A Computationally Efficient Framework for Modeling Microscale and Rarefied Gas Flows Based on New Constitutive Relations

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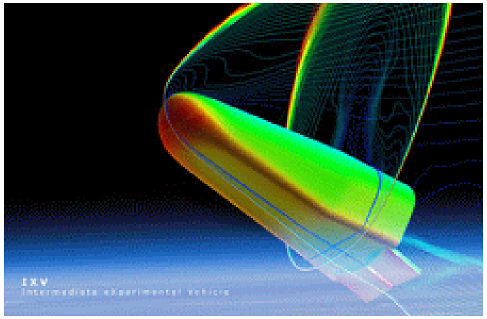
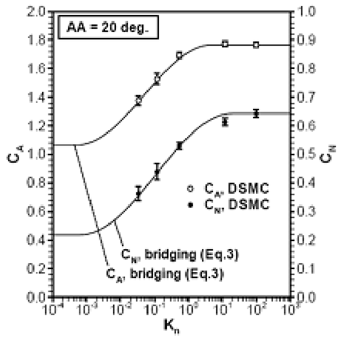
Rarefied and micro/nanoscale gases

Compression-dominated

High *M*, low Kn

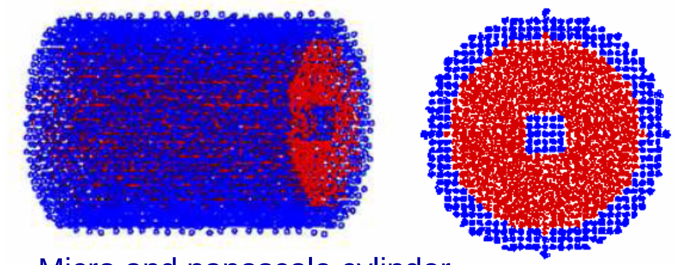
Intermediate Experimental Vehicle





Shear-dominated

Low *M*, high Kn



Micro and nanoscale cylinder

An overview of rarefied and micro/nanoscale gases

- Rarefied (hypersonic) gases

  Gas flow + hypersonic vehicle flying at high altitude

- Micro/nano devices:

  Gas (liquid) flow + MN solid devices

  1) Molecular interaction between gas (liquid) particles and solid atoms

  2) Gas (liquid) flows in thermal nonequilbrium regimes

  3) Electrokinetics, surface tension etc.

  MN solid + MN solid devices => Interface heat transfer etc.

- Micro/nano particles:

  MN particles in gas => Aerosol etc.

  MN particles in liquid => Suspension etc.

  MN gas in liquid => Micro bubble etc.

  Production of MN particles

Modeling micro and nanomechanics of fluids and rarefied gases

Top-down: the classical linear (fluid mechanics) theories can account for virtually everything about materials (fluids).

$$\rho \frac{D}{Dt}\begin{bmatrix} 1/\rho \\ \mathbf{u} \\ E_t \end{bmatrix} + \nabla \cdot \begin{bmatrix} \mathbf{u} \\ p\mathbf{I} + \mathbf{\Pi} \\ \left(p\mathbf{I} + \mathbf{\Pi}\right)\cdot \mathbf{u} + \mathbf{Q} \end{bmatrix} = \mathbf{0}$$

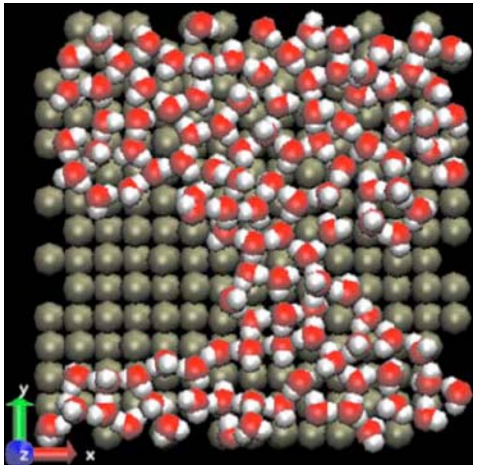
$$\mathbf{\Pi} = -\eta\left[\nabla \mathbf{u}\right]^{(2)}, \quad \mathbf{Q} = -k\nabla T$$

Navier **Fourier**

Linear uncoupled constitutive relations

$$\text{Example.} \quad \dot{m} = \frac{H^3 W p_{out}^2}{24\eta LRT}\left(p_{in}^2 - 1\right)$$

Bottom-up: only a molecular-statistical theory of the structure of fluids can provide understanding of their true behavior.



A critical observation on how to combine two approaches: an efficient way to include the molecular nature of gases is to develop full (nonlinear coupled) constitutive relations but to retain the conservation laws.

Modelling of nonequilibrium gas system (I)

Molecular (Probabilistic)

Thermodynamics (Reduction of Information)

$$\beta = \frac{1}{k_B T}$$

Continuum (Hydrodynamic)

Phase Space

$$f\left(t, \mathbf{r}; \mathbf{v}\right)$$

$$\left(\rho, \mathbf{u}, T, \Pi, \mathbf{Q}, \cdots\right)\left(t, \mathbf{r}\right)$$

Thermodynamic Space

Boltzmann

$$\left(\frac{\partial}{\partial t} + \mathbf{v} \cdot \nabla\right) f\left(t, \mathbf{r}; \mathbf{v}\right) = C\left[f, f_2\right]$$

$$\rho = \left\langle m f\left(t, \mathbf{r}; \mathbf{v}\right)\right\rangle$$

$$\rho \mathbf{u} = \left\langle m \mathbf{v} f\left(t, \mathbf{r}; \mathbf{v}\right)\right\rangle$$

$$\left\langle \cdots \right\rangle = \iiint \cdots dv_x dv_y dv_z$$

$$\rho \frac{D\mathbf{u}}{Dt} + \nabla \cdot \left(p\mathbf{I} + \Pi\right) = 0$$

Conservation Laws

Moment Equation

Not far from LTE

Navier-Stokes-Fourier

Modelling of nonequilibrium gas system (II): The moment method

$$\rho = \langle mf(t,\mathbf{r};\mathbf{v})\rangle, \quad \rho\mathbf{u} = \langle m\mathbf{v}f(t,\mathbf{r};\mathbf{v})\rangle, \quad \left(\frac{\partial}{\partial t} + \mathbf{v}\cdot\nabla + \mathbf{a}\cdot\nabla_v\right) f(t,\mathbf{r};\mathbf{v}) = C[f, f_2]$$

Differentiating the statistical definition $\rho \equiv \langle mf(t,\mathbf{r};\mathbf{v})\rangle$ *with time* and *then combining* with the Boltzmann equation

$$\frac{\partial}{\partial t}\rho = \frac{\partial}{\partial t}\langle mf(t,\mathbf{r};\mathbf{v})\rangle = \left\langle m\frac{\partial f}{\partial t}\right\rangle = \langle mC[f, f_2]\rangle - \langle m\mathbf{v}\cdot\nabla f\rangle$$

$$\frac{\partial \rho}{\partial t} + \langle m\mathbf{v}\cdot\nabla f\rangle = \langle mC[f, f_2]\rangle = 0$$

$$\frac{\partial \rho}{\partial t} + \langle m\nabla\cdot(f\mathbf{v})\rangle - \langle mf\nabla\cdot\mathbf{v}\rangle = \frac{\partial \rho}{\partial t} + \langle m\nabla\cdot(f\mathbf{v})\rangle = 0$$

$$\frac{\partial \rho}{\partial t} + \nabla\cdot\langle mf\mathbf{v}\rangle = 0$$

$$\frac{\partial \rho}{\partial t} + \nabla\cdot(\rho\mathbf{u}) = 0$$

The moment method (I)

$$\rho \frac{D}{Dt}\left(\frac{\langle h^{(k)} f \rangle}{\rho} \right) + \nabla \cdot \langle \mathbf{c} h^{(k)} f \rangle = \left\langle f \left(\frac{D}{Dt} + \mathbf{c} \cdot \nabla + \mathbf{a} \cdot \nabla_{\mathrm{v}} \right) h^{(k)} \right\rangle + \langle h^{(k)} C[f] \rangle$$

$$\rho \frac{D}{Dt} \begin{bmatrix} [1, \rho\mathbf{u}, \rho E_t]^T / \rho \\ \boldsymbol{\Pi} / \rho \\ \mathbf{Q} / \rho \end{bmatrix} + \nabla \cdot \begin{bmatrix} [\mathbf{u}, p\mathbf{I} + \boldsymbol{\Pi}, (p\mathbf{I} + \boldsymbol{\Pi}) \cdot \mathbf{u} + \mathbf{Q}]^T \\ \boldsymbol{\Psi}^{(\Pi)} \\ \boldsymbol{\Psi}^{(Q)} \end{bmatrix} = \begin{bmatrix} [\mathbf{0}, \rho\mathbf{a}, \rho\mathbf{a} \cdot \mathbf{u}]^T \\ \mathbf{Z}^{(\Pi)} + \boldsymbol{\Lambda}^{(\Pi)} \\ \mathbf{Z}^{(Q)} + \boldsymbol{\Lambda}^{(Q)} \end{bmatrix}$$

$$\rho \frac{D}{Dt} \begin{pmatrix} \text{non-conserved} \\ \text{variable} \end{pmatrix} + \nabla \cdot \begin{pmatrix} \text{high-order} \\ \text{variable} \end{pmatrix} = \textbf{kinematic term } \mathbf{Z}$$

$$+ \textbf{ dissipation term (Boltzmann collision) } \boldsymbol{\Lambda}$$

Main parameter $\Pi / p \sim \mathrm{Kn} \cdot M$ **(not Kn alone)**

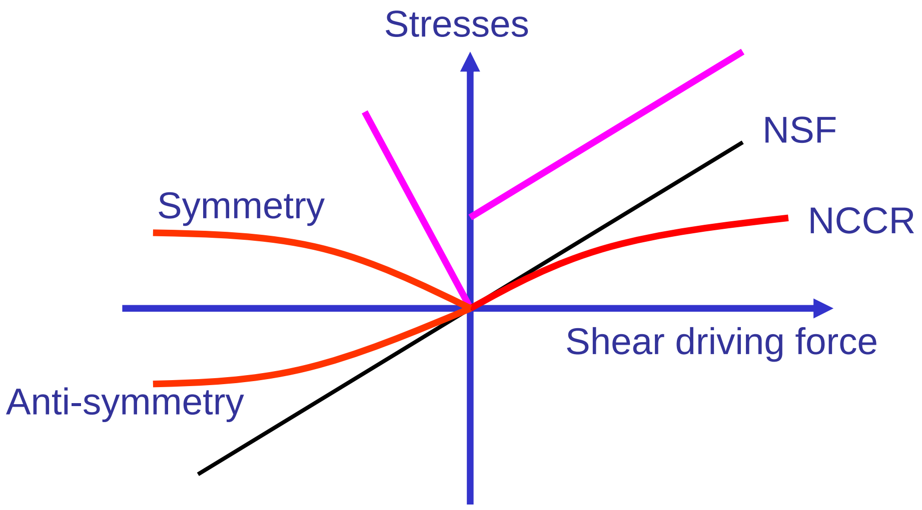
The moment method (II): Closure problem

The mathematician plays a game in which he himself invents the rules, while the physicist plays a game in which **the rules are provided by nature**. [P. Dirac, 1939]

Physically motivated closure

$$\rho \frac{D}{Dt}\begin{bmatrix} \mathbf{\Pi}/\rho \\ \mathbf{Q}/\rho \end{bmatrix} + \nabla \cdot \begin{bmatrix} \mathbf{\Psi}^{(\Pi)} \\ \mathbf{\Psi}^{(Q)} \end{bmatrix} = \begin{bmatrix} 0 \\ 0 \end{bmatrix}$$

$$\text{where} \quad \begin{bmatrix} \mathbf{\Psi}^{(\Pi)} \\ \mathbf{\Psi}^{(Q)} \end{bmatrix} \equiv \begin{bmatrix} \left\langle m[\mathbf{cc}]^{(2)}\,\mathbf{c}f \right\rangle \\ \left\langle \frac{1}{2} m c^2 \mathbf{cc}f \right\rangle \end{bmatrix}$$



⇨ Nonlinear coupled constitutive relations (NCCR),

but algebraic unlike differential in other theories

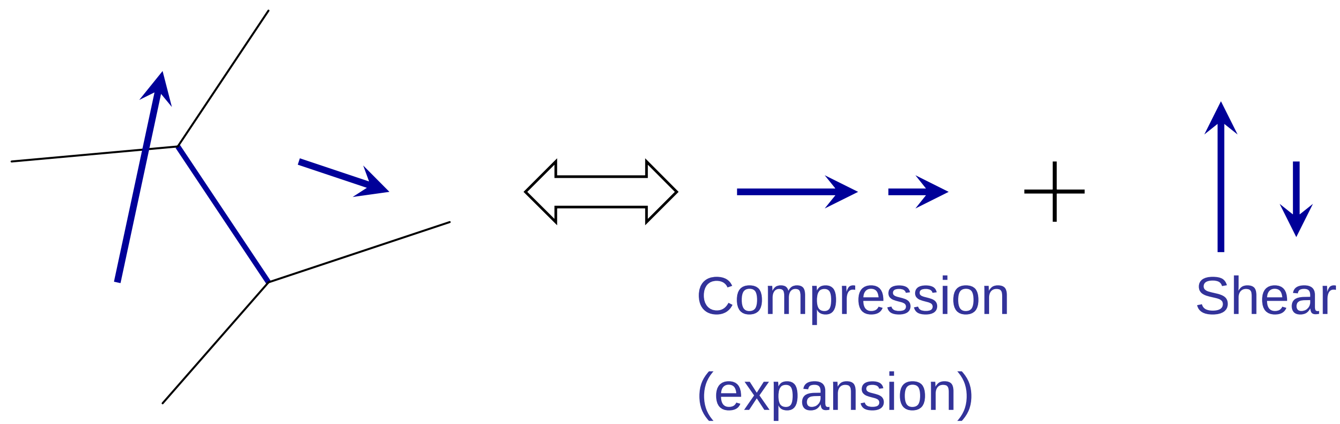
A computational framework based on nonlinear coupled constitutive relations

$$\rho \frac{D}{Dt}\begin{bmatrix} 1/\rho \\ \mathbf{u} \\ E_t \end{bmatrix} + \nabla \cdot \begin{bmatrix} \mathbf{u} \\ p\mathbf{I} + \mathbf{\Pi} \\ \left(p\mathbf{I} + \mathbf{\Pi}\right) \cdot \mathbf{u} + \mathbf{Q} \end{bmatrix} = \mathbf{0}$$

and

$$\mathbf{\Pi} = F_{\Pi}(\mathbf{\Pi}_{\mathrm{NSF}}, \mathbf{Q}_{\mathrm{NSF}}, p, T),\ \mathbf{Q} = F_{Q}(\mathbf{\Pi}_{\mathrm{NSF}}, \mathbf{Q}_{\mathrm{NSF}}, p, T)$$

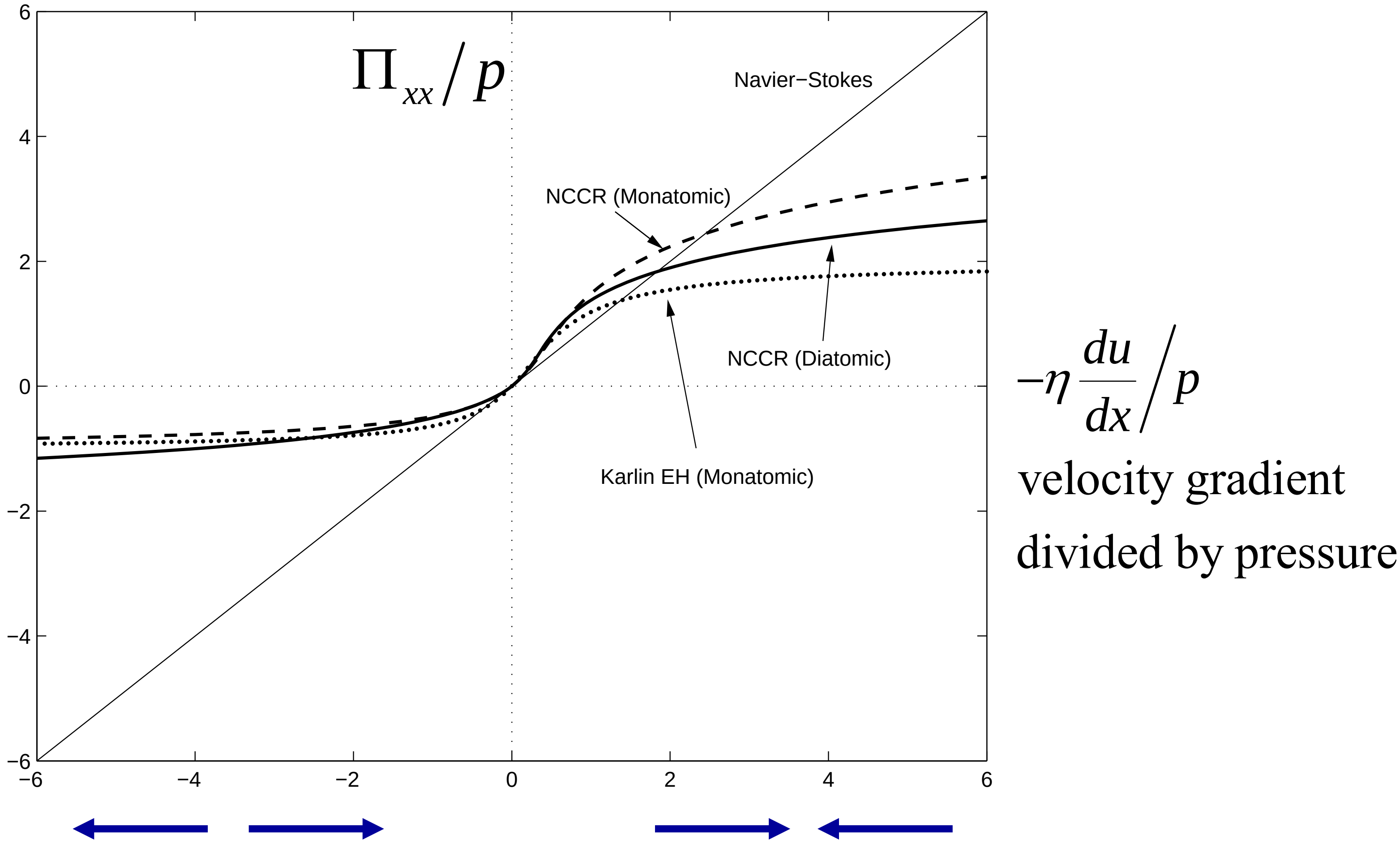
nonlinear coupled constitutive algebraic relations



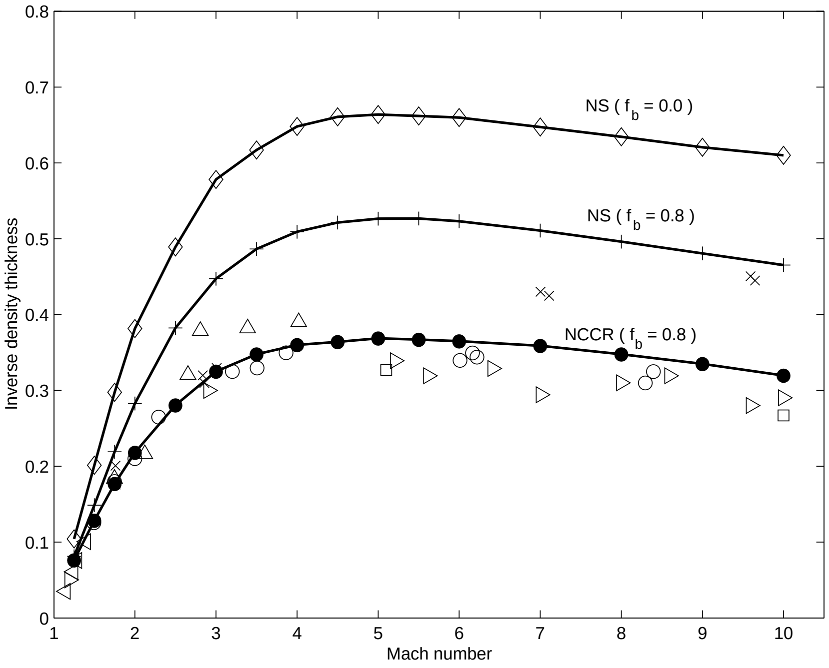
⇨ Computationally efficient at the same level of NS CFD solvers

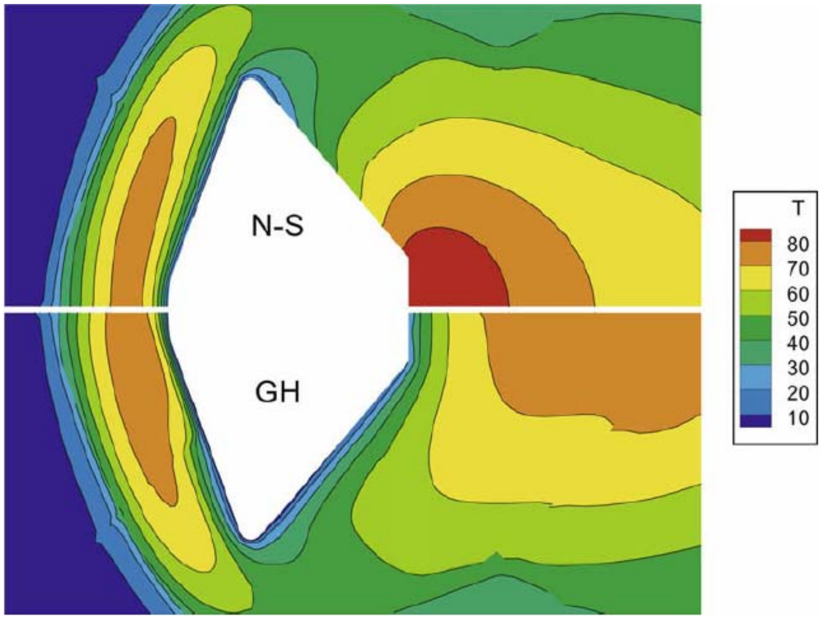
Nonlinear coupled constitutive relations in shock wave (stresses vs strain rate/*p*)

Non-Navier (viscoelastic) behavior!



Validation in compression-dominated flow





*S*hock structure

(Monatomic & diatomic)

(R. S. Myong, JCP 2004)

M=23.47 at altitude 105 km

(5 species)

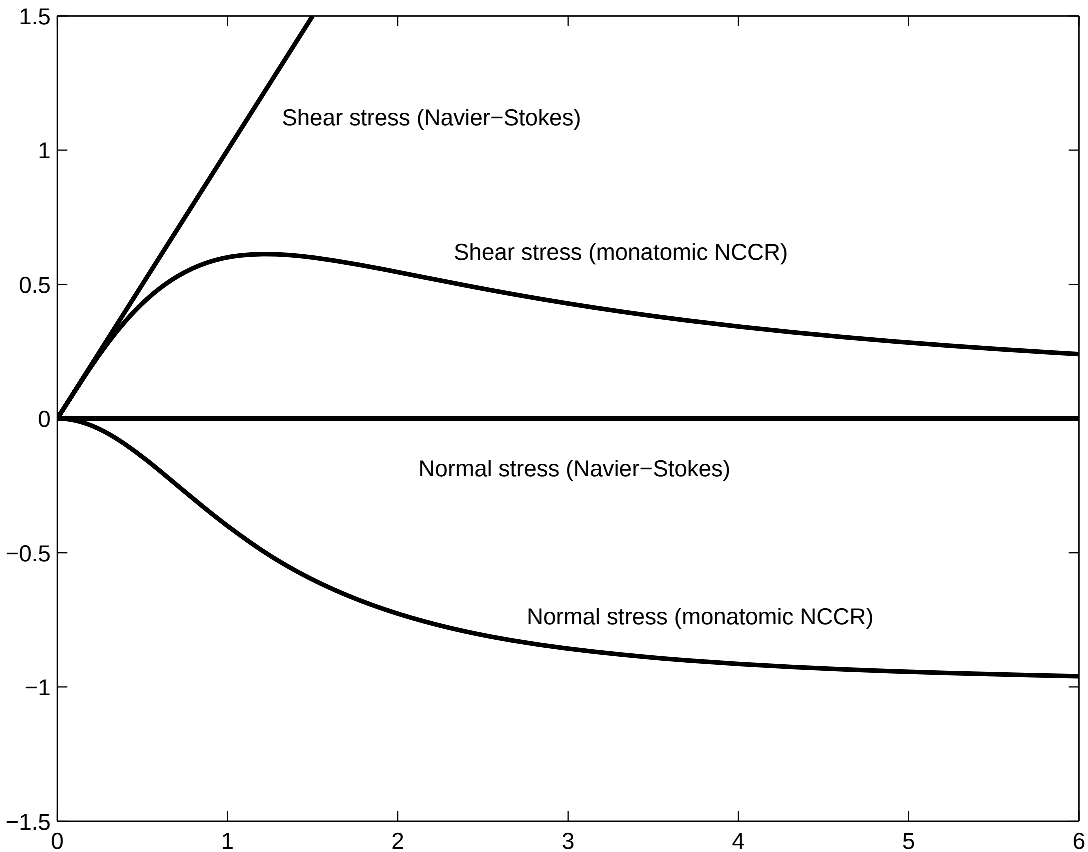
(J. W. Ahn et. al, JCP 2009)

Nonlinear coupled constitutive relations in shear flow (stresses vs strain rate/*p*)

Shear-thinning non-Navier (viscoelastic) behavior! (cross fluid in rheology)

Coupled since normal stress is generated by shear velocity gradient

$\Pi_{xx,\,xy} / p$



$-\eta \dfrac{du}{dy} \Big/ p$

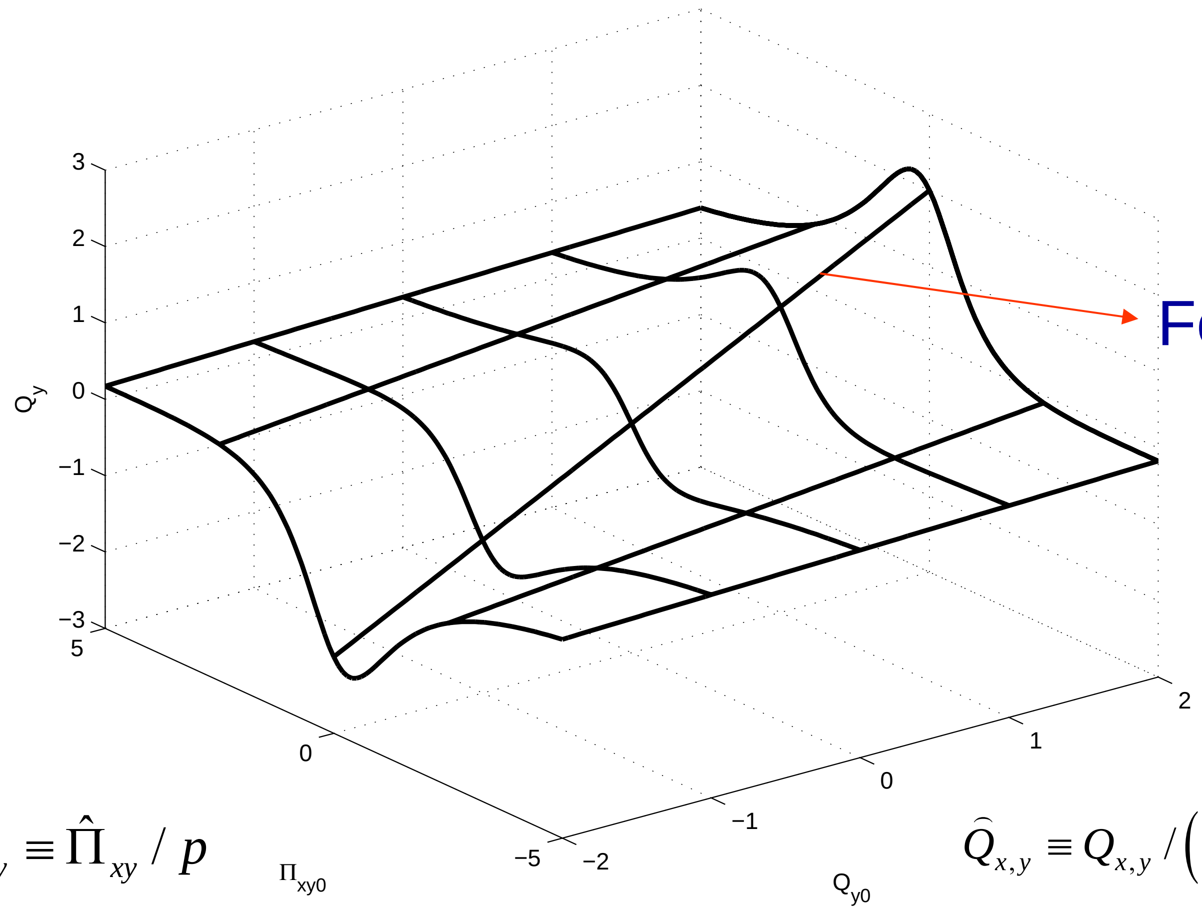
velocity (shear) gradient divided by pressure

Cf. negative axis

Nonlinear coupled constitutive relations in force-driven shear gas flow (heat flux vs temp. gradient)

Non-Fourier behavior!

$$\hat{Q}_y = \frac{3}{\left(3 + 2\hat{\Pi}_{xy_0}^2\right)}\left(\hat{Q}_{y_0} + \hat{a}\hat{\Pi}_{xy_0}\right) \text{ where } a \text{ is force.}$$



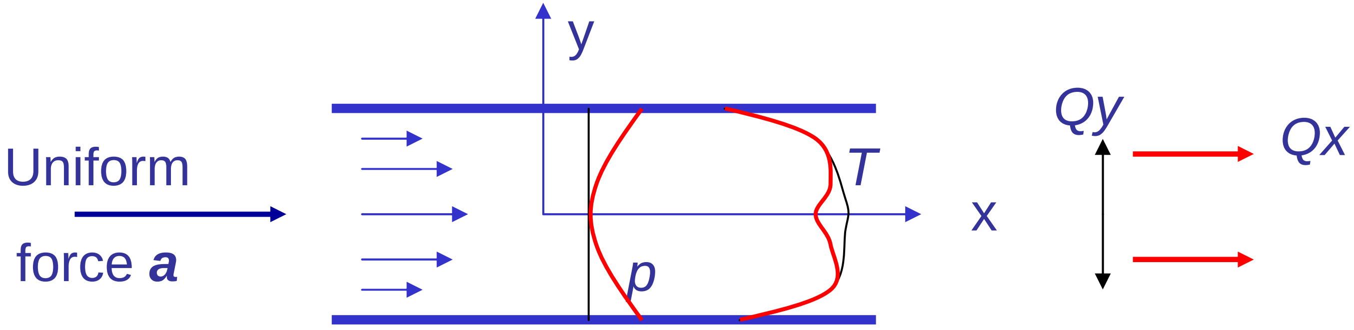
$$\hat{Q}_y = \hat{Q}_{y_0}$$

$$\hat{\Pi}_{xy} \equiv \hat{\Pi}_{xy} / p$$

$$\hat{Q}_{x,y} \equiv Q_{x,y} / \left(p\sqrt{C_p T / (2\,\mathrm{Pr})}\right)$$

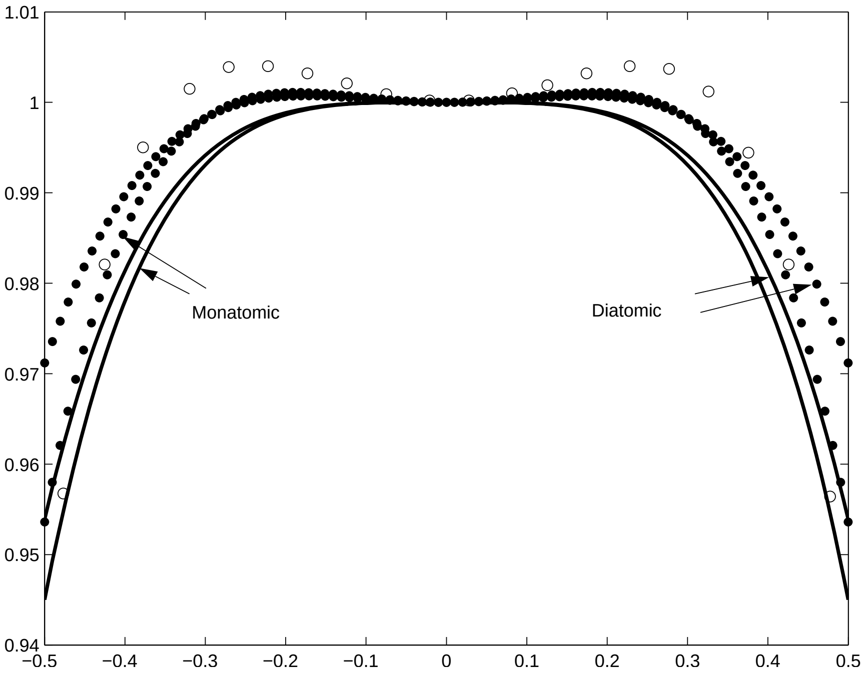
Force (gravity)-driven Poiseuille 1-d gas flow (I)

- Identified as one of three surprising hydrodynamic results discovered by DSMC (1994)
- Global failure of the NSF theory in predicting non-uniform pressure profile and the central minimum in the temperature profile ⇨ Hydrodynamic theories in trouble



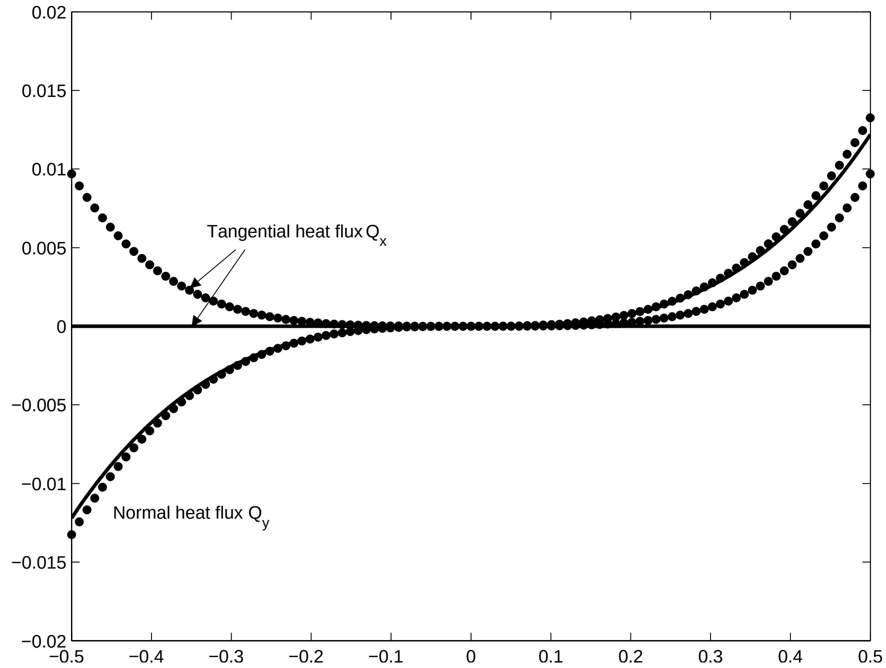
$$\frac{d}{dy}\begin{bmatrix}\Pi_{xy}\\ p+\Pi_{yy}\\ \Pi_{xy}u+Q_y\end{bmatrix}=\begin{bmatrix}\rho a\\ 0\\ \rho au\end{bmatrix},\quad \begin{bmatrix}0\\0\\0\\0\end{bmatrix}=-\begin{bmatrix}(p+\Pi_{yy})\Pi_{xy_0}/\eta\\ -2\Pi_{xy}\Pi_{xy_0}/(3\eta)\\ \Pi_{xy}C_pQ_{y_0}/k+C_pQ_y\Pi_{xy_0}/(\Pr k)+a\Pi_{xx}\\ (p+\Pi_{yy})C_pQ_{y_0}/k+a\Pi_{xy}\end{bmatrix}+\begin{bmatrix}p\Pi_{xy}/\eta\\ p\Pi_{yy}/\eta\\ pC_pQ_x/k\\ pC_pQ_y/k\end{bmatrix}$$

Force-driven Poiseuille flow (II): An analytical solution for constant force (Kn=0.1)



Temperature profile across channel

(○-DSMC, ●-NCCR, —— NSF)

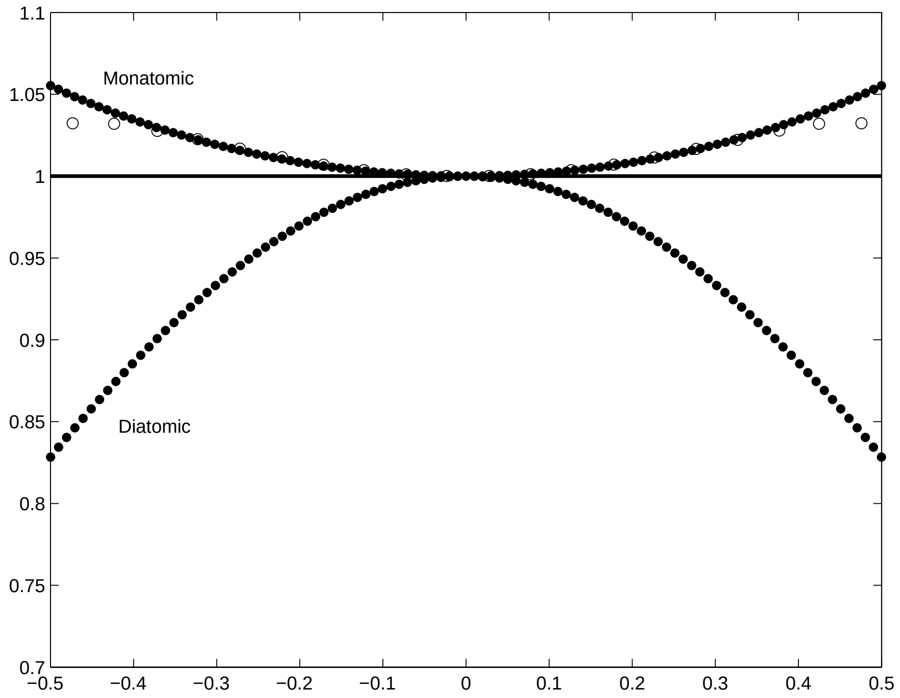


Normal and tangential heat flux profile across channel

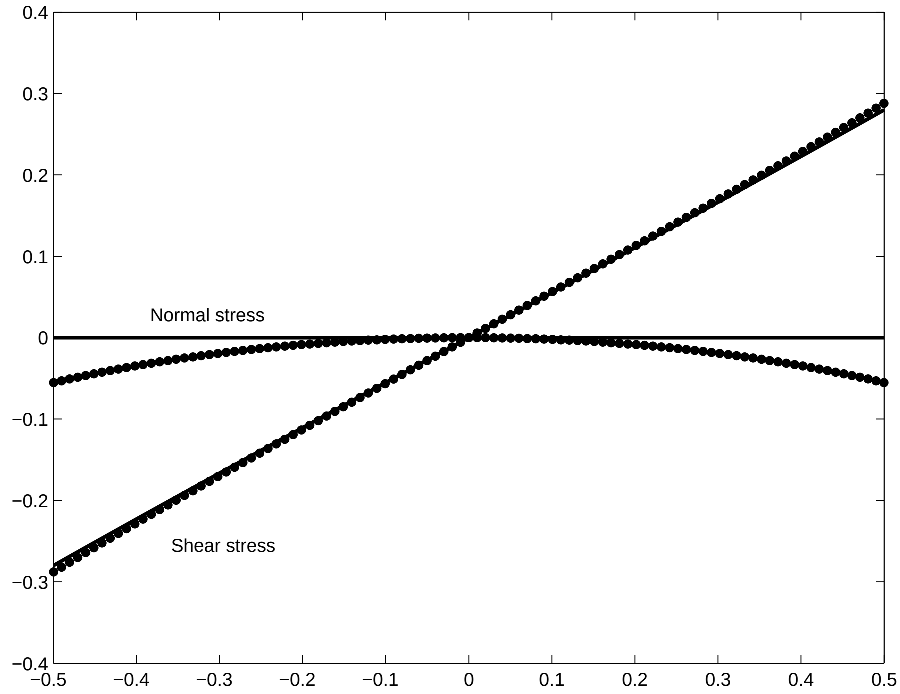
Not only confirming the temperature minimum due to non-Fourier relation,

but also showing a heat transfer from the cold region to the hot region near the centerline

Force-driven Poiseuille flow (III): An analytical solution for constant force (Kn=0.1)



Pressure profile across channel



Stress profile across channel

Not only confirming the non-uniform pressure and the non-zero normal stress due to non-Navier relations,

but also showing its reversal (from concave to convex) in case of diatomic gases

Summary

- New constitutive relations (NCCR):
  - multi-axial, viscoelastic flow in stress/pressure domain (similar to rheology) and in heat flux $\hat{Q}_{x,y} \equiv Q_{x,y} / \left(p\sqrt{C_p T/(2\,\mathrm{Pr})} \right)$
  - mathematically coupled nonlinear (algebraic)
  - computationally efficient

- Solving challenging problems that render the classical hydrodynamic theories (NSF) a global failure.

- Describing how coupled and nonlinear relationship affects the prediction of gas flow and heat transfer in rarefied and micro/nano-system

Acknowledgements

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