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Boundary Conditions for Regularized 13-Moment-Equations

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Compressible Viscous Gas Flow

- gas variables: density, velocity and temperature $U = \{\rho,\, \mathbf{v},\, T\}$

$$
\begin{aligned}
\partial_t \rho \quad & + \operatorname{div} \rho\mathbf{v} && = 0 \\
\partial_t \rho\mathbf{v} \quad & + \operatorname{div}\left(\rho\mathbf{v}\,\mathbf{v}^T + p\mathbf{I} + \boldsymbol{\sigma}\right) && = 0 \\
\partial_t \rho\left(e + \tfrac{1}{2}\mathbf{v}^2\right) & + \operatorname{div}\left(\left(\rho\left(e + \tfrac{1}{2}\mathbf{v}^2\right) + p\right)\mathbf{v} + \boldsymbol{\sigma}\,\mathbf{v} + \mathbf{q}\right) && = 0
\end{aligned}
$$

- ideal monatomic gas, internal energy $e(T) = \frac{3}{2}\frac{k}{m}T$, and pressure $p(\rho, T) = \rho\,\frac{k}{m}\,T$

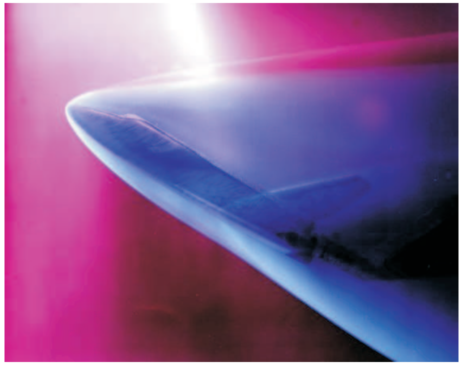
Empirical Consititutive Relations

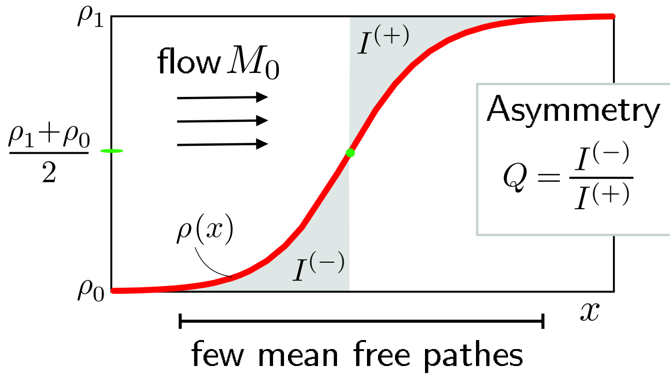
$$
\sigma_{ij} = -2\mu(T)\frac{\partial v_{\langle i}}{\partial x_{j\rangle}}
\qquad\qquad
q_i = -\lambda(T)\frac{\partial T}{\partial x_i}
$$

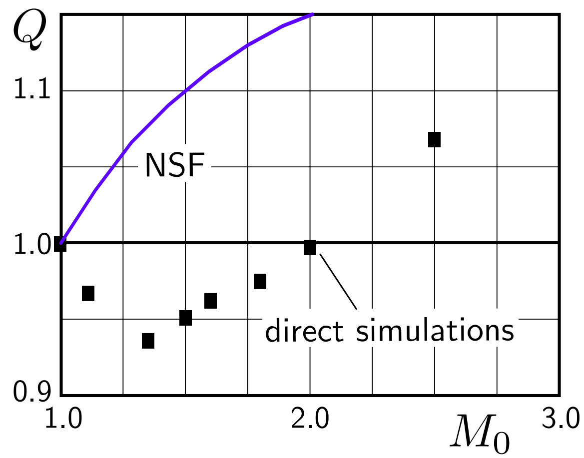
Navier (1822) and Stokes (1845) — Fourier (1822)

Failure of NSF Models

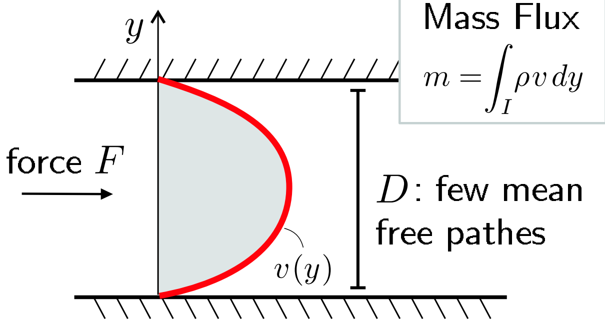
- asymmetry of density shock wave profiles

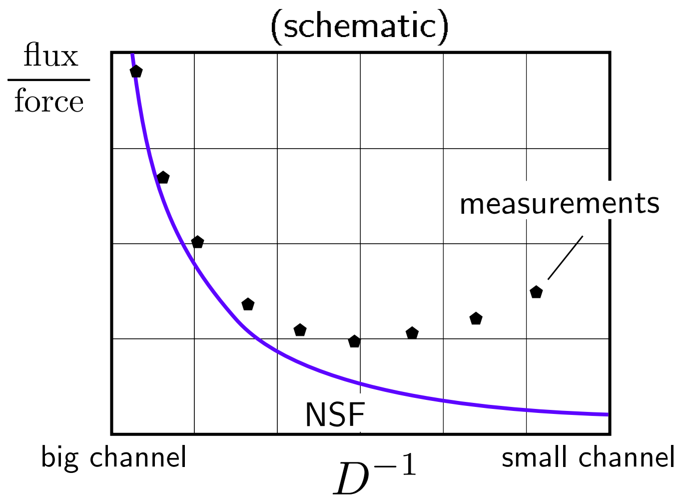






- micro-channel mass flux





Kinetic Gas Theory

- stochastic description based on velocity distribution function $f : \Omega \times [0, \mathcal{T}] \times \mathbb{R}^3 \to \mathbb{R}$

$$\frac{\partial f}{\partial t} + c_i \frac{\partial f}{\partial x_i} = \frac{1}{\varepsilon} \int_{\mathbb{R}^5} \left(f' \, f'^1 - f \, f^1 \right) \, g \, b \, db \, d\omega \, d\mathbf{c}_1$$

BOLTZMANN (1872)

- moments of the distribution function: $F_{ij\cdots k} = m \int c_i c_j \cdots c_k \, f \, d\mathbf{c}$
- fluid variables $F = \rho, \; F_i = \rho v_i, \; F_{ii} = 3\rho T + \rho v_i^2 \;, \; F_{ij} \sim \; \sigma_{ij} \;, \; F_{ijj} \sim \; q_i$
- moments satisfy an equation hierarchy with closure problem
- scaling parameter: Knudsen number $\varepsilon \;\widehat{=}\; \frac{\text{mean-free-path}}{\text{observation scale}}$
- limit $\varepsilon \to 0$, equilibrium flow $f \to f_M$, Maxwell distribution
- non-equilibrium modelling $0 < \varepsilon < 1$

Find partial differential equations that approximate the multi-scale behavior in a continuum model

Classical Approximations

Chapman-Enskog

- asymptotic analysis: $f_{CE} = f_M + \varepsilon\, f^{(1)} + \varepsilon^2\, f^{(2)} + \ldots$

  leads to e.g. $q_i = q_i^{(0)} + \varepsilon\, q_i^{(1)} + \varepsilon^2 q_i^{(2)} + \ldots$ for non-equilibrium variables

  $q_i^{(0)}$: 0; $q_i^{(1)}$: Fourier; $q_i^{(2)}$: Burnett; $\ldots$: super-Burnett

- parabolic systems including higher order derivatives

! Burnett and super-Burnett are linearly unstable, see BOBYLEV (1982)

Grad

- Hermite series of the distribution function: $f_G = f_M \left(1 + \sum^N \Lambda_{ij\ldots k}\, c_i c_j \cdots c_k\right)$

  with relation $\Lambda_{ij\ldots k} \leftrightarrow F_{ij\ldots k}$ for a fixed number of N moments

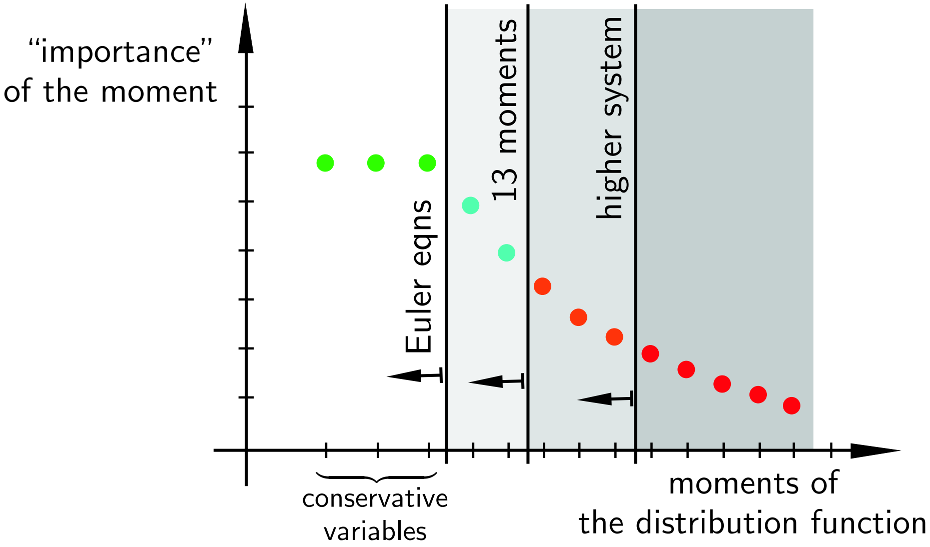
- Grad considers evolution equations for a large set of N moments, e.g. 13

- large first order hyperbolic systems in divergence form, always stable

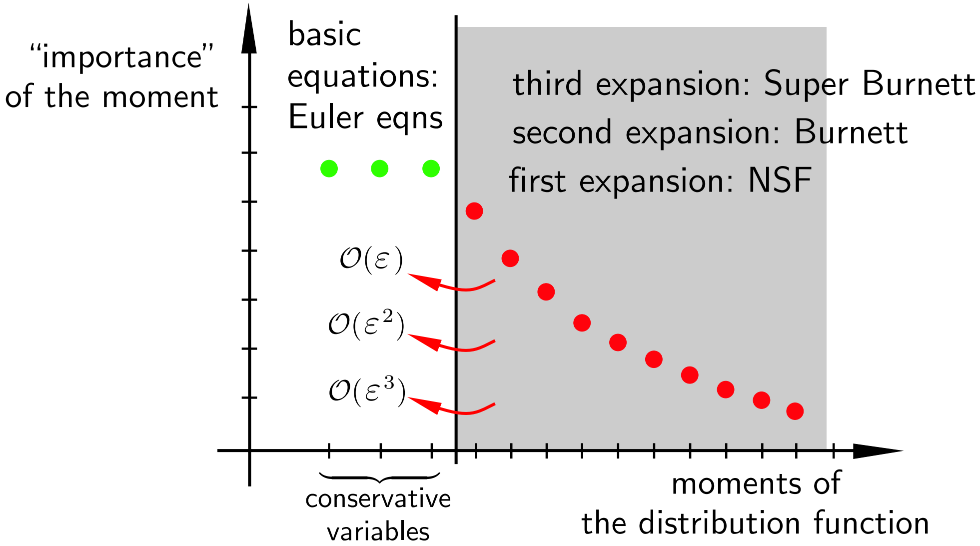
! introduces subshocks into shock structure, see GRAD (1952), WEISS (1995)

Regularization of Moment Equations

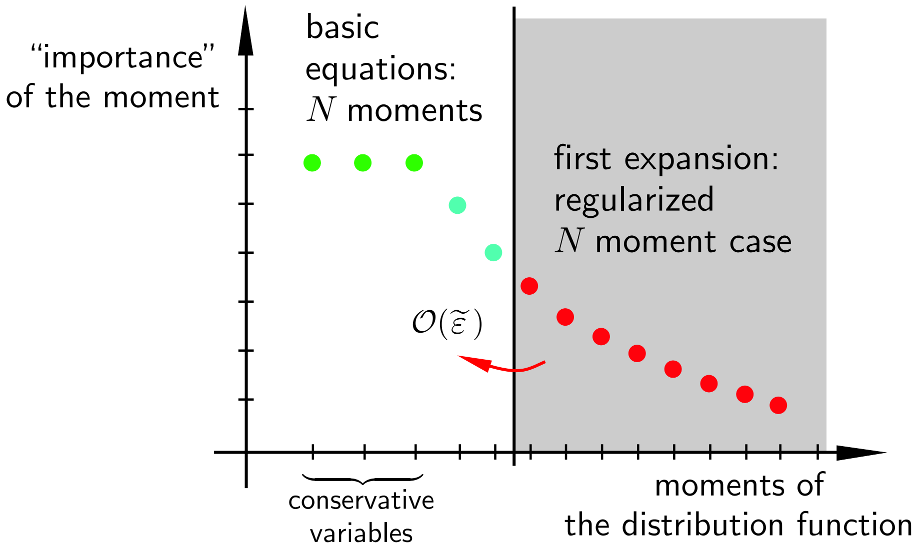
STRUCHTRUP/TORRILHON (2003)



Grad's moment approach



Chapman-Enskog expansion



Regularized 13-Moment-Equations

- basic conservation equation

$$
\begin{aligned}
&\partial_t \rho && + \operatorname{div} \rho \mathbf{v} && = 0 \\
&\partial_t \rho \mathbf{v} && + \operatorname{div} \left(\rho \mathbf{v}\, \mathbf{v}^T + p\mathbf{I} + \boldsymbol{\sigma}\right) && = 0 \\
&\partial_t \rho \left(e + \tfrac{1}{2}\mathbf{v}^2\right) && + \operatorname{div} \left(\left(\rho \left(e + \tfrac{1}{2}\mathbf{v}^2\right) + p\right) \mathbf{v} + \boldsymbol{\sigma}\, \mathbf{v} + \mathbf{q}\right) && = 0
\end{aligned}
$$

Extended Consititutive Relations (Regularized 13-Moment-Equation, linearized)

- stress/heatflux follow a driven wave equation system with relaxation and dissipation

$$
\frac{\partial \sigma_{ij}}{\partial t} + \tfrac{4}{5}\frac{\partial q_{\langle i}}{\partial x_{j\rangle}} + 2p\frac{\partial v_{\langle i}}{\partial x_{j\rangle}} = -\tfrac{p}{\mu}\sigma_{ij} + 2\,\frac{\partial}{\partial x_k}\Big(T\tfrac{\mu}{p}\frac{\partial \sigma_{\langle ij}}{\partial x_{k\rangle}}\Big)
$$

$$
\frac{\partial q_i}{\partial t} + T\frac{\partial \sigma_{ij}}{\partial x_j} + \tfrac{5}{2}p\frac{\partial T}{\partial x_i} = -\tfrac{2}{3}\tfrac{p}{\mu}q_i + \tfrac{12}{5}\,\frac{\partial}{\partial x_k}\Big(T\tfrac{\mu}{p}\frac{\partial q_{\{i}}{\partial x_{k\}}}\Big)
$$

STRUCHTRUP and TORRILHON (2003)

- R13 is highly accurate and fully stable continuum model with smooth shock profiles
- earlier attempts: GRAD (1958), KARLIN ET AL. (1998), JIN & SLEMROD (2001), MÜLLER ET AL. (2002)

Full Regularized 13-Moment-Equations

- full nonlinear 3d-equations for stress and heat flux:

$$\partial_t \sigma_{ij} + \partial_k (\sigma_{ij} v_k + m_{ijk}) + \tfrac{4}{5} \partial_{\langle i} q_{j\rangle} + 2p \partial_{\langle i} v_{j\rangle} + 2 \partial_k v_{\langle i}\, \sigma_{j\rangle k} = -\frac{p}{\mu} \sigma_{ij}$$

$$\partial_t q_i + \partial_k (q_i v_k + \tfrac{1}{2} \hat{R}_{ik}) + p \partial_k (\sigma_{ik}/\rho) + \tfrac{5}{2} (p \delta_{ik} + \sigma_{ik}) \partial_k \theta$$
$$- (\sigma_{ij}/\rho) \partial_k \sigma_{kj} + q_k \partial_k v_i + (m_{ijk} + \tfrac{6}{5} q_{(i} \delta_{jk)}) \partial_k v_i = -\frac{2p}{3\mu} q_i$$

- regularization terms ($\hat{R}_{ij} = R_{ij} + \frac{1}{3} R \delta_{ij}$):

$$m_{ijk} = -2\mu\, \partial_{\langle i} (\sigma_{jk\rangle}/\rho) + \frac{8}{10p} q_{\langle i} \sigma^{(\mathrm{NSF})}_{jk\rangle}$$

$$R_{ij} = -\frac{24}{5} \mu\, \partial_{\langle j} (q_{j\rangle}/\rho) + \frac{32}{25p} q_{\langle i} q^{(\mathrm{NSF})}_{j\rangle} + \frac{24}{7\rho} \sigma_{k\langle i} \sigma^{(\mathrm{NSF})}_{j\rangle k}$$

$$R = -12\mu\, \partial_k (q_k/\rho) + \frac{8}{p} q_k q^{(\mathrm{NSF})}_k + \frac{6}{\rho} \sigma_{ij} \sigma^{(\mathrm{NSF})}_{ij}$$

- abbreviations: $\sigma^{(\mathrm{NSF})}_{ij} = -2\mu\, \partial_{\langle i} v_{j\rangle}$

$$q^{(\mathrm{NSF})}_i = -\frac{15}{4} \mu\, \partial_i \theta$$

Accuracy and Knudsen Order

- **Definition : (Knudsen order)** *Assume $U^{(Boltz)}$ and $U^{(model)}$ are the respective solutions expanded in ε and the difference satisfies*

$$\left\| \boldsymbol{\sigma}^{(\mathrm{model})} - \boldsymbol{\sigma}^{(\mathrm{Boltz})} \right\| + \left\| \mathbf{q}^{(\mathrm{model})} - \mathbf{q}^{(\mathrm{Boltz})} \right\| = \mathcal{O}\left(\varepsilon^{n+1}\right)$$

Then the Knudsen order or accuracy of the model is $n \in \mathbb{N}$.

- all continuum models can be assigned a Knudsen order
- equilibrium flow: $n\,(\text{Euler}) = 0$
- classical theory: $n\,(\text{NSF}) = 1$
- Burnett expansion: $n\,(\text{Burnett}) = 2$ (unstable!!)
- Grad's 13-moment-equations: $n\,(\text{Grad}) = 2$ (subshocks!!)

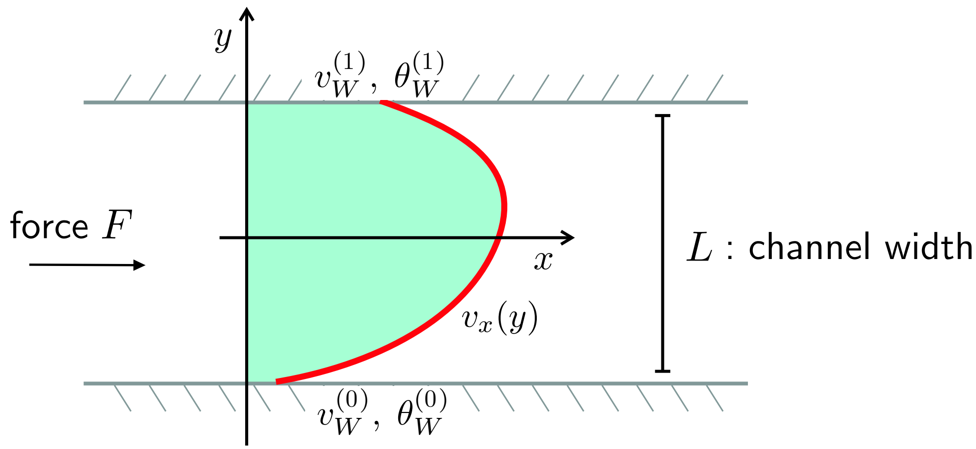
- **Theorem : (R13 Accuracy)** *The regularized 13-moment-equations provide a Knudsen order*

$$n\,(\text{R13}) = 3,$$

hence, they are of super-Burnett order. Higher terms inside the equation stabilize the system.

Boundary Value Problems

- consider plane channel flow between infinite plates
- plates can be heated and moved independently with $v_W^{(0,1)}$, $\theta_W^{(0,1)}$
- force represent homogeneous pressure gradient



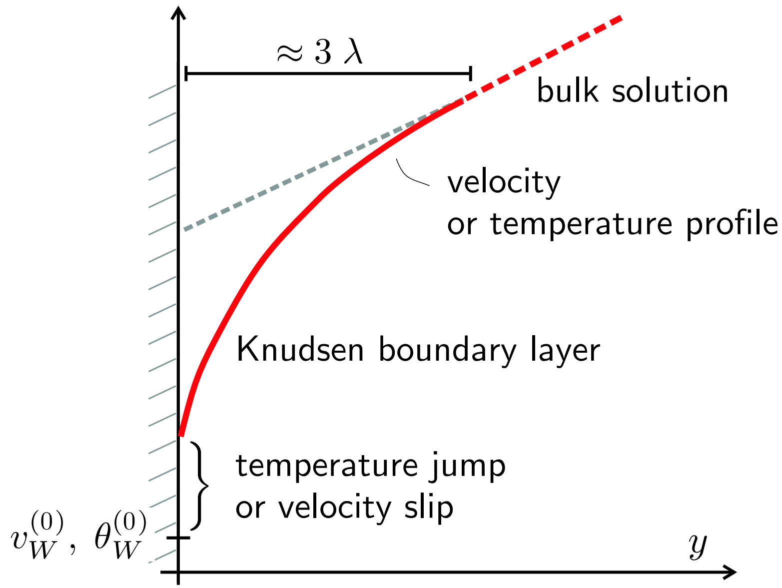
- write steady R13-equations as first order system in channel geometry:

$$\mathbf{A}\left(\mathbf{U}\right)\partial_y\mathbf{U} = \mathbf{P}\left(\mathbf{U}\right)$$

- 10 relevant R13-variables for channel flow:

$$\mathbf{U} = \Big\{ \underbrace{v_x, \sigma_{xy}, q_x, m_{xyy}, R_{xy}}_{\text{velocity part}} \Big| \underbrace{\theta, q_y, \sigma_{yy}, \hat{R}_{yy}, m_{yyy}}_{\text{temperature part}} \Big\}$$

Knudsen layer phenomenon:



Kinetic Boundary Conditions

- Maxwell accommodation model for the distribution function at the wall

$$\tilde{f}(\mathbf{c}) = \begin{cases} \chi f_W(\mathbf{c}) + (1-\chi) f_{\text{gas}}^{(*)}(\mathbf{c}) & \mathbf{n}\cdot(\mathbf{c}-\mathbf{v}_W) > 0 \\ f_{\text{gas}}(\mathbf{c}) & \mathbf{n}\cdot(\mathbf{c}-\mathbf{v}_W) < 0 \end{cases}$$

- R13 distribution function + integration gives boundary relations for moments
- continuity for $\chi \to 0$ implies: only odd (in y) moments should be prescribed
- consistency implies: only fluxes of the variable set should be prescribed

$$\Rightarrow \quad \sigma_{xy} = -\sqrt{\frac{2}{\pi\theta}}\frac{\chi}{2-\chi}\left(P\,V_W + \frac{1}{2}m_{xyy} + \frac{1}{5}q_x\right)$$

$$R_{xy} = \sqrt{\frac{2}{\pi\theta}}\frac{\chi}{2-\chi}\left(P\,\theta\,V_W - \frac{1}{2}\theta\,m_{xyy} - \frac{11}{5}\theta\,q_x - P\,V_W^3 + 6P(\theta-\theta_W)V_W\right)$$

$$q_y = -\sqrt{\frac{2}{\pi\theta}}\frac{\chi}{2-\chi}\left(2P(\theta-\theta_W) + \frac{5}{28}\hat{R}_{yy} + \frac{1}{2}\theta\,\sigma_{yy} - \frac{1}{2}P\,V_W^2\right)$$

$$m_{yyy} = \sqrt{\frac{2}{\pi\theta}}\frac{\chi}{2-\chi}\left(\frac{2}{5}P(\theta-\theta_W) - \frac{1}{14}\hat{R}_{yy} - \frac{7}{5}\theta\,\sigma_{yy} - \frac{3}{5}P\,V_W^2\right)$$

4 boundary conditions on both walls not enough...

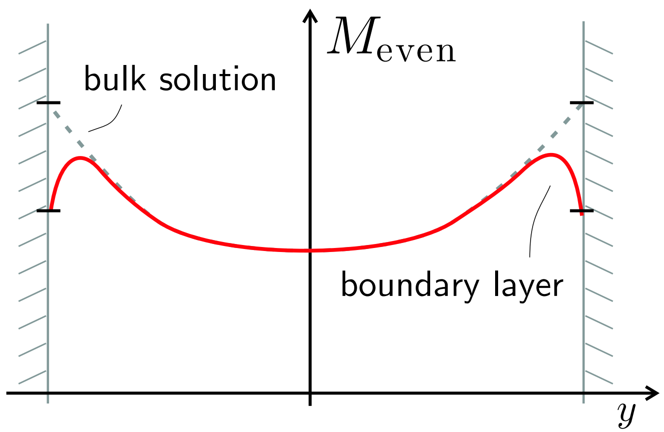
with $V_W = v_x - v_W$

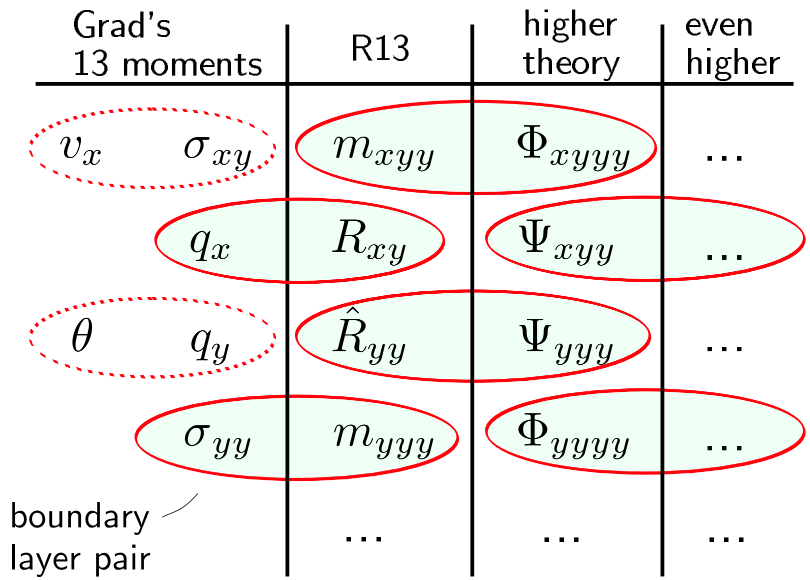
Boundary Layer Reduction

- in an infinite moment hierarchy all higher variables produce boundary layers
- an even moment M_{even} together with an odd higher moment F_{odd} forms a boundary layer pair, with kinetic boundary condition for F_{odd}

$$\left.\begin{aligned} \{\text{other terms}\} + \partial_y F_{\text{odd}} &= -\frac{1}{\varepsilon} M_{\text{even}} \\ F_{\text{odd}} &= -\varepsilon\, \partial_y M_{\text{even}} \end{aligned}\right\} \rightsquigarrow \exp(\pm y/\varepsilon)$$

- any truncated theory produces cut pairs, single variables are reduced to their bulk solution
- bulk values imply boundary conditions





Nullspace Conditions

- consider the R13 system in first order form with variable vector $\mathbf{U} \in \mathbb{R}^N$

$$\mathbf{A}\left(\mathbf{U}\right)\partial_y \mathbf{U} = \mathbf{P}\left(\mathbf{U}\right)$$

- reduction of boundary layer pair from a larger system produces a singular matrix $\mathbf{A}(\mathbf{U})$, thus eigenvalues $\lambda_i = 0$ and left eigenvectors

$$\{\mathbf{x}_i\}_{i=1,\ldots\alpha} \text{ with } \mathbf{x}_i \cdot \mathbf{A}(\mathbf{U}) = 0$$

- on the differential equations, this produces intrinsic relations of the variables for $i = 1, \ldots\alpha$

$$\mathbf{x}_i \cdot \mathbf{P}(\mathbf{U}) = 0$$

- intrinsic relations correspond to bulk solutions and supplement boundary conditions

- $\alpha = 2$ for R13 with linear constitutive equations:

$$\mathbf{x}_1 \cdot \mathbf{P}(\mathbf{U}) = 0 \quad \Rightarrow \quad m_{xyy} = -\frac{16}{15}\mu F$$

$$\mathbf{x}_2 \cdot \mathbf{P}\left(\mathbf{U}\right) = 0 \quad \Rightarrow \quad \hat{R}_{yy} = \frac{6}{5}\sigma \frac{R_{xy} - 6\theta\,\sigma}{p + \sigma_{yy}}$$

Order-Preserving Transformation

- fully non-linear R13 system fails to exhibit zero eigenvalues
- coherence implies: transformation necessary to find bulk solutions
- order preserving transformation: $\left\|\boldsymbol{\sigma}^{(\widetilde{\mathrm{R13}})}-\boldsymbol{\sigma}^{(\mathrm{Boltz})}\right\|+\left\|\mathbf{q}^{(\widetilde{\mathrm{R13}})}-\mathbf{q}^{(\mathrm{Boltz})}\right\| \overset{!}{=} \mathcal{O}\left(Kn^4\right)$
- constitutive relations may be altered within an error $\mathcal{O}\left(Kn^2\right)$

  e.g., by replacing: $\mu\,\partial_y v_x = -\sigma_{xy}^{(\mathrm{NSF})} = -\sigma_{xy} + \mathcal{O}\left(Kn^2\right)$
- algebraisation: $\hat{R}_{yy} = -\frac{36}{5}\,\mu\,\partial_y q_y - \frac{66}{5p}\,q_y \underbrace{\mu\,\partial_y\theta}_{\sim q_y} - \frac{36}{7\rho}\,\sigma_{xy}\underbrace{\mu\,\partial_y v_x}_{\sim \sigma_{xy}} + \ldots$
- final system exhibits nullspaces as before

$$\mathbf{x}_1 \cdot \mathbf{P}\left(\mathbf{U}\right) = 0 \quad \Rightarrow \quad m_{xyy} = \frac{32}{45p}\sigma\, q_y - \frac{16}{15}\mu\, F$$

$$\mathbf{x}_2 \cdot \mathbf{P}\left(\mathbf{U}\right) = 0 \quad \Rightarrow \quad \hat{R}_{yy} = \frac{136}{25p}q_y^2 - \frac{72}{35\rho}\sigma^2$$

Complete Set of Boundary Conditions

- kinetic boundary conditions on both sides of the channel

$$\sigma_{xy} = -\sqrt{\frac{2}{\pi\theta}}\ \beta_1 \left(P\,V_W + \frac{1}{2} m_{xyy} + \frac{1}{5} q_x \right)$$

$$R_{xy} = \sqrt{\frac{2}{\pi\theta}}\ \beta_2 \left(P\,\theta\,V_W - \frac{1}{2}\theta\,m_{xyy} - \frac{11}{5}\theta\,q_x - P\,V_W^3 + 6P(\theta - \theta_W)V_W \right)$$

$$q_y = -\sqrt{\frac{2}{\pi\theta}}\ \beta_3 \left(2P(\theta - \theta_W) + \frac{5}{28}\hat{R}_{yy} + \frac{1}{2}\theta\,\sigma_{yy} - \frac{1}{2}P\,V_W^2 \right)$$

$$m_{yyy} = \sqrt{\frac{2}{\pi\theta}}\ \beta_4 \left(\frac{2}{5}P(\theta - \theta_W) - \frac{1}{14}\hat{R}_{yy} - \frac{7}{5}\theta\,\sigma_{yy} - \frac{3}{5}P\,V_W^2 \right)$$

- specific accommodation coefficients $\{\beta_1, \beta_2, \beta_3, \beta_4\}$ are fitted to be $\{0.9, 0.5, 0.9, 0.5\}$

- bulk solution values supplement conditions on both sides

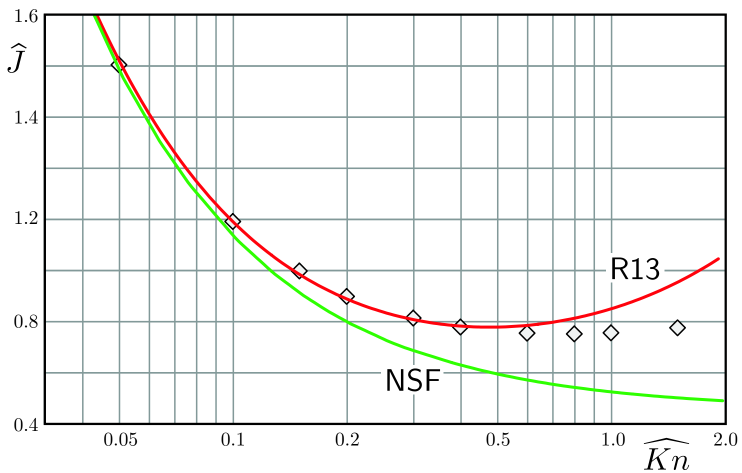
$$m_{xyy} = \frac{32}{45p}\sigma\,q_y - \frac{16}{15}\mu\,F$$

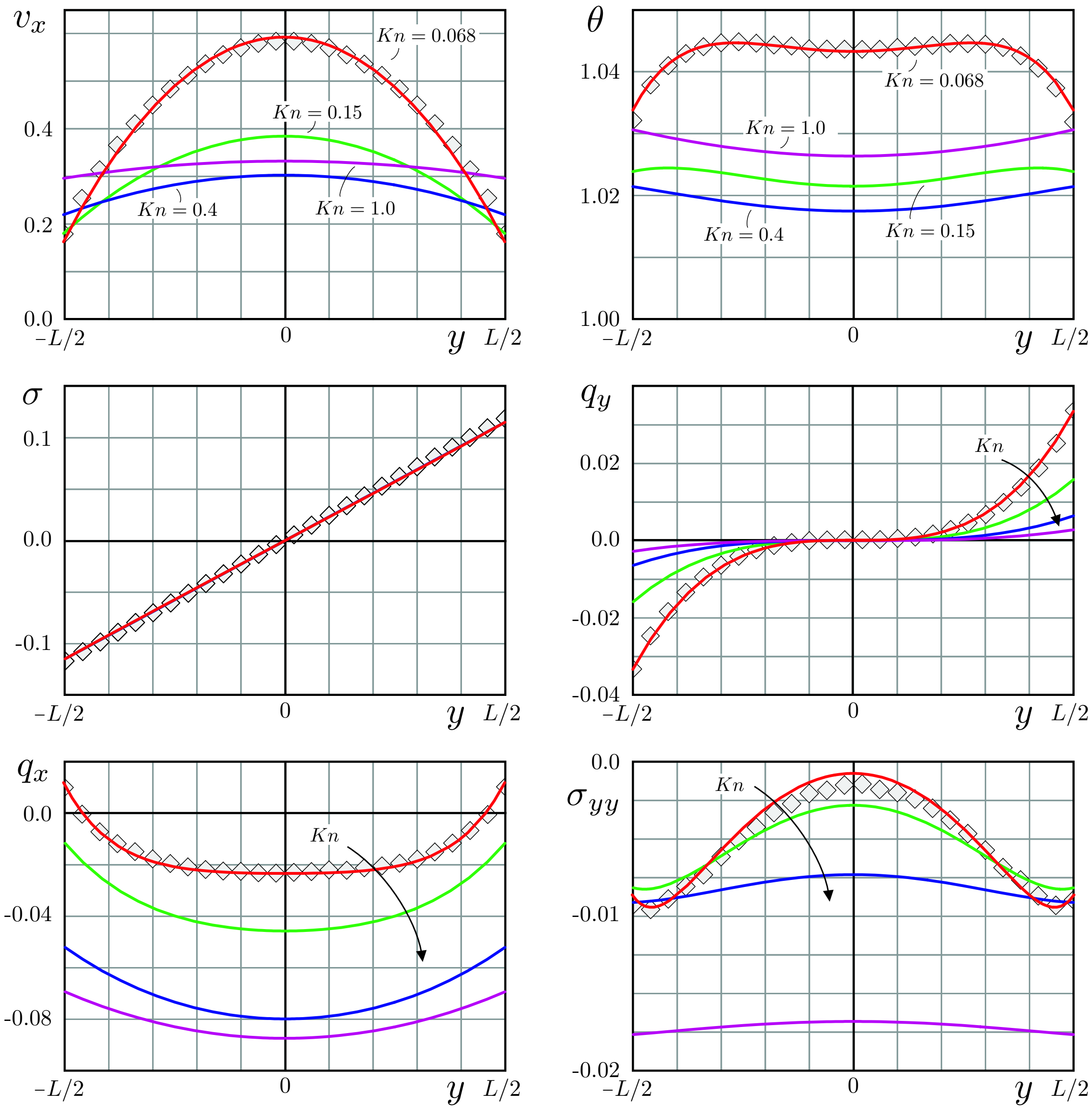
$$\hat{R}_{yy} = \frac{136}{25p}q_y^2 - \frac{72}{35\rho}\sigma^2$$

- larger values of Kn seem to require larger values of accommodation coefficients

Poiseuille Channel Flow

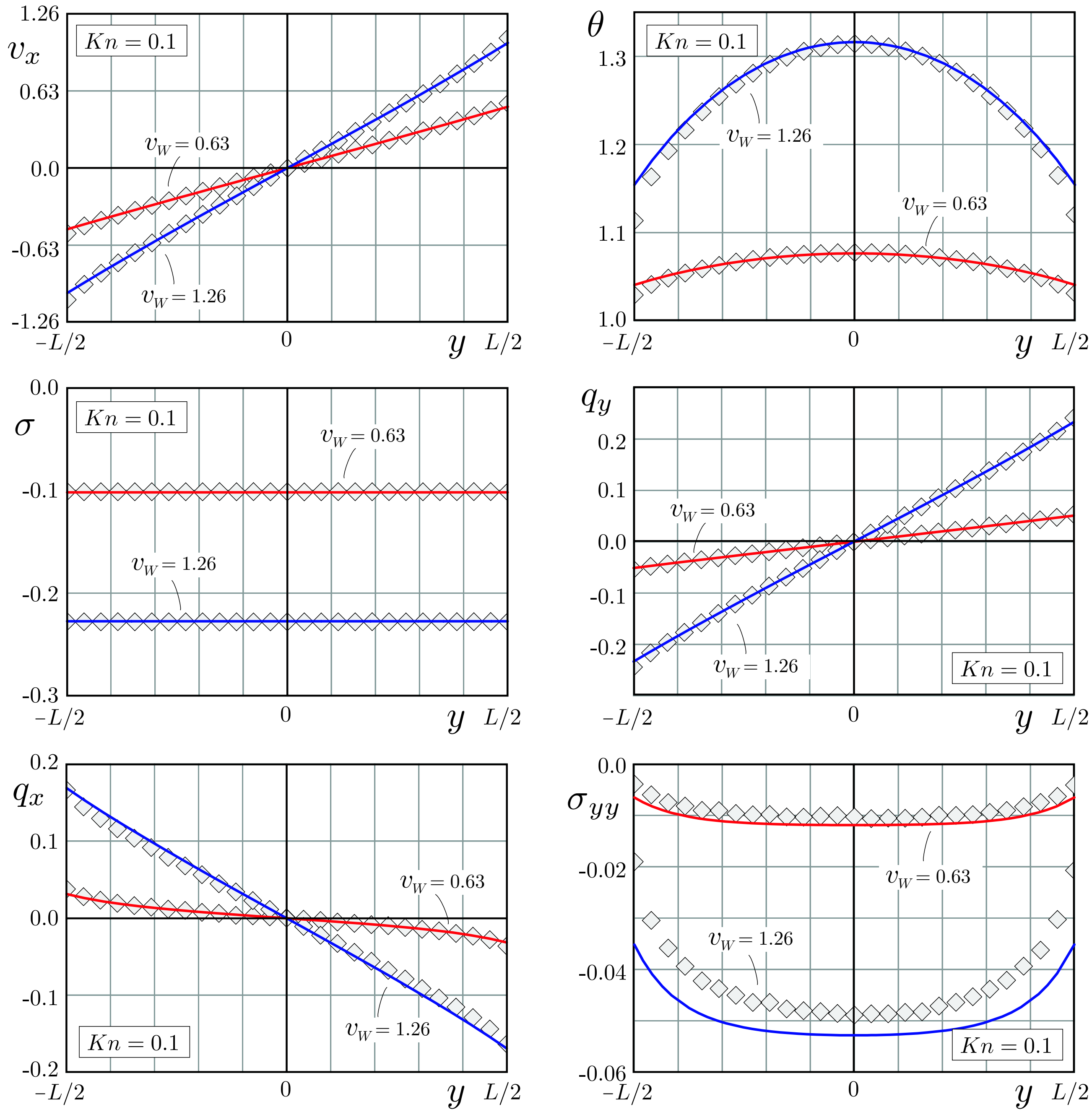
- channel flow with walls at rest and same temperature
- given force $F = 0.23$ corresponds to homogeneous pressure gradient
- the case $Kn = 0.068$ is compared to DSMC results
- R13 produces Knudsen minmum in total mass flux





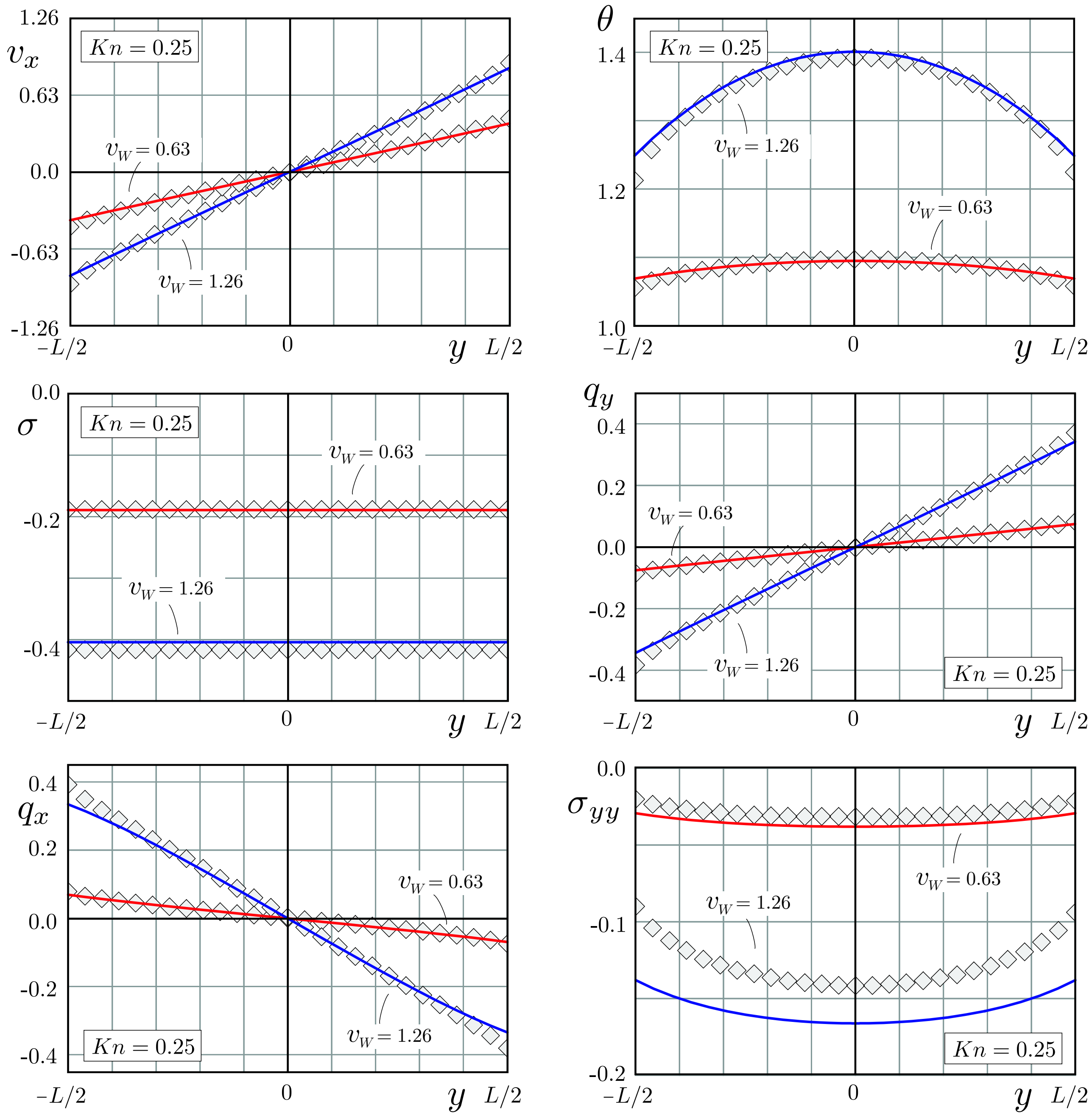
R13 Couette Channel Flow I

- channel flow with walls at opposite velocities and same temperature
- two different cases of velocities $v_W = 1.26$ and $v_W = 0.63$ at different Kn
- here: $Kn = 0.1$



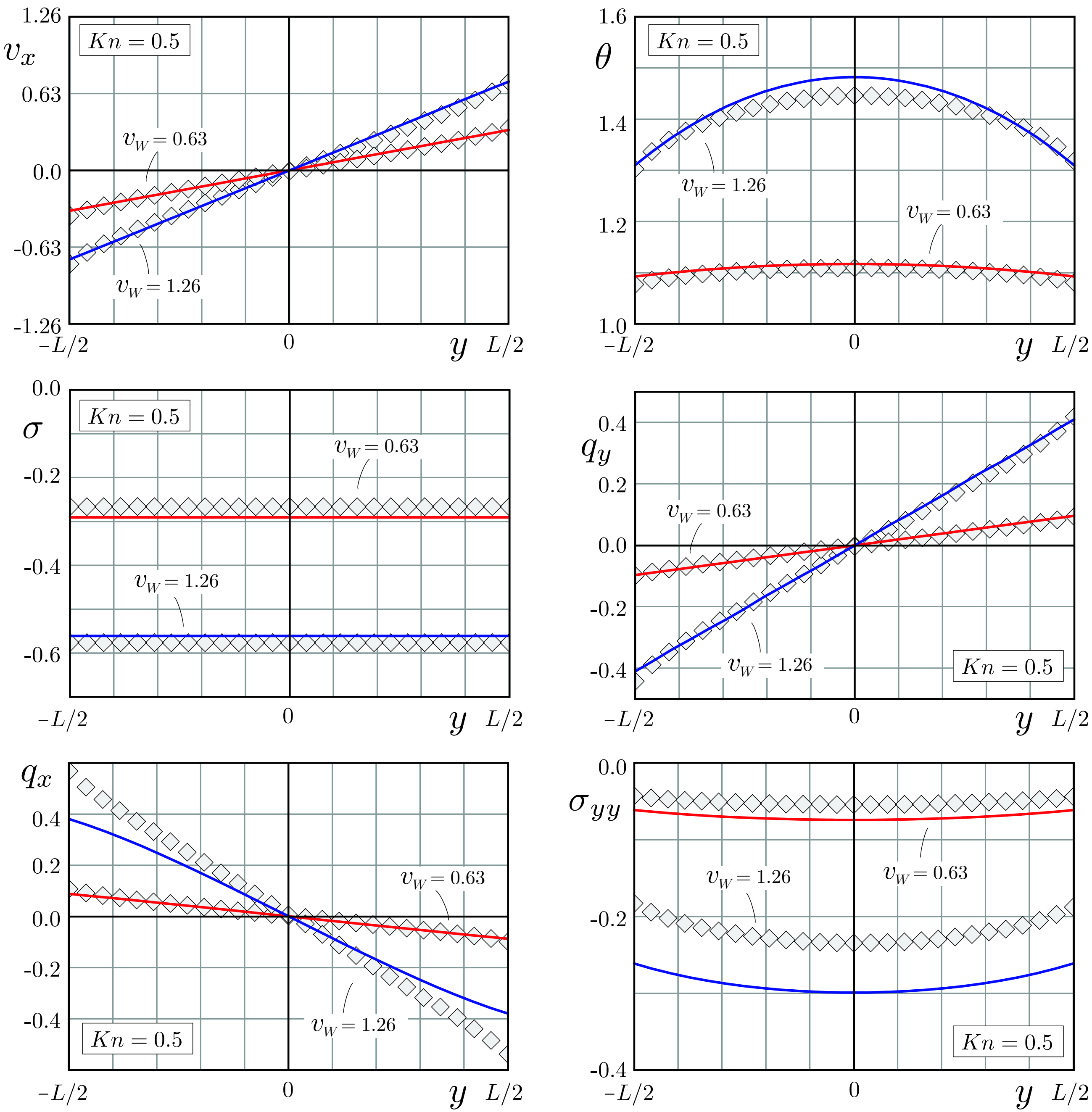
R13 Couette Channel Flow II

- channel flow with walls at opposite velocities and same temperature
- two different cases of velocities $v_W = 1.26$ and $v_W = 0.63$ at different Kn
- here: $Kn = 0.25$



R13 Couette Channel Flow III

- channel flow with walls at opposite velocities and same temperature
- two different cases of velocities $v_W = 1.26$ and $v_W = 0.63$ at different Kn
- here: $Kn = 0.5$



Achievements with R13

- accuracy of super-Burnett order in full non-linear, multidimensional setting (MT & HS 2004)

$$\left\|\boldsymbol{\sigma}^{(\mathrm{R13})}-\boldsymbol{\sigma}^{(\mathrm{Boltz})}\right\|+\left\|\mathbf{q}^{(\mathrm{R13})}-\mathbf{q}^{(\mathrm{Boltz})}\right\|=\mathcal{O}\left(Kn^{4}\right)$$

- linearly stable for all wave numbers and frequencies (HS & MT 2003)
- follows from an order-of-magnitude argument without expansion (HS 2004)
- good agreement with dynamic form factors of light scattering (MT 2006)
- smooth shock wave profiles with improved quantitative agreement (MT & HS 2004)
- allows efficient numerical multi-dimensional simulations (MT 2006)
- comes with entropy law in the linear case (HS & MT 2007)
- channel micro-flow simulations possible (Gu & Emerson 2007)