$

conservation laws

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

$$\rho\frac{Dv_i}{Dt} + \rho\frac{\partial \theta}{\partial x_i} + \theta\frac{\partial \rho}{\partial x_i} + \mathrm{Kn}^1\left[\frac{\partial \sigma_{ik}}{\partial x_k}\right] = 0$$

$$\frac{3}{2}\rho\frac{D\theta}{Dt} + \rho\theta\frac{\partial v_k}{\partial x_k} + \mathrm{Kn}^1\left[\frac{\partial q_k}{\partial x_k} + \sigma_{kl}\frac{\partial v_k}{\partial x_l}\right] = 0$$

equations for pressure deviator and heat flux

$$\mathrm{Kn}^2\mu\left[\frac{D\sigma_{ij}}{Dt} + \frac{4}{5}\frac{\partial q_{\langle i}}{\partial x_{j\rangle}} + 2\sigma_{k\langle i}\frac{\partial v_{j\rangle}}{\partial x_k} + \sigma_{ij}\frac{\partial v_k}{\partial x_k}\right] + \mathrm{Kn}^3\mu\left[\frac{\partial u^0_{ijk}}{\partial x_k}\right] = -\rho\theta\mathrm{Kn}^1\left[\sigma_{ij} + 2\mu\frac{\partial v_{\langle i}}{\partial x_{j\rangle}}\right]$$

$$\mathrm{Kn}^2\kappa\left[\frac{Dq_i}{Dt} + \frac{5}{2}\sigma_{ik}\frac{\partial \theta}{\partial x_k} - \sigma_{ik}\theta\frac{\partial \ln\rho}{\partial x_k} + \theta\frac{\partial \sigma_{ik}}{\partial x_k} + \frac{7}{5}q_i\frac{\partial v_k}{\partial x_k} + \frac{7}{5}q_k\frac{\partial v_i}{\partial x_k} + \frac{2}{5}q_k\frac{\partial v_k}{\partial x_i}\right]$$
$$+\mathrm{Kn}^3\kappa\left[\frac{1}{2}\frac{\partial w^1_{ij}}{\partial x_k} + \frac{1}{6}\frac{\partial w^2}{\partial x_i} + u^0_{ikl}\frac{\partial v_k}{\partial x_l} - \frac{\sigma_{ik}}{\rho}\frac{\partial \sigma_{kl}}{\partial x_l}\right] = -\frac{5}{2}\rho\theta\mathrm{Kn}^1\left[q_i + \kappa\frac{\partial \theta}{\partial x_i}\right]$$

+ higher moment equations for u^0_{ijk}, $w^1_{ij} = u^1_{ij} - \mu_1\sigma_{ij}$, $w^2 = u^2 - u^2_{|E}$

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)

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

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

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

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

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

Linear stability [HS & MT 2003]

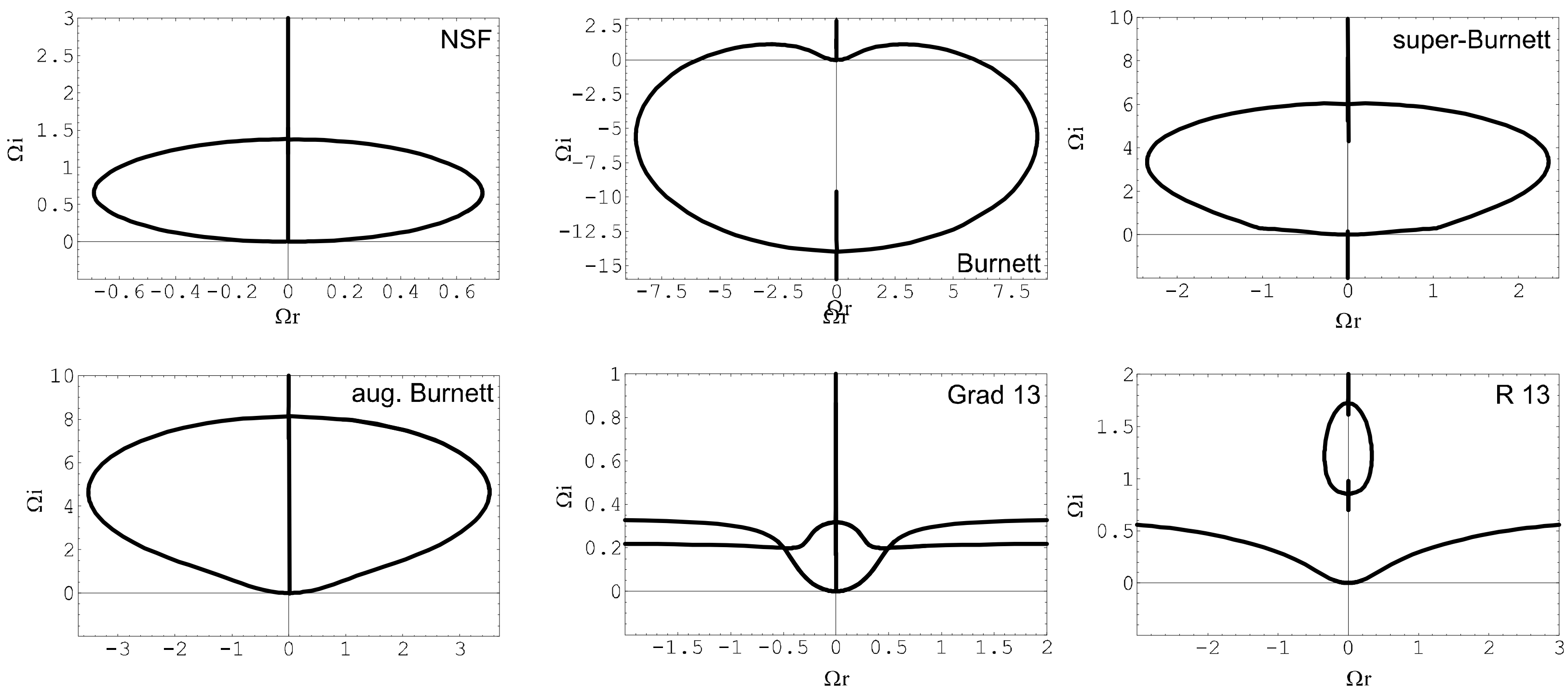
disturbance in space k real, $\Omega = \Omega_r(k) + i\Omega_i(k)$ complex

$$u_A = \tilde{u}_A \exp[-\alpha t] \exp[ik(v_{ph}t - x)]$$

phase velocity and damping

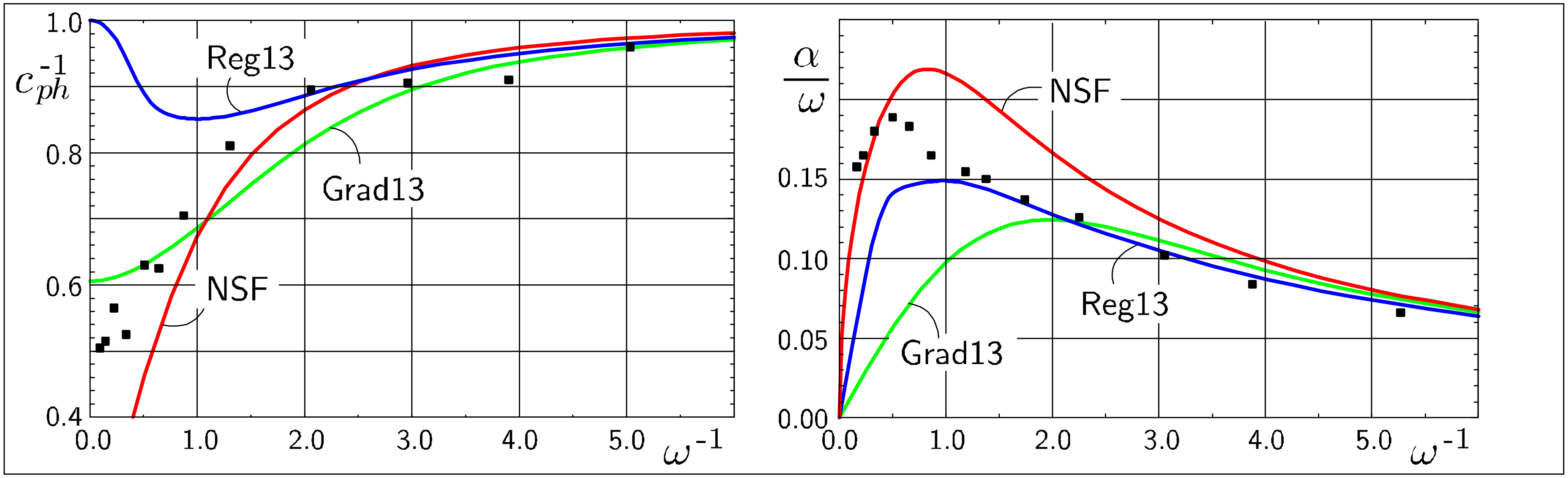
$$v_{ph} = \frac{\Omega_r(k)}{k} \quad \text{and} \quad \alpha = \Omega_i(k)$$

stability $\Omega_i(k) \geq 0$



Dispersion and Damping [HS & MT 2003]

phase speed and damping measured by Meyer and Sessler



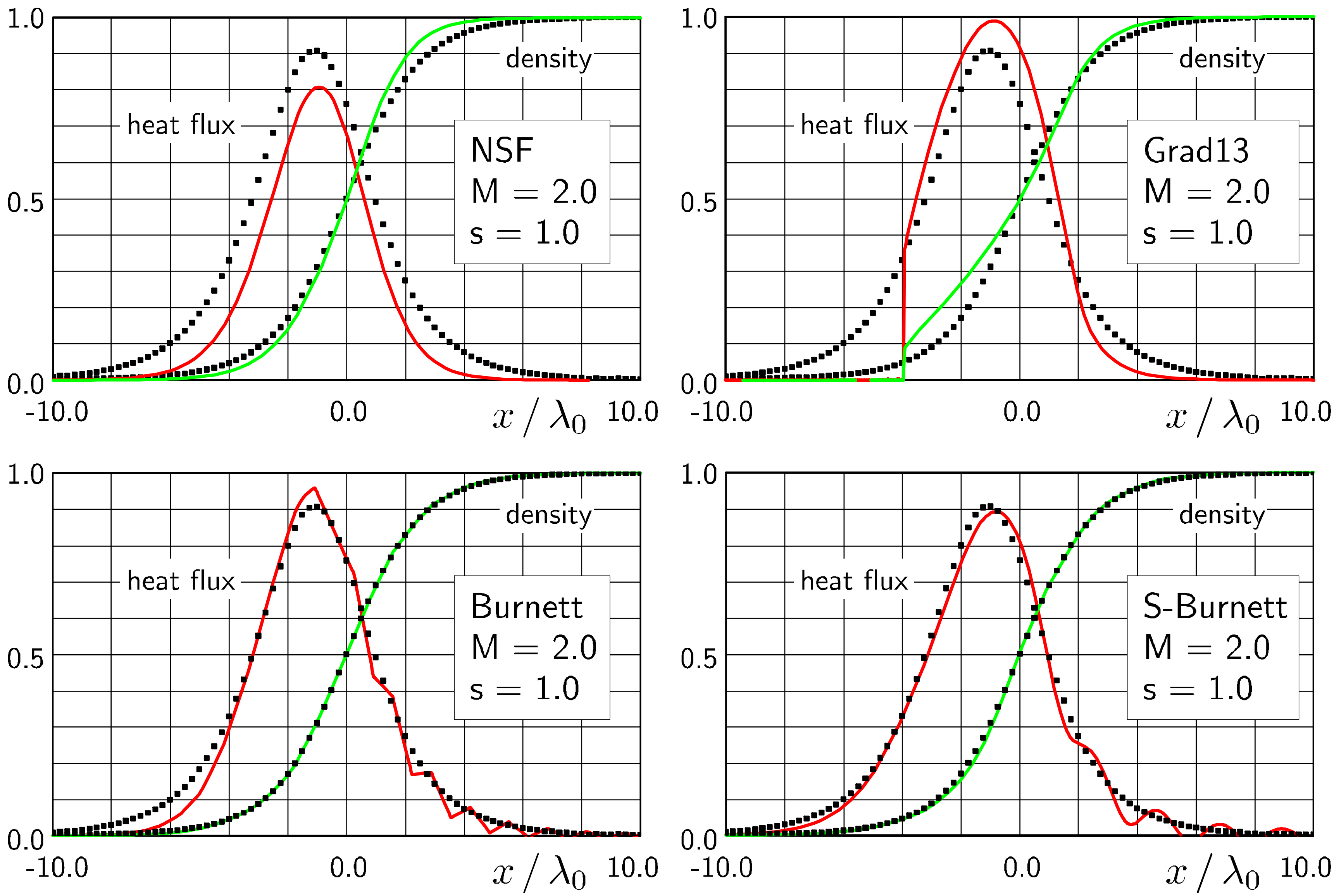
proper Knudsen number for oscillation

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

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

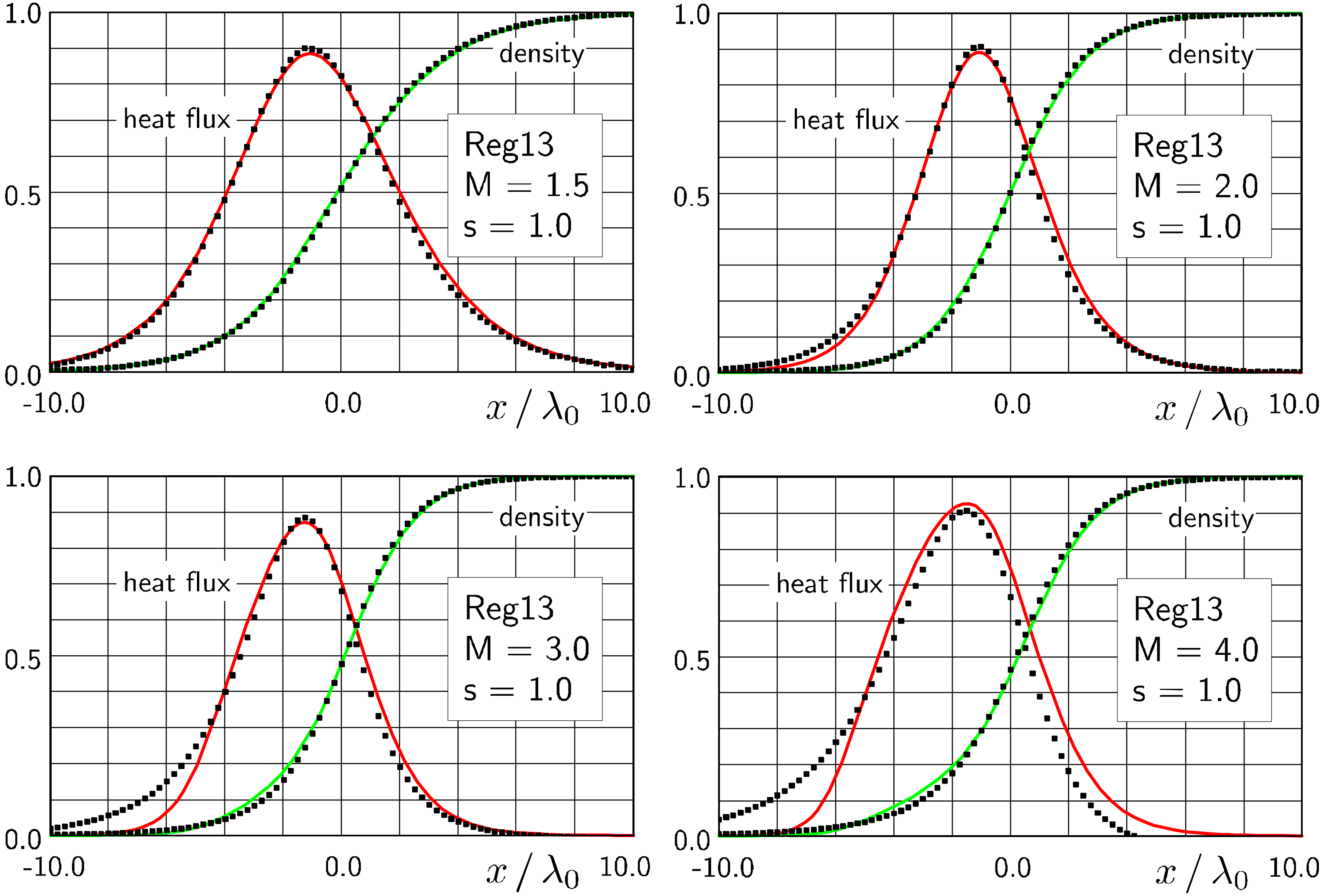
Shocks: Comparison with DSMC results [MT & HS 2004]

Failure of NSF, Burnett, super-Burnett, and Grad13



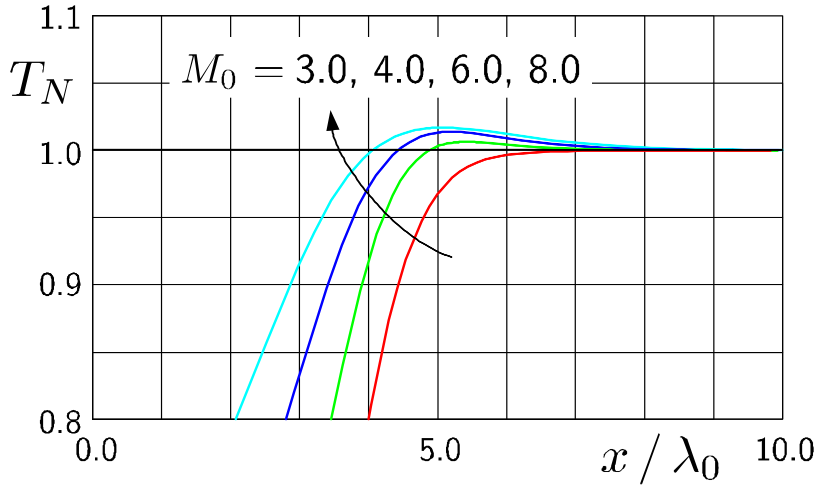
Shocks: Comparison with DSMC results [MT & HS 2004]

Success of R13



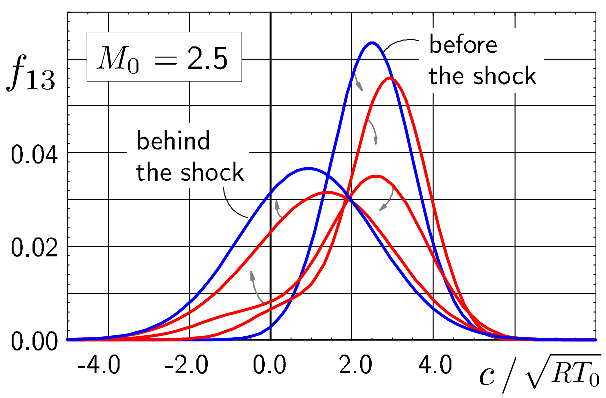
Shocks: Temperature overshoot

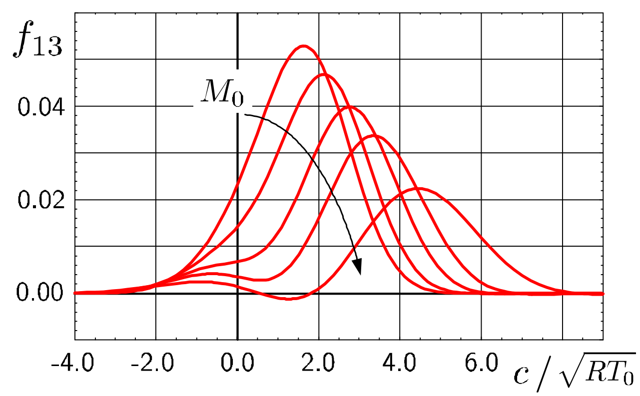
R13: overshoot in agreement with DSMC, NSF: no overshoot



Shocks: Positivity of distribution function

Grad's distribution: $$f_{13} = f_M \left(1 + \frac{\sigma}{4\rho T^2}\left(3C_x^2 - C^2\right) - \frac{q}{\rho T^2} C_x \left(1 - \frac{1}{5T} C^2\right)\right)$$





H-Theorem for linear equations [HS & MT 2007]

entropy balance

$$\frac{D\eta}{Dt} + \frac{\partial \phi_k}{\partial x_k} = \Sigma \geq 0$$

convex dimensionless entropy density similar to [Bobylev 2007]

$$\eta = \eta_0 - \frac{1}{2}\rho^2 - \frac{1}{2}v_i v_i - \frac{3}{4}\theta^2 - \frac{1}{4}\sigma_{ij}\sigma_{ij} - \frac{1}{5}q_i q_i$$

entropy flux

$$\phi_k = -(\rho + \theta)\, v_k - v_i \sigma_{ik} - \theta q_k - \frac{2}{5} q_i \sigma_{ik} - \frac{1}{2}\sigma_{ij} u^0_{ijk} - \frac{1}{5} q_i w_{ik}$$

bulk entropy generation rate

$$\Sigma = \frac{\sigma_{ij}\sigma_{ij}}{2\mathrm{Kn}} + \frac{4}{15}\frac{q_i q_i}{\mathrm{Kn}} - \frac{1}{2}u^0_{ijk}\frac{\partial \sigma_{\langle ij}}{\partial x_{k\rangle}} - \frac{1}{5} w_{ik}\frac{\partial q_i}{\partial x_k} \overset{!}{\geq} 0$$

regularizing constitutive equations guarantee $\Sigma \geq 0$ and linear stability

$$w_{ij} = w^1_{ij} + \frac{1}{3}w^2\delta_{ij} = -\frac{24}{5}\mathrm{Kn}\frac{\partial q_{\langle i}}{\partial x_{j\rangle}} - 4\mathrm{Kn}\frac{\partial q_k}{\partial x_k}\delta_{ij} \quad , \quad u^0_{ijk} = -2\mathrm{Kn}\frac{\partial \sigma_{\langle ij}}{\partial x_{k\rangle}}$$

H-Theorem & boundary conditions [HS & MT 2007]

first and second law for solid wall at rest, temperature θ_W

$$c_v \frac{\partial \theta_W}{\partial t} + \frac{\partial q_k}{\partial x_k} = 0 \quad , \qquad \frac{\partial \eta_W}{\partial t} + \frac{\partial \phi_k^W}{\partial x_k} = \Sigma_W$$

with $\eta_W = \eta_W^0 - \frac{c_v}{2}\theta_W^2$, $\phi_k^W = -\theta_W q_k$, $\Sigma_W = -q_k \frac{\partial \theta_W}{\partial x_k}$

entropy generation at wall: $\Sigma_W = \left(\phi_k^W - \phi_k\right) n_k \geq 0$

$$\Sigma_W = \bar{\sigma}_{ni}\left[v_i - v_i^W + \left(\frac{2}{5} - \alpha\right)\bar{q}_i + u_{inn}^0\right] + \bar{q}_i\left[\alpha\bar{\sigma}_{ni} + \frac{1}{5}w_{in}\right]$$
$$+ q_n\left[\theta - \theta_W + \left(\frac{2}{5} - \beta\right)\sigma_{nn} + \frac{1}{5}w_{nn}\right] + \sigma_{nn}\left[\beta q_n + \frac{3}{4}u_{nnn}^0\right] + \frac{1}{2}\bar{\sigma}_{ij}u_{ijn}^0 \geq 0$$

phenomenological boundary conditions guarantee $\Sigma_W \geq 0$

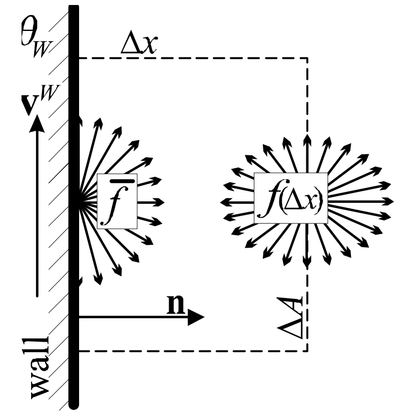
$$\bar{\sigma}_{ni} = \gamma_1\left[v_i - v_i^W + \left(\frac{2}{5} - \alpha\right)\bar{q}_i + u_{inn}^0\right] \qquad \bar{q}_i = \gamma_2\left[\alpha\bar{\sigma}_{ni} + \frac{1}{5}w_{ni}\right]$$

$$q_n = \gamma_4\left[\theta - \theta_W + \left(\frac{2}{5} - \beta\right)\sigma_{nn} + \frac{1}{5}w_{nn}\right] \qquad \sigma_{nn} = \gamma_3\left[\beta q_n + \frac{1}{2}u_{nnn}^0\right] \qquad \bar{\sigma}_{ij} = \gamma_5\left[\frac{1}{2}m_{ijn}\right]$$

with phenomenological coefficients $\gamma_1 - \gamma_5$, α, β

Kinetic boundary conditions

Maxwell's boundary condition for phase density:



$$\bar{f} = \begin{cases} \chi f_W + (1-\chi)\, f_{gas}\left(-C_k^W n_k\right) & ,\ C_k^W n_k \geq 0 \\ f_{gas}\left(C_k^W n_k\right) & ,\ C_k^W n_k \leq 0 \end{cases}$$

χ – accommodation coefficient, n_k– wall normal, f_{gas} – incoming particles, $C_k^W = c_k - v_k^W$

wall Maxwellian

$$f_W = \frac{\rho_W}{m}\sqrt{\frac{1}{2\pi\theta_W}}^3 \exp\left[-\frac{C_W^2}{2\theta_W}\right]$$

kinetic BC for moments continuity of fluxes

$$\bar{F}_{Ak} n_k = F_{Ak}^{gas} n_k$$

so that

$$F_{Ak} n_k = \frac{\chi}{1-\chi}\int_{C_k^W n_k \geq 0} \Psi_A C_k^W n_k \left(f_W - f_{gas}\right) d\mathbf{c}$$

Boundary conditions for moments [MT & HS 2008]

Rule 1:

Continuity: meaningful BC for all accommodation coefficients $\chi \in [0,1]$

$\Longrightarrow$ **only "odd fluxes"** [Grad 1949]

Rule 2:

Consistency: kinetic BC only for fluxes that appear in equations

Rule 3:

Coherence: same number of BC for linearized and non-linear equations

Rules 1 and 2 are straightforward

Rule 3 requires algebraization: e.g.,

$$u_{tnn}^{0} = -\mu \left[\frac{16}{15} \frac{\partial \sigma_{tn}/\rho}{\partial n} + \underline{\frac{32}{75} \frac{q_n}{p} \frac{\partial v_t}{\partial n}} \right] \Longrightarrow u_{tnn}^{0} = -\mu \left[\frac{16}{15} \frac{\partial \sigma_{tn}/\rho}{\partial n} - \underline{\frac{32}{75} \frac{q_n \sigma_{tn}}{p\mu}} \right] + \mathcal{O}\left(\mathrm{Kn}^3\right)$$

Order of Magnitude in Kn is preserved!!

Boundary condition for moments [MT & HS 2008]

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

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

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

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

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

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

bulk equation (at left and right boundary)

$$u^0_{tnn} = \frac{32}{45}\frac{\sigma_{tn}q_n}{p}$$

mass conservation

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

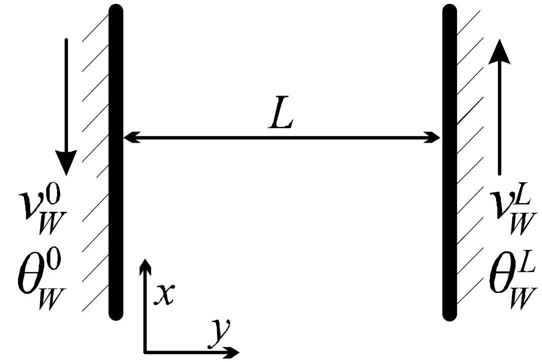
with $V_t = v_t - v_t^W$, $P = \left(\rho\theta + \frac{1}{2}\sigma_{nn} - \frac{1}{28}\frac{w_{nn}}{\theta} - \frac{1}{120}\frac{w_{kk}}{\theta}\right)$

indices n, t indicate normal/tangential components

Channel flow - 13 BC for 13 ODE's $\Longrightarrow$ well-posed problem!

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

Couette flow with R13 [HS 2005, HS & MT 2008]



$\mathcal{O}\left(\mathrm{Kn}^2\right)$ expansion of Grad13/R13/Burnett: bulk equations

$$\sigma_{12} = \mathrm{const} \quad , \quad p + \sigma_{22} = P_0 = \mathrm{const} \quad , \quad \frac{dq_2}{dy} = -\sigma_{12}\frac{dv}{dy}$$

$$\sigma_{12} = -\mu\frac{dv}{dy} \quad , \quad q_2 = -\frac{15}{4}\mu\frac{d\theta}{dy} \quad , \quad \sigma_{22} = -\frac{6}{5}\frac{\sigma_{12}\sigma_{12}}{P_0} \quad , \quad q_1 = \frac{7}{2}\frac{\sigma_{12}q_2}{P_0}$$

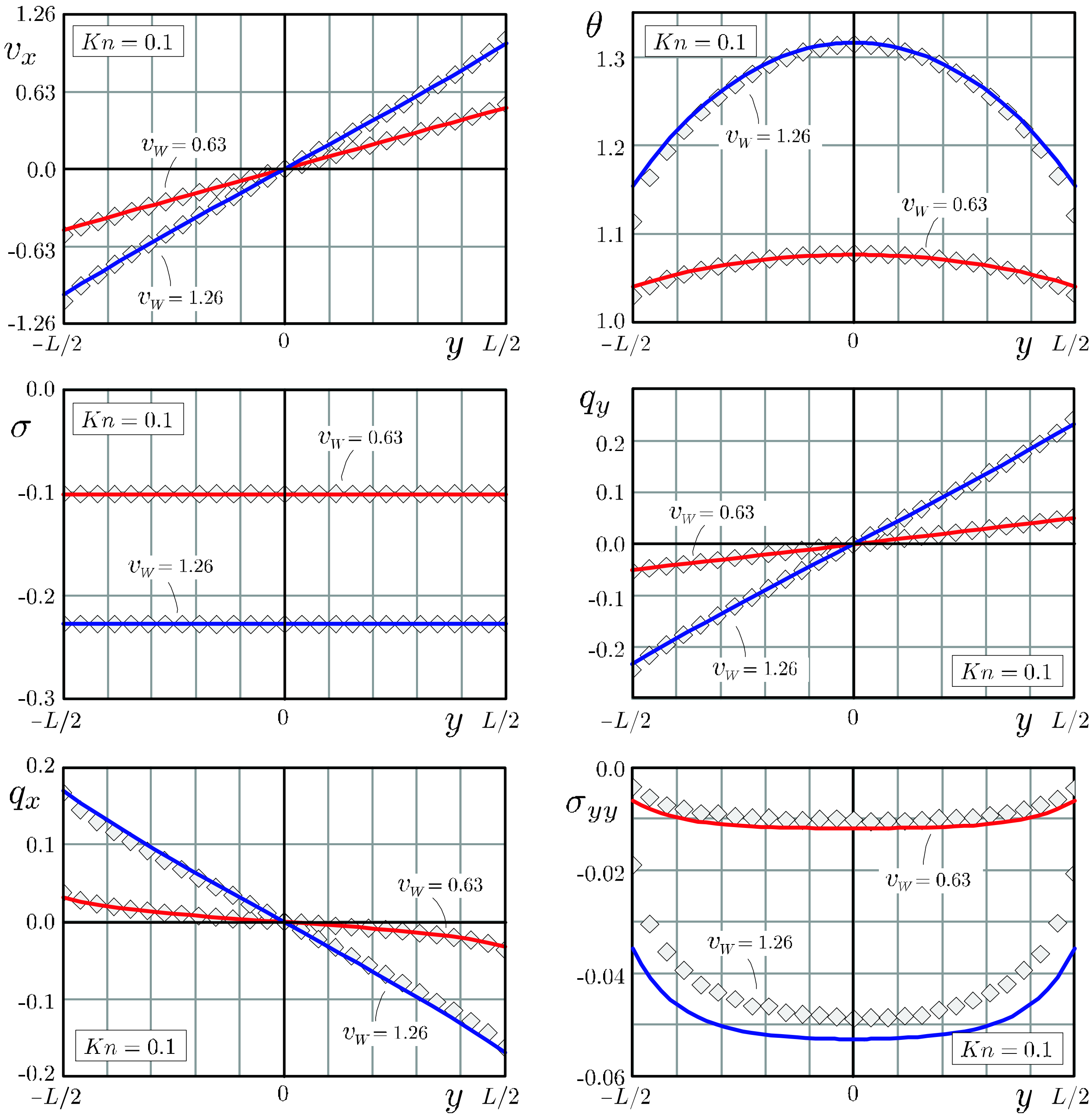
Linear R13 equations: Knudsen boundary layers

$$v\left(x\right) = v_0 - \sigma_{12}\frac{y}{\mathrm{Kn}} - \frac{2}{5}q_1\left(y\right) \quad \text{with} \quad q_1\left(y\right) = A\sinh\left[\sqrt{\frac{5}{9}}\frac{y}{\mathrm{Kn}}\right] + B\cosh\left[\sqrt{\frac{5}{9}}\frac{y}{\mathrm{Kn}}\right]$$

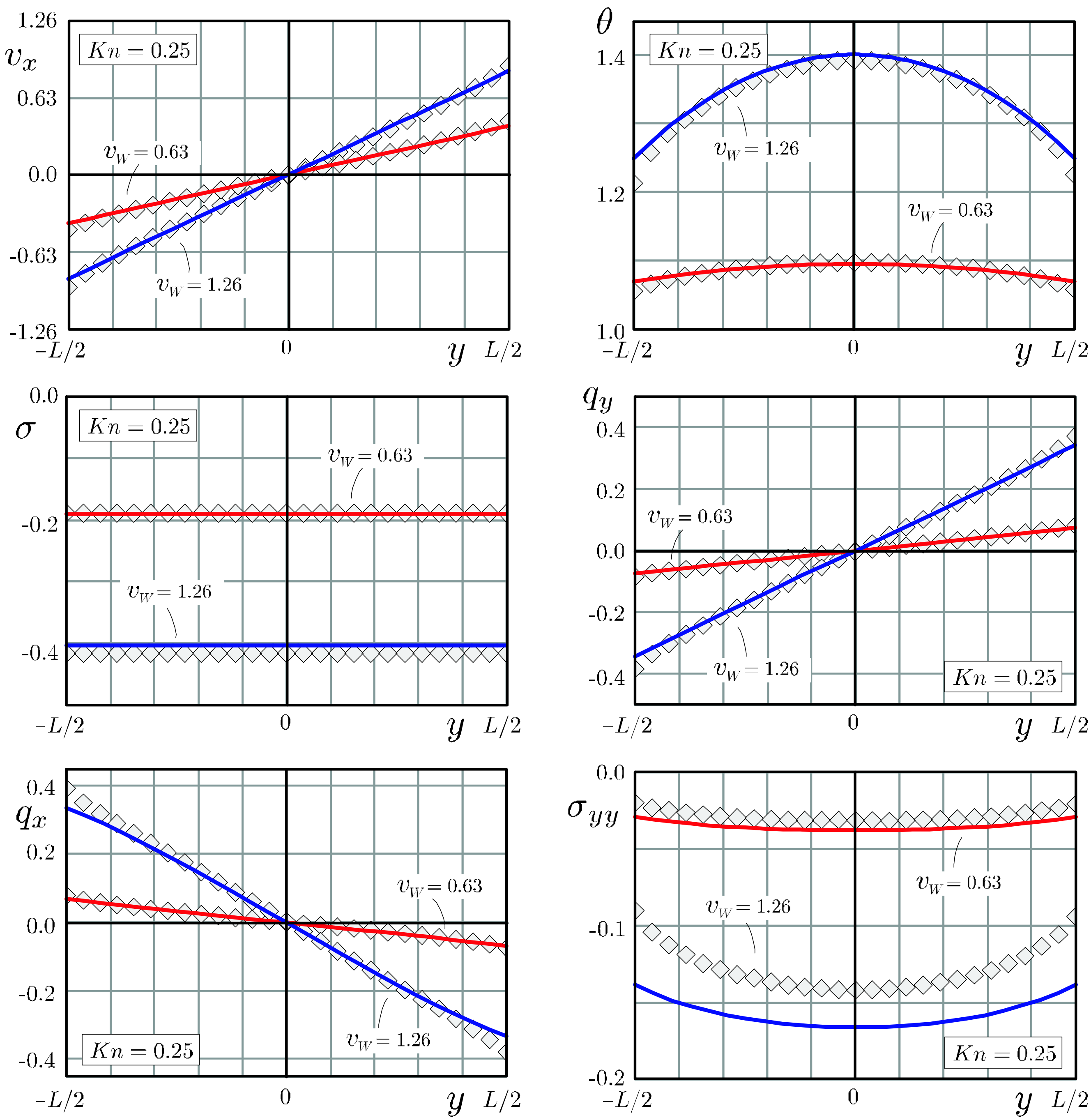
$$T\left(x\right) = T_0 - \frac{4q_1}{15}\frac{y}{\mathrm{Kn}} - \frac{2}{5}\sigma_{22}\left(y\right) \quad \text{with} \quad \sigma_{22}\left(y\right) = C\sinh\left[\sqrt{\frac{5}{6}}\frac{y}{\mathrm{Kn}}\right] + D\cosh\left[\sqrt{\frac{5}{6}}\frac{y}{\mathrm{Kn}}\right]$$

analytical/numerical solutions are superpositions of bulk solutions and Knudsen layers

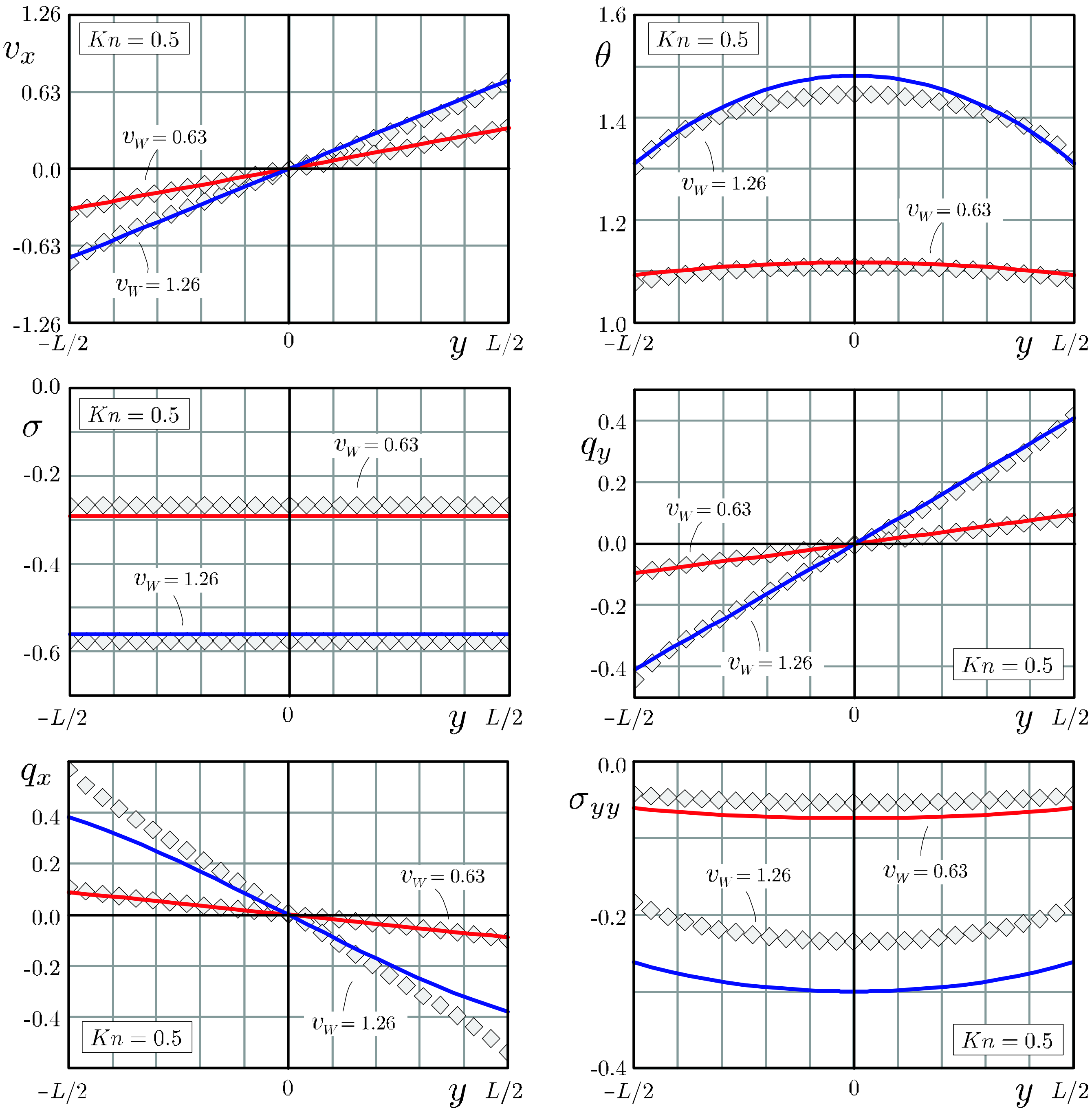
Couette flow: $\mathrm{Kn} = 0.1$ compared to DSMC [MT & HS 2008]



Couette flow: $\mathrm{Kn} = 0.25$ compared to DSMC [MT & HS 2008]



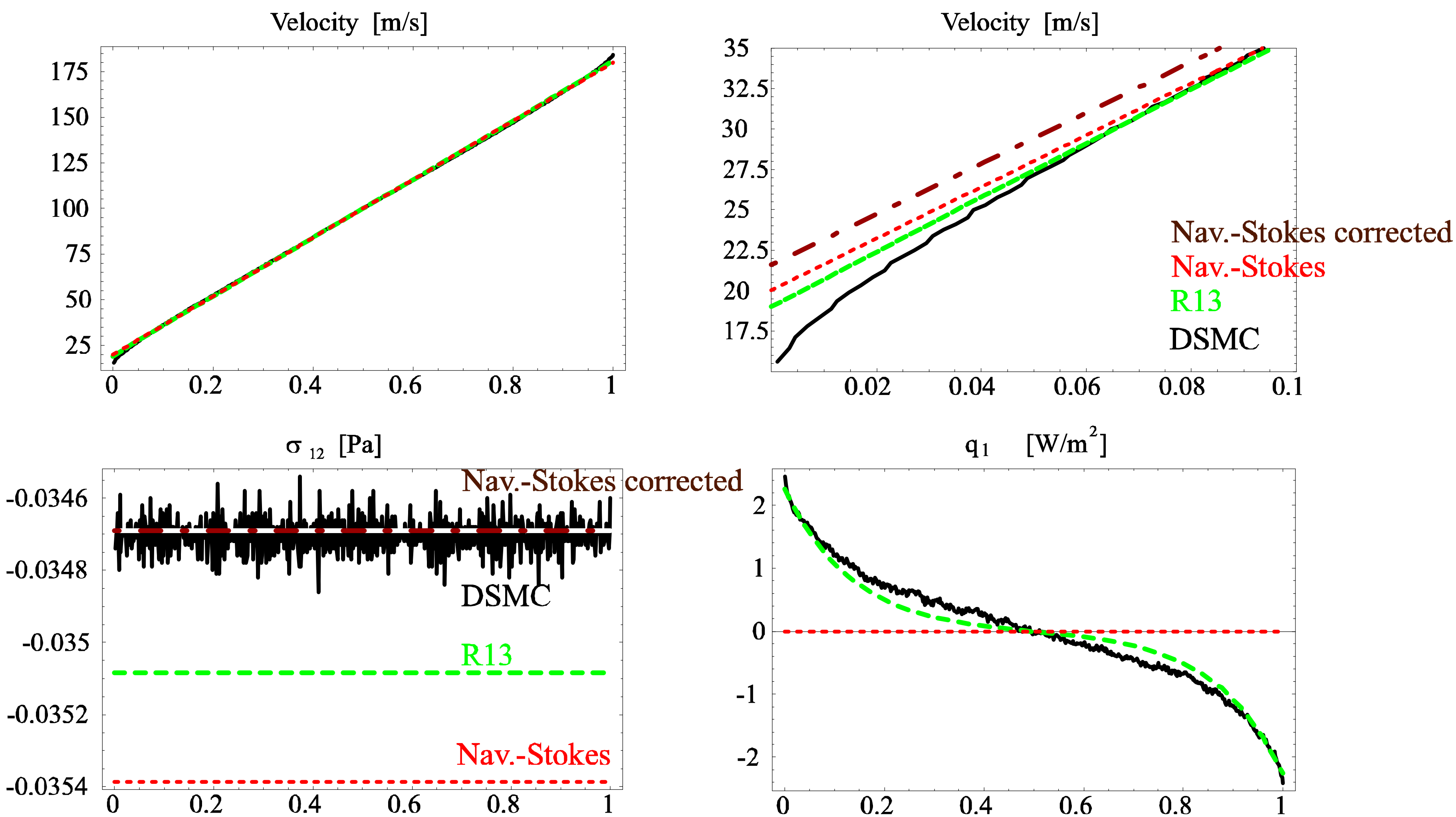
Couette flow: $\mathrm{Kn} = 0.5$ compared to DSMC [MT & HS 2008]



Couette flow: $\mathrm{Kn} = 0.1$, DSMC, R13, Navier-Stokes [HS & MT 2008]

1st order jump condition for Navier-Stokes with Knudsen layer correction coefficient α

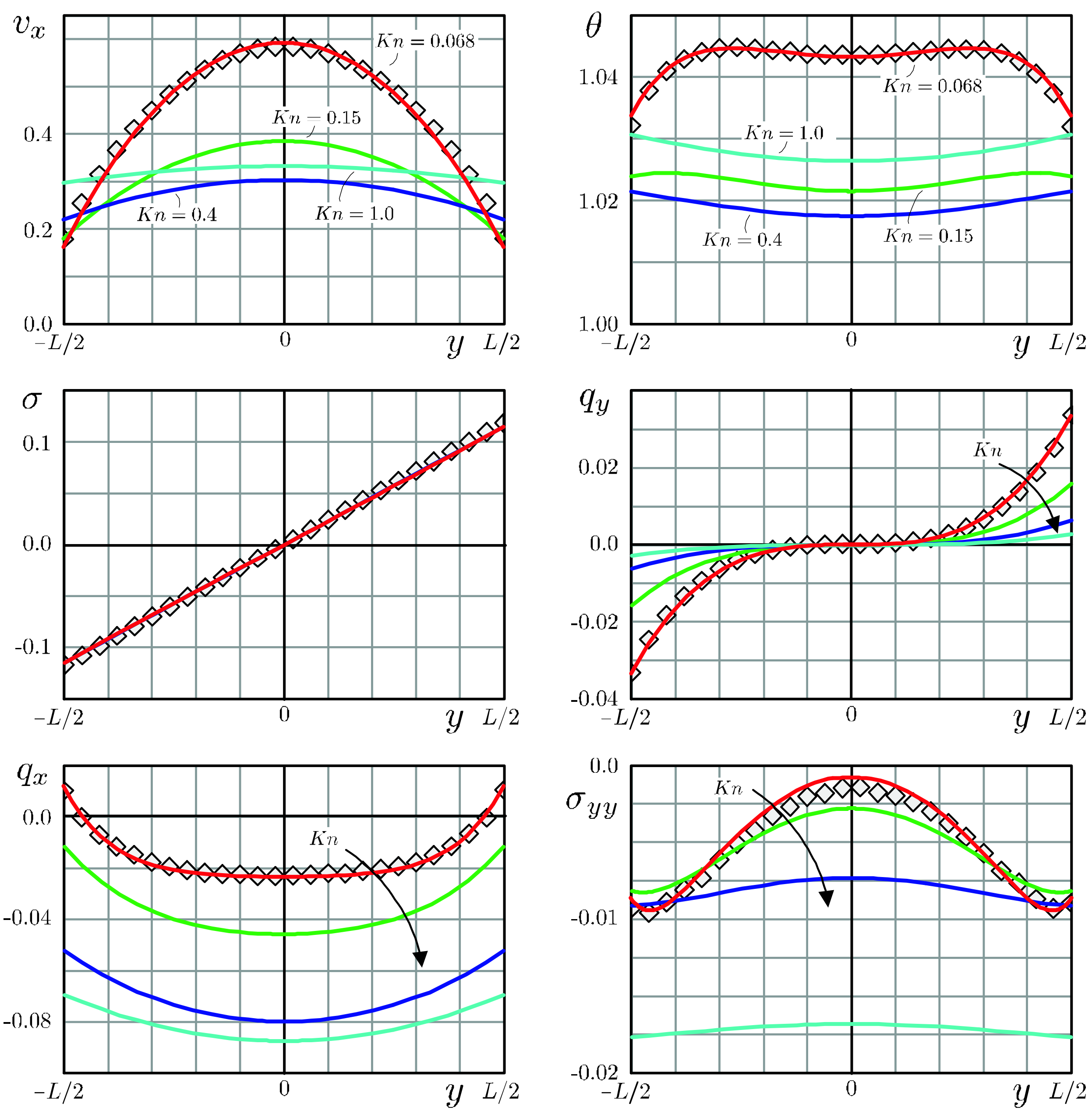
$$v - v_W = \alpha \frac{2-\chi}{\chi} \mathrm{Kn} \sqrt{\frac{\pi}{2}} \frac{\partial v}{\partial y} n_2$$



original Nav.-St.: $\alpha = 1$, corrected Nav.-St.: $\alpha = 1.1$

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

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



$$\theta = \mathsf{C}_8 - \frac{G_1^2}{\mathrm{Kn}^2}\left[\frac{y^4}{45} - \frac{488}{525}\,\mathrm{Kn}^2 y^2\right]$$

$$+\ \mathsf{C}_3\,\frac{956}{375}\,G_1\,\mathrm{Kn}\cosh\left[\frac{\sqrt{5}y}{3\mathrm{Kn}}\right]$$

$$+\ \mathsf{C}_3\,\frac{32}{35\sqrt{5}}\,\sigma_{12}\sinh\left[\frac{\sqrt{5}y}{3\mathrm{Kn}}\right]$$

$$-\ \mathsf{C}_6\,\frac{2}{5}\cosh\left[\frac{\sqrt{5}y}{\sqrt{6}\mathrm{Kn}}\right]$$

superposition of

bulk solution

Knudsen layers

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

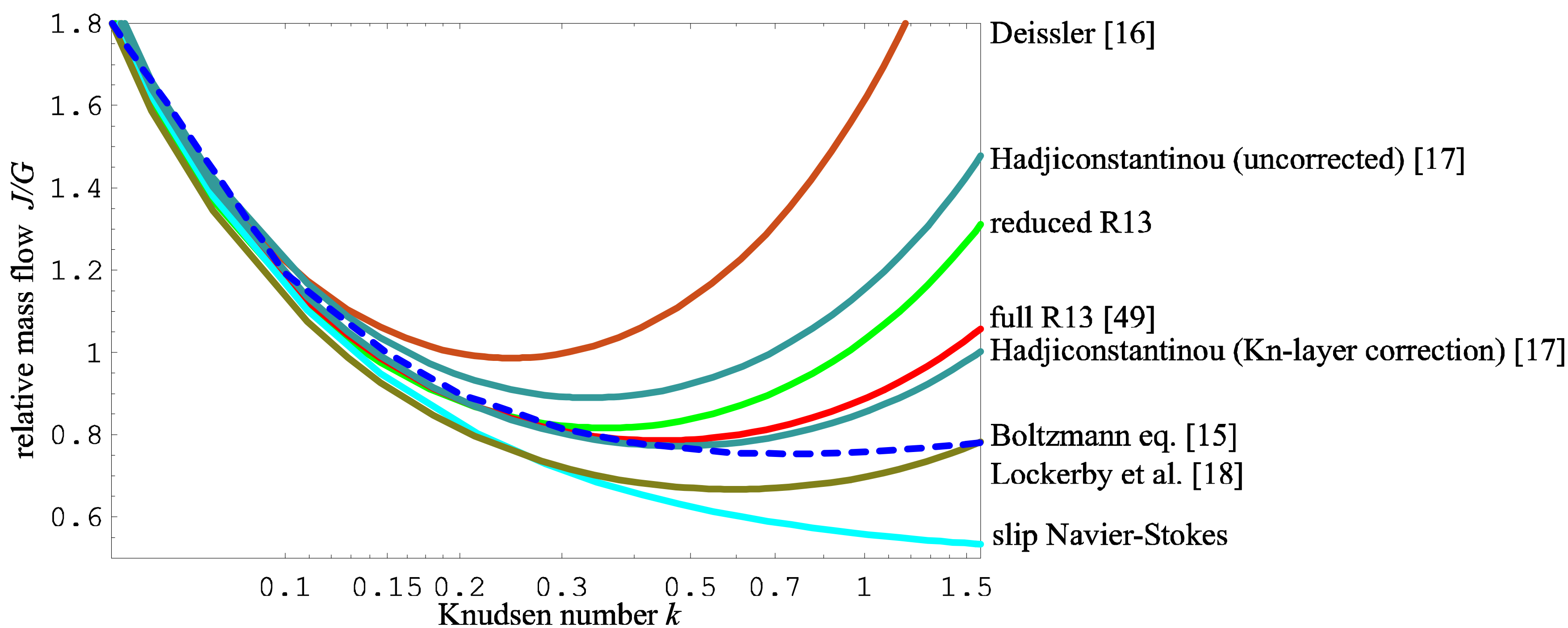
linearized Navier-Stokes with 2nd order slip (values for α and β vary between authors)

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

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 (analog to Knudsen minimum) [HS & MT 2008]

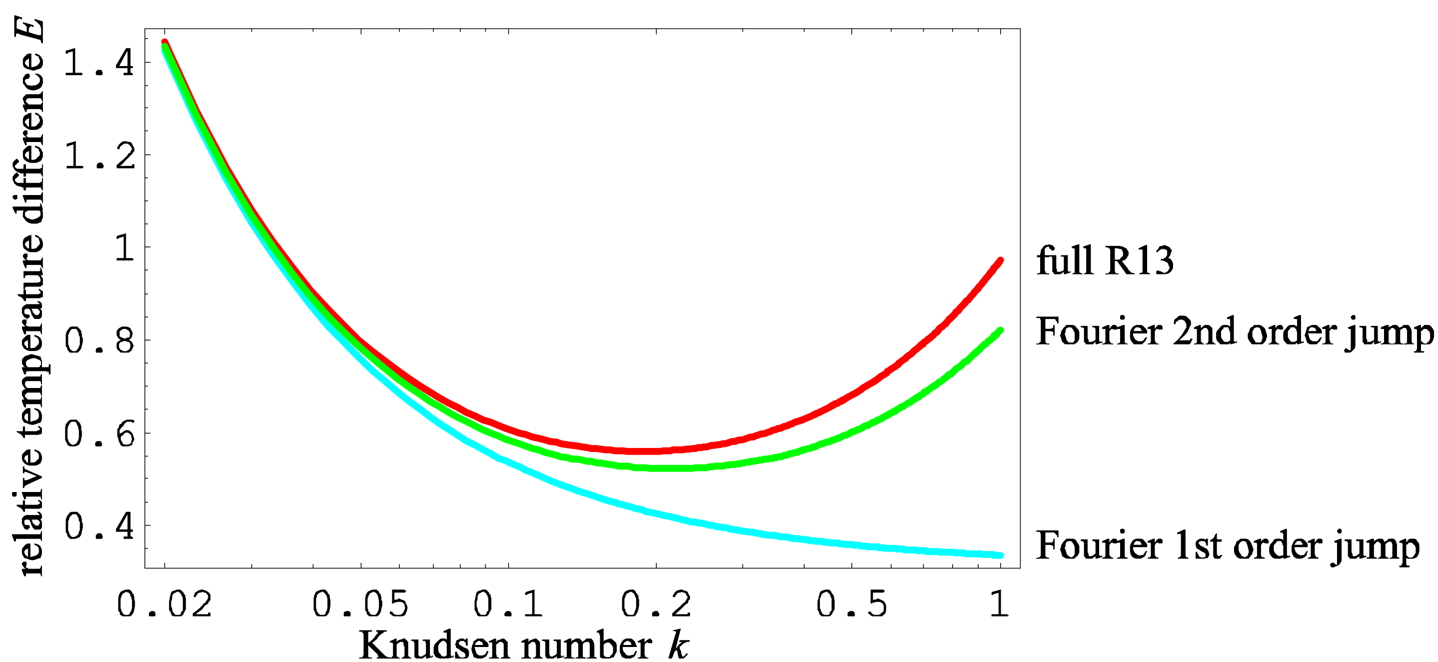
gas heated by radiation: gas at rest, walls at θ_W, energy absorbed S

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

Fourier and R13 (second order jump condition)

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

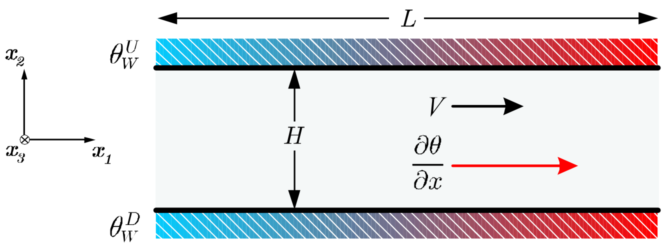
$$E_{R13} = \frac{1}{45}\frac{1}{\mathrm{Kn}} + \frac{13}{50}\sqrt{\frac{\pi}{2}} + \frac{18}{25}\mathrm{Kn} + \frac{\sqrt{\frac{6}{5}}\left(7\pi + 160\mathrm{Kn}\sqrt{\frac{\pi}{2}} + 384\mathrm{Kn}^2\right)}{140\left(15\coth\left[\sqrt{\frac{5}{6}}\frac{1}{2\mathrm{Kn}}\right] + 2\sqrt{15\pi}\right)}$$

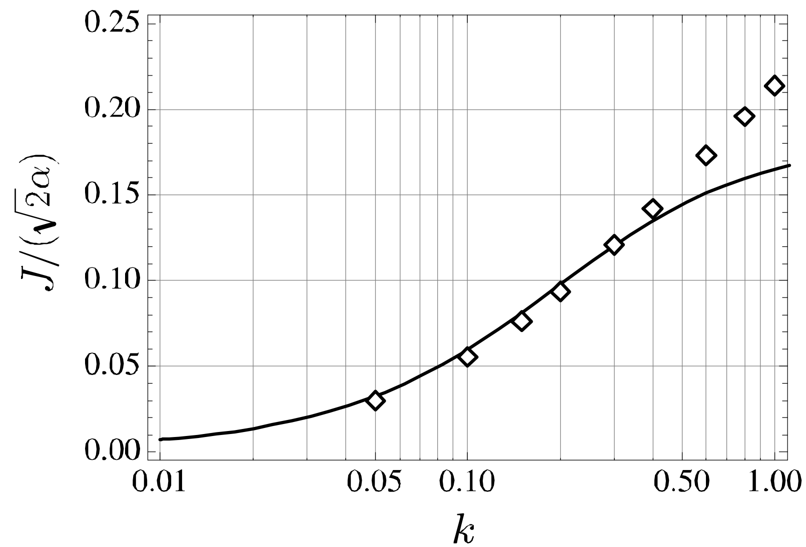


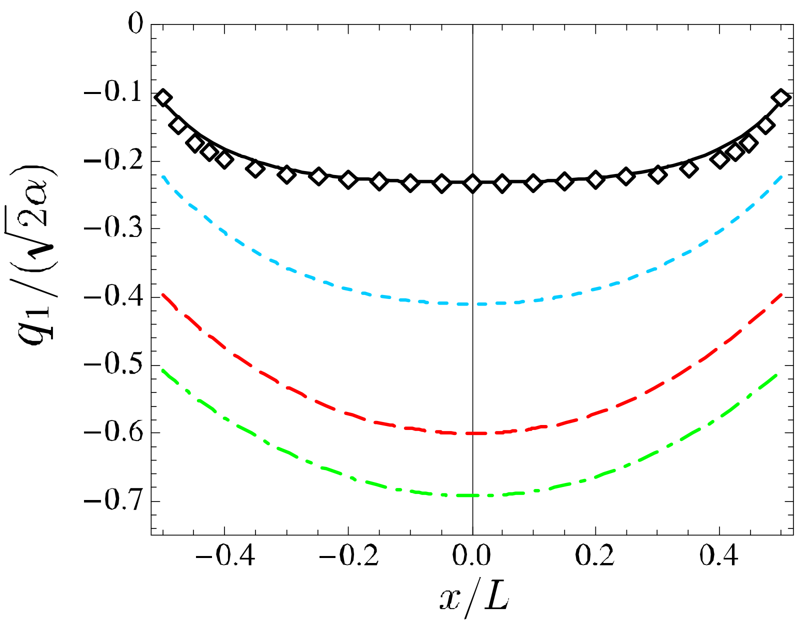
Thermal transpiration flow [PT & HS 2008]

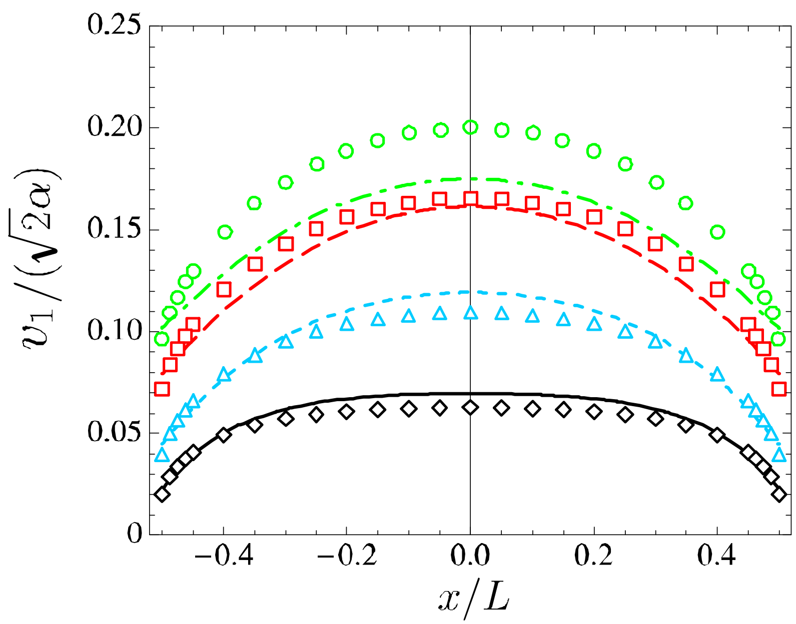
Flow driven by T-gradient in wall $\mathrm{Kn} = 0.09, 0.18, 0.35, 0.53$

mass flow, heat flux, velocity (R13, linear Boltzmann)



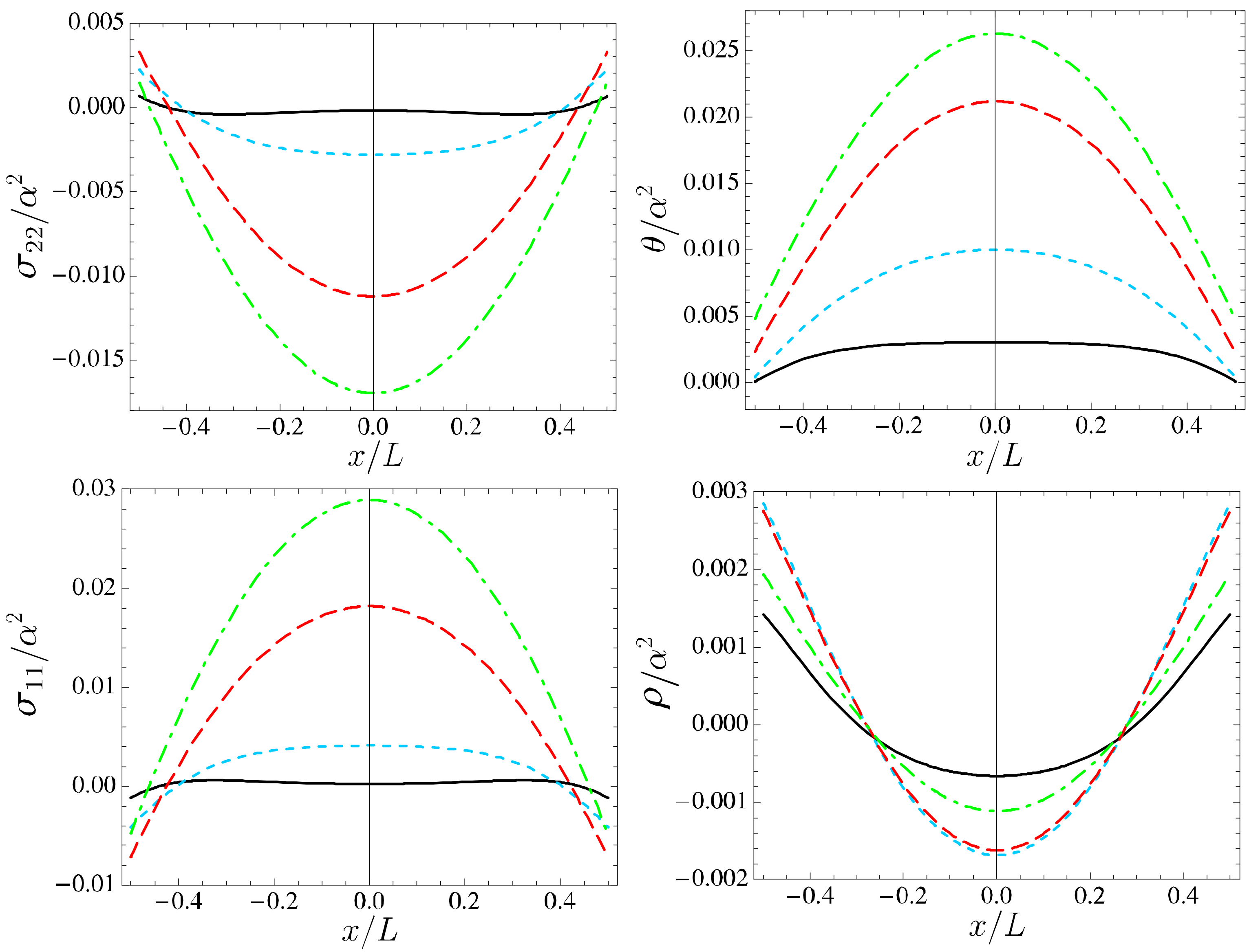






Thermal transpiration flow [PT & HS 2008]

temperature profile and other non-linear effects (R13 prediction)



Knudsen layers and moments [HS 2003, 2008]

heat transfer with many moments(simplified linear model)

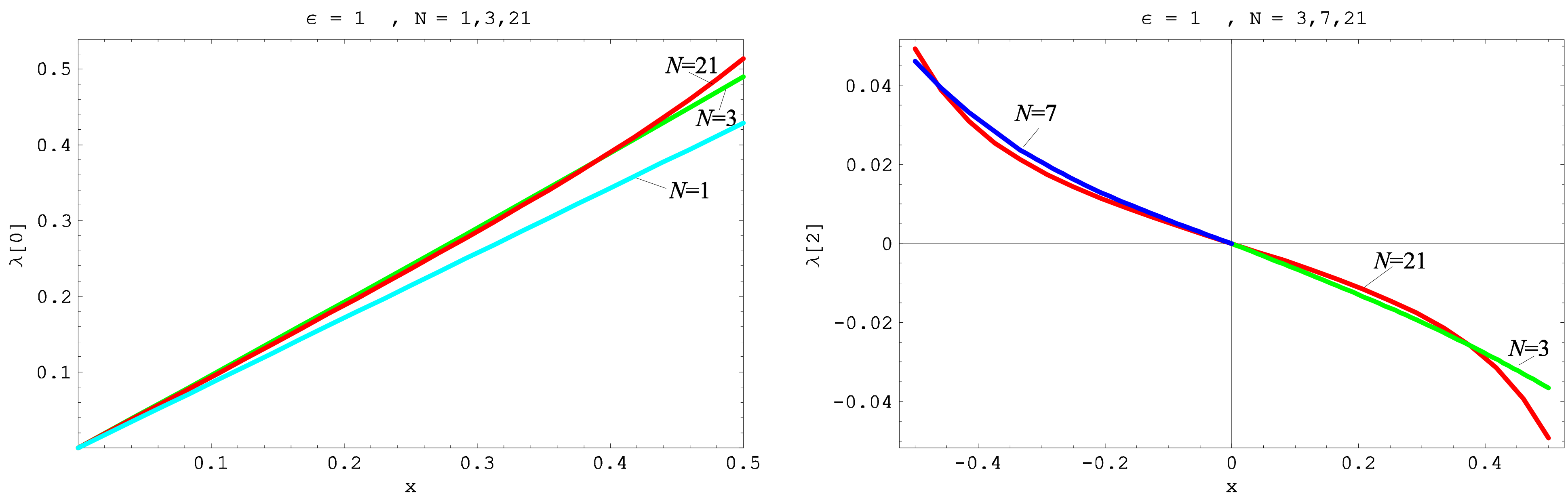
energy: linear plus Knudsen layers

$$q_0 = K - \frac{3}{\mathrm{Kn}}\lambda_1 x - 2\lambda_2 \quad , \quad q_1 = const.$$

Knudsen layer moments ($b^{(m)}$, Φ_{nm} from eigenvalue problem)

$$\lambda_n = \sum_{m=2} \Phi_{nm}\Gamma^0_m \exp\left[-\frac{x}{\mathrm{Kn}b^{(m)}}\right] \quad (n \geq 2)$$

energy density, second moment in transition regime $\mathrm{Kn} = 1$



marked Knudsen layers, already $N = 3$ **gives good agreement!!**

$N = 1$: **no Knudsen layer, large deviation**

Knudsen layers and moments [HS 2003, 2008]

heat transfer with many moments(simplified linear model)

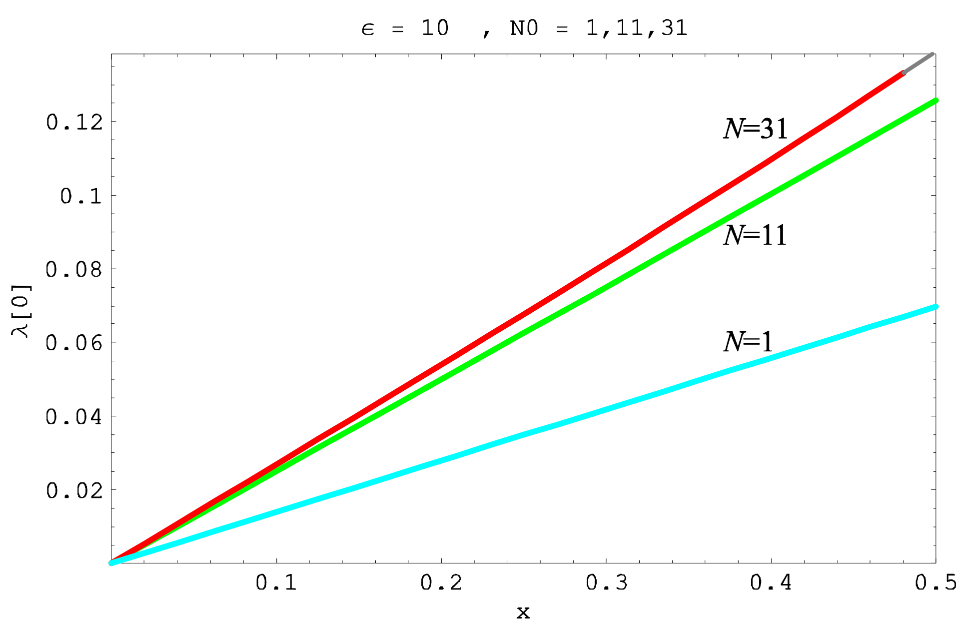
energy: linear plus Knudsen layers

$$q_0 = K - \frac{3}{\mathrm{Kn}}\lambda_1 x - 2\lambda_2 \quad , \quad q_1 = const.$$

Knudsen layer moments ($b^{(m)}$, Φ_{nm} from eigenvalue problem)

$$\lambda_n = \sum_{m=2} \Phi_{nm}\Gamma^0_m \exp\left[-\frac{x}{\mathrm{Kn}b^{(m)}}\right] \quad (n \geq 2)$$

energy density, second moment in free molecular flow $\mathrm{Kn} = 10$



marked Knudsen layers, T-jump, N **must be large** $(N \geq 31)$ **!!**

Knudsen layers and moments [HS 2003, 2008]

examination of equation, boundary conditions, solutions shows

- **Knudsen layer amplitudes flow from BC**
- Kn-**expansion of equations** (CE, order of magnitude, ...) **not appropriate for Kn-layers**
- **Knudsen layers are 2nd order effects** (amplitude $\sim \mathrm{Kn}^2$)
- **high resolution of Knudsen layers requires many moments** (independent of CE-order!)
- **equations with few Knudsen layers better than eqs. without**

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

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

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)

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

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

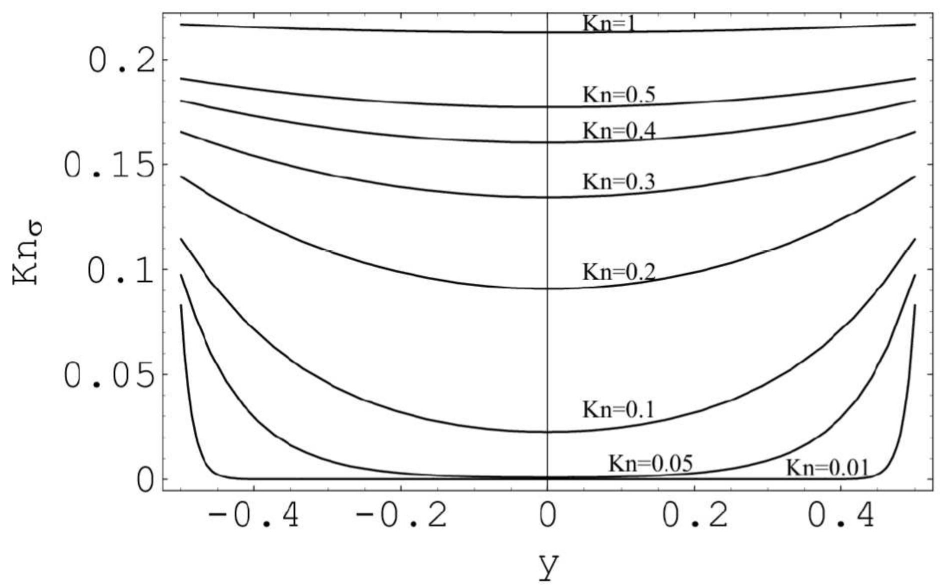
Example III: Linear Poiseuille flow with the R13 equations

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

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

Summary: Regularized 13 moment equations

- rational derivation from Boltzmann equation
- contain Burnett and super-Burnett in CE expansion
- linearly stable
- phase speeds and damping match experiments better than NSF, Grad13
- smooth shock structures for all Ma, accurate for $\mathrm{Ma} < 3$
- H-theorem for linear case, including boundary conditions !
- furnished with complete theory of boundary conditions
- just enough moments to exhibit Knudsen boundary layers
- excellent agreement to DSMC simulations for all rarefaction effects
- accessible to other moment sets: R20 [Mizzi-Gu-Emerson], R10 [McDonald-Groth]

Future work

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

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but . . . the more the merrier ?