The Subtle Interplay of Kinematics and Dissipation Terms in the Constitutive Equations of Rarefied and Microscale Gases

Nov. 7, 2008

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Presented at the Workshop on Moment Methods in Kinetic Gas Theory in ETH Zurich

Theoretical modeling for gas flows in thermal nonequilibrium

- Hydrodynamic theories in thermodynamic space:

  Linear: Navier-Stokes-Fourier (suitable for preliminary calculation; very efficient and powerful; question of applicability)

  High order: Chapman-Enskog method (Burnett etc.), Grad's and Eu's modified moment methods, (rational) extended irreversible thermodynamics, information entropy maximization method, resummation technique (Karlin) etc => Achieving economy of thoughts and description (**constitutive relations** between microscopic and macroscopic physics specific to a substance); computational issues

- Molecular description in phase space: Boltzmann equation, DSMC, MD, etc

  Valid for whole flow regimes; non-trivial issue in computational efficiency

Modelling of nonequilibrium gas system (I)

Molecular (Deterministic)

Equation of Motion

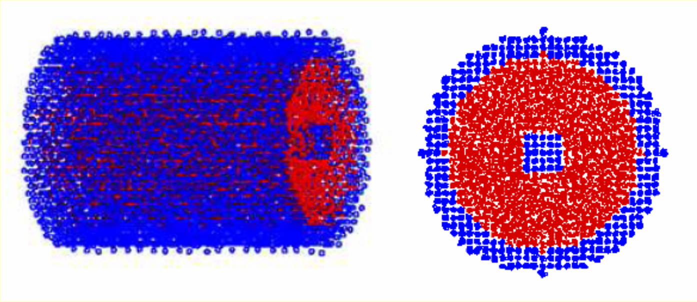
(Molecular Dynamics)

⟺

Molecular (Probabilistic)

Liouville Equation

(Monte Carlo)



⇓ **Molecular Chaos**

Molecular (Probabilistic)

(Generalized) Boltzmann Eq.

(Direct CFD, DSMC)

Modelling of nonequilibrium gas system (II)

Molecular (Probabilistic)

Thermodynamics (Reduction of Information)

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

Continuum (Hydrodynamic)

Phase Space

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

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

Thermodynamic Space

Boltzmann

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

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

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

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

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

Conservation Laws

Moment Equation

Not far from LTE

Navier-Stokes-Fourier

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

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

$$\text{Diatomic}: \left(\frac{\partial}{\partial t} + \mathbf{v}\cdot\nabla + \frac{j}{I}\frac{\partial}{\partial\psi}\right) f(t,\mathbf{r},\mathbf{j},\psi;\mathbf{v}) = R[f, f_2]$$

$$\rho \equiv \langle mf(t,\mathbf{r};\mathbf{v})\rangle$$

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

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

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

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

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

The moment method (I)

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

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

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

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

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

Weissenberg No.= $\dfrac{\tau}{T} = \dfrac{l/a}{L/V} \sim \mathrm{Kn}\cdot M$

No approximations (no explicit $C[f, f_2]$ **except for the dissipation term)**

The moment method (II)

By differentiating $\mathbf{\Pi} = \left\langle m[\mathbf{cc}]^{(2)} f(t,\mathbf{r};\mathbf{v}) \right\rangle$ with time and combining with the BTE

$$\rho \frac{D}{Dt}\left(\frac{\mathbf{\Pi}}{\rho}\right) + \nabla \cdot \boldsymbol{\psi}^{(\Pi)} = \mathbf{Z}^{(\Pi)} + \mathbf{\Lambda}^{(\Pi)}$$

$$\rho \frac{D}{Dt}\left(\frac{\mathbf{\Pi}}{\rho}\right) + \nabla \cdot \left\langle m\mathbf{c}[\mathbf{cc}]^{(2)} f \right\rangle = \left\langle f\left(\frac{D}{Dt} + \mathbf{c}\cdot\nabla\right) m[\mathbf{cc}]^{(2)} \right\rangle + \left\langle m[\mathbf{cc}]^{(2)} C[f] \right\rangle$$

$$\text{Material derivative} + \text{high-order flux} = -2[\mathbf{\Pi}\cdot\nabla\mathbf{u}]^{(2)} - 2p[\nabla\mathbf{u}]^{(2)} - \frac{\mathbf{\Pi}}{\eta/p}\boxed{fn(p,T,\mathbf{\Pi},\mathbf{Q},\cdots)}$$

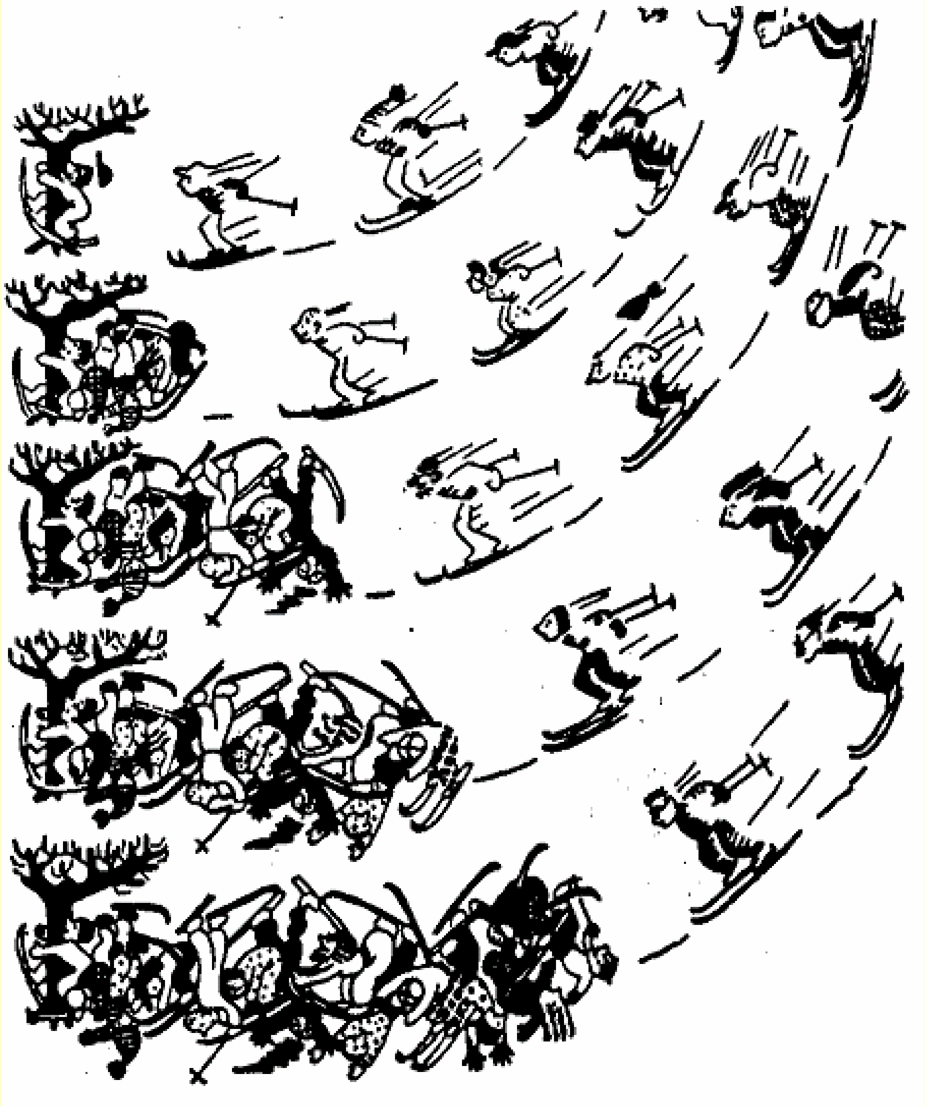
Juggleling of four terms is difficult. By assuming the left-hand term small, we have

$$\frac{\mathbf{\Pi}}{\eta/p} fn(p,T,\mathbf{\Pi},\mathbf{Q},\cdots) = -2[\mathbf{\Pi}\cdot\nabla\mathbf{u}]^{(2)} - 2p[\nabla\mathbf{u}]^{(2)}$$: **Nonlinear algebraic equations**

Constitutive equations for multi-axial (9-dimensional) states of stress and heat flux

Challenging problems in which the NSF theory shows a global failure : Shock structure and force-driven Poiseuille flows

Shock wave structure



The modified moment method: Shock structure

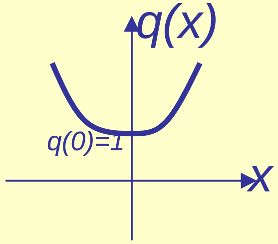
$$\frac{\mathbf{\Pi}}{\eta / p} q(\kappa) = -2\left[\mathbf{\Pi} \cdot \nabla \mathbf{u}\right]^{(2)} - 2p\left[\nabla \mathbf{u}\right]^{(2)}$$

There exists a mathematical singularity when

$$q(\kappa) = 1$$

A remedy by B. C. Eu (1980) assumes

$$q(\kappa) \equiv \frac{\sinh \kappa}{\kappa} \quad \text{where} \; \kappa = \frac{(mk_B T)^{1/4}}{\sqrt{2}pd}\left(\frac{\mathbf{\Pi} : \mathbf{\Pi}}{2\eta} + \frac{\mathbf{Q} \cdot \mathbf{Q}}{\lambda}\right)^{1/2}$$



f in an exponential form; cumulant expansion for $C[f, f_2]$

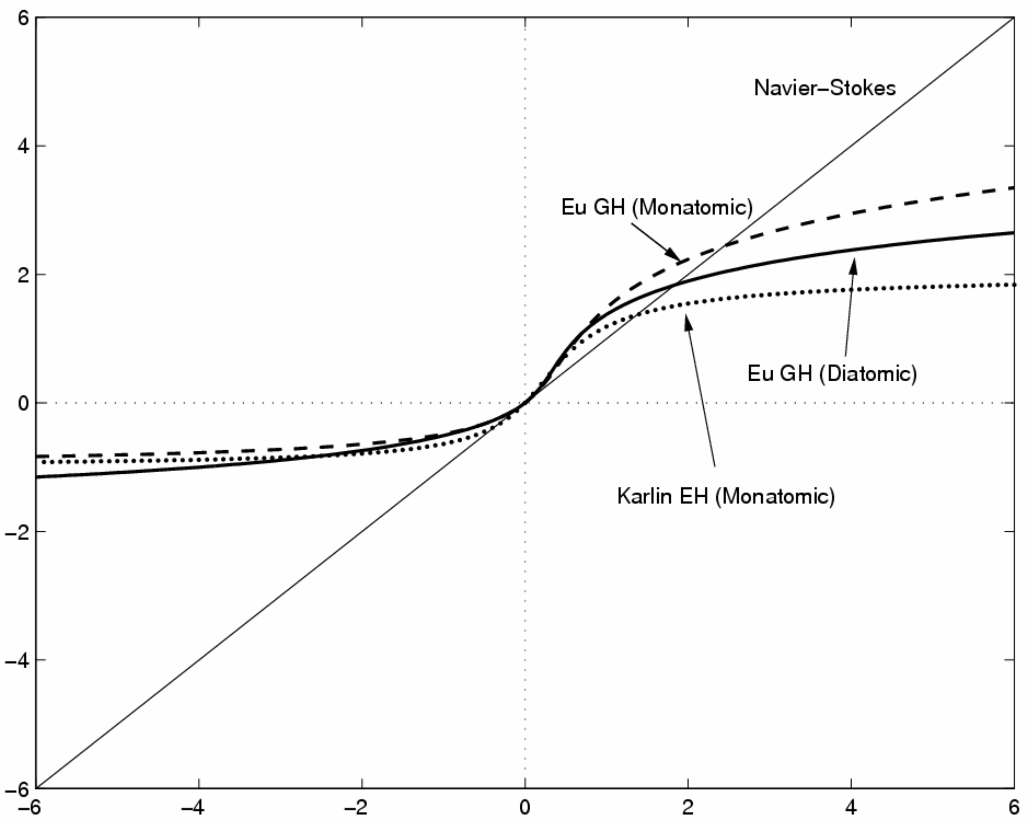
and can remove the mathematical singularity.

This may indicate that the dissipation term $q(\kappa)$ **plays a critical role in the shock structure problem.**

Cf. $q(\kappa) = 1 + \frac{1}{6}\kappa^2 + O(\kappa^4)$

Constitutive relations for shock structure

Stress



Thermodynamic Force $\hat{\Pi}_{xx_0}$

New implicit model

$$\hat{\Pi}_{xx} q(\hat{\Pi}_{xx}) = \hat{\Pi}_{xx_0} + \hat{\Pi}_{xx} \hat{\Pi}_{xx_0}$$

Dissipation = Therm. Force + Kinematics

Nonlinearity **Asymmetry**

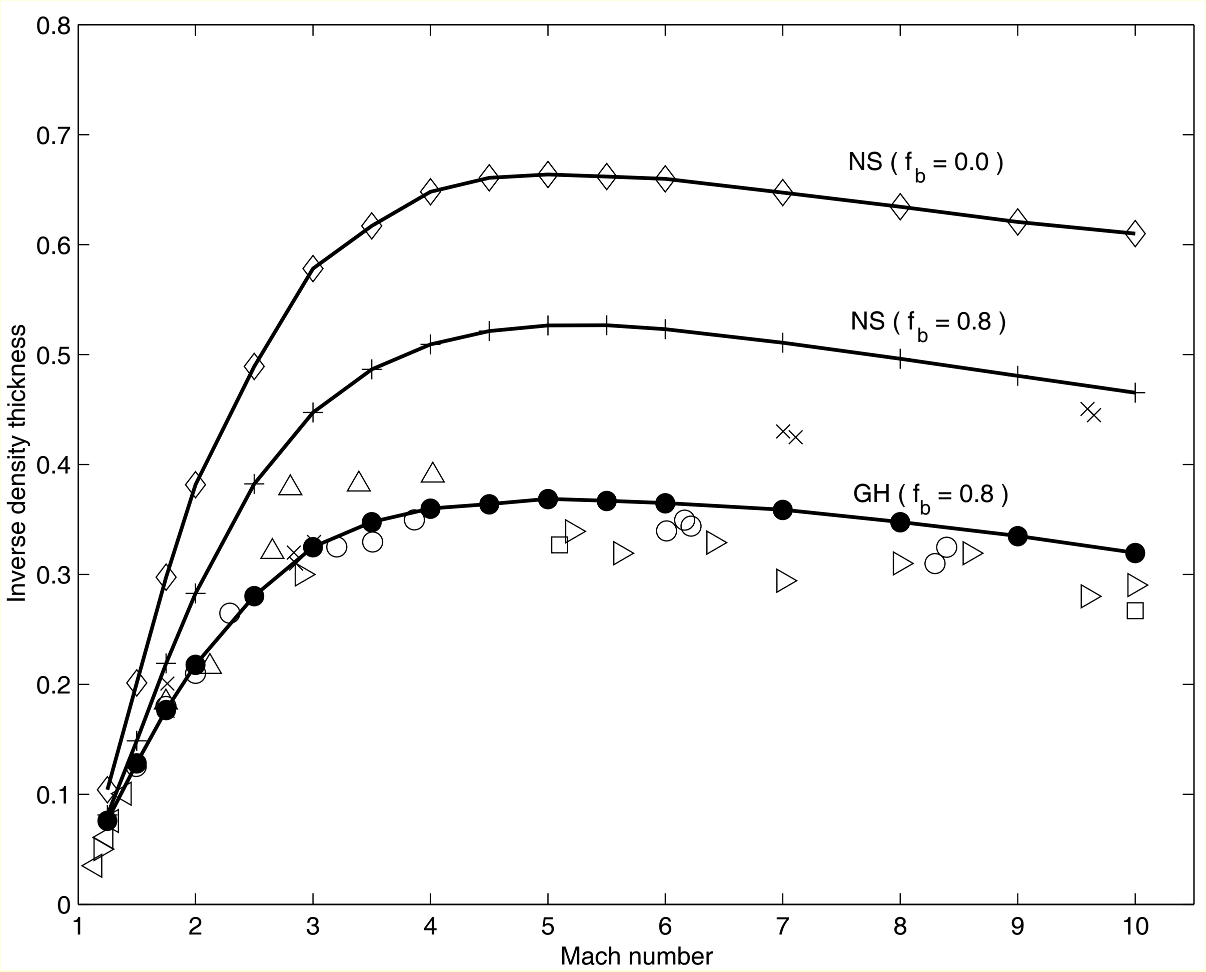
Cf. Navier-Stokes' model

$$\hat{\Pi}_{xx} = \hat{\Pi}_{xx_0} = -2\eta [\nabla \mathbf{u}]^{(2)}$$

Cf. Karlin's explicit model (1997) based on the resummation technique

$$\hat{\Pi}_{xx} = \frac{-3 + 2\hat{\Pi}_{xx_0} + 3\sqrt{1 - 4\hat{\Pi}_{xx_0} / 3 + 4\hat{\Pi}^2_{xx_0}}}{4\hat{\Pi}_{xx_0}}$$

An example of shock structure solution: Monatomic and diatomic gases



Myong (JCP 2004) by a model constitutive equation

Constitutive relations in one-dimensional shear flow (I)

$$0 = -2\left[\mathbf{\Pi}\cdot\nabla\mathbf{u}\right]^{(2)} - 2p\left[\nabla\mathbf{u}\right]^{(2)} - \frac{\mathbf{\Pi}}{\eta/p}q(\kappa)$$

In dimensionless form

$$0 = \left[\hat{\mathbf{\Pi}}\cdot\nabla\hat{\mathbf{u}}\right]^{(2)} + \hat{\mathbf{\Pi}}_0 - \hat{\mathbf{\Pi}}q(\hat{R}) \quad \text{where } \hat{R}^2 \equiv \hat{\mathbf{\Pi}}:\hat{\mathbf{\Pi}} + \hat{\mathbf{Q}}\cdot\hat{\mathbf{Q}}$$

Cf. $0 = \hat{\mathbf{\Pi}}_0 - \hat{\mathbf{\Pi}}q(\hat{\mathbf{\Pi}}) \Rightarrow \hat{\mathbf{\Pi}} = \sinh^{-1}\hat{\mathbf{\Pi}}_0$: Eyring-Ree emprical formula in rheology

When only shear velocity dv/dx exists,

$$\hat{\Pi}_{xx}q(\hat{R}) = -\frac{2}{3}\hat{\Pi}_{xy}\hat{\Pi}_{xy_0}$$

$$\hat{\Pi}_{xy}q(\hat{R}) = (1+\hat{\Pi}_{xx})\hat{\Pi}_{xy_0} \quad \text{where } \hat{R}^2 = 3\hat{\Pi}_{xx}(\hat{\Pi}_{xx}-1)$$

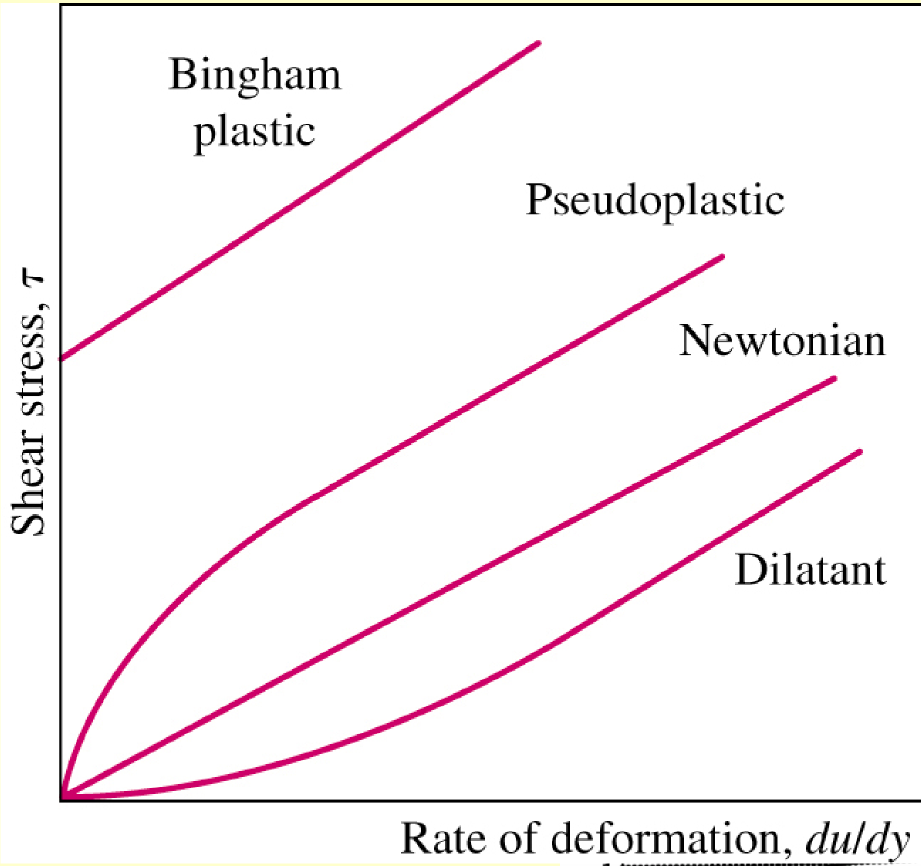
I) Symmetric, but **nonlinear and coupled ($\hat{\mathbf{\Pi}}_{\mathbf{xx}}$ induced by $\hat{\mathbf{\Pi}}_{\mathbf{xy}_0}$)**

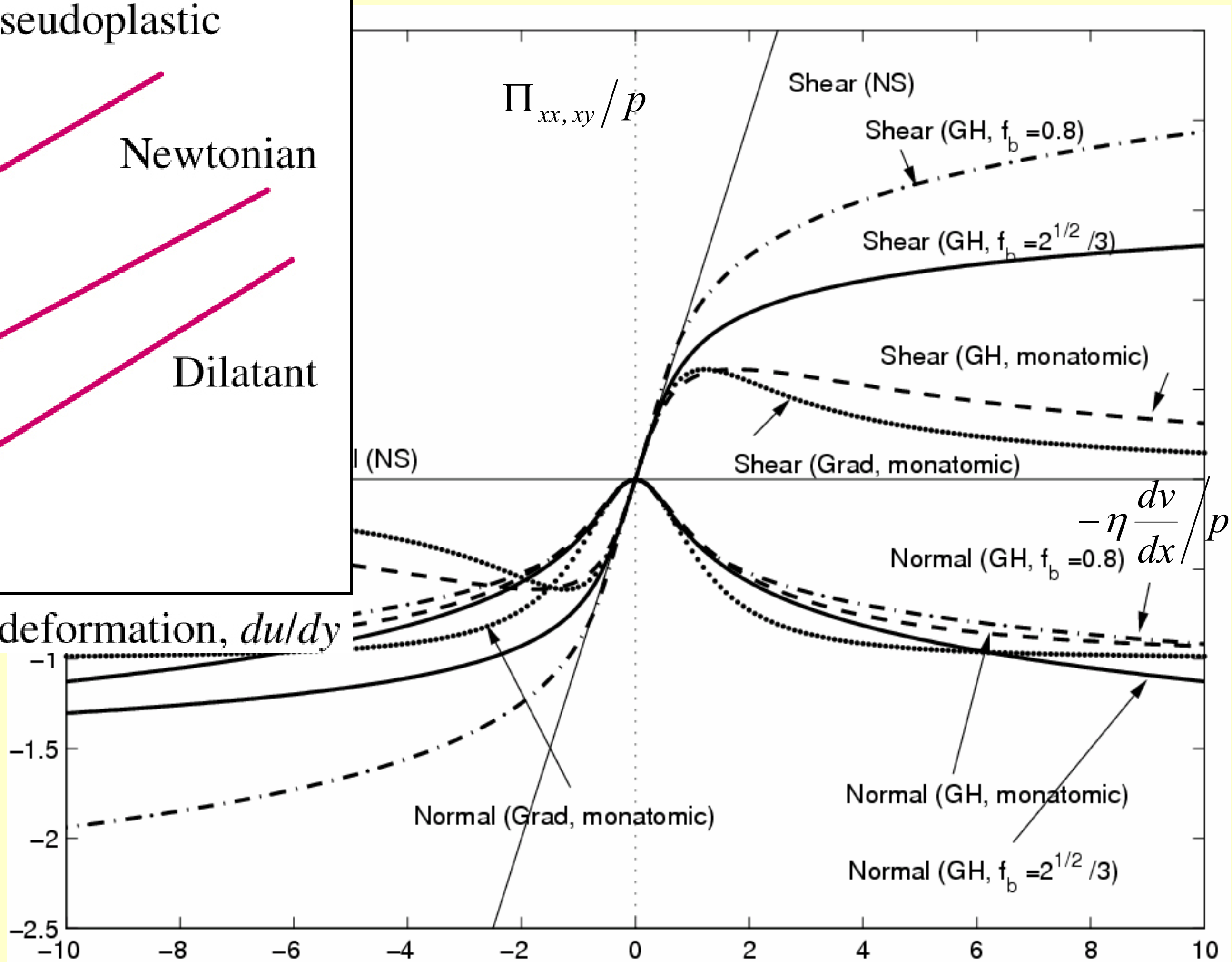
II) Yielding **a stress constraint** $\hat{\Pi}^2_{xy} = -1.5(1+\hat{\Pi}_{xx})\hat{\Pi}_{xx}$

Constitutive relations in one-dimensional shear flow (II)

Shear-thinning (viscoelastic) behavior!

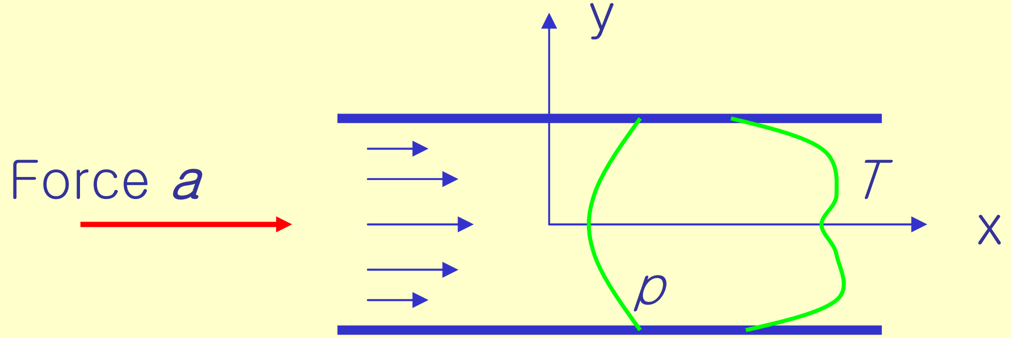
(Cross fluid in rheology)





Force-driven Poiseuille 1-d gas flow: An analytical solution (I)

- Identified as one of three surprising hydrodynamic results discovered by DSMC (A.L. Garcia, 1997)
- Global failure of the NSF theory in predicting *non-uniform pressure profile and the central minimum in the temperature profile* -> Hydrodynamic theories in trouble
- Further studied numerically by K. Xu (2003; Super-Burnett) and Torrilhon & Struchtrup (2008; Regularized 13-moment equations)



Force-driven Poiseuille 1-d gas flow: An analytical solution (II)

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

By applying pure 1-d assumption, a closure relation, and q(k)=1

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

$$\frac{d}{dy}\begin{bmatrix}p\mathbf{I}+\mathbf{\Pi}\\ \left(p\mathbf{I}+\mathbf{\Pi}\right)\cdot\mathbf{u}+\mathbf{Q}\\ \mathbf{0}\\ \mathbf{0}\end{bmatrix}=\begin{bmatrix}\rho\mathbf{a}\\ \mathbf{0}\\ \mathbf{Z}^{(\Pi)}-\dfrac{\mathbf{\Pi}}{\eta/p}\\ \mathbf{Z}^{(Q)}-\dfrac{\mathbf{Q}}{k/C_p p}\end{bmatrix}$$

Force-driven Poiseuille 1-d gas flow: An analytical solution (III)

The analytical solutions are

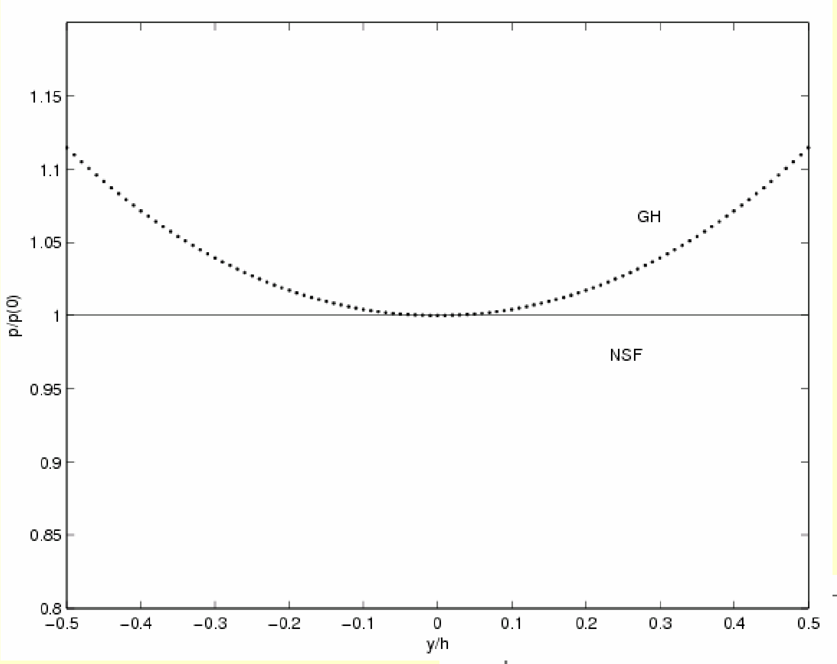
$$\frac{p(y)}{p_{y=0}} = 1 + \tan^2\left(\sqrt{\tfrac{2}{3}}\varepsilon_h \frac{y}{h}\right), \quad \frac{\Pi_{xy}(y)}{p_{y=0}} = \sqrt{\tfrac{3}{2}}\tan\left(\sqrt{\tfrac{2}{3}}\varepsilon_h \frac{y}{h}\right)$$

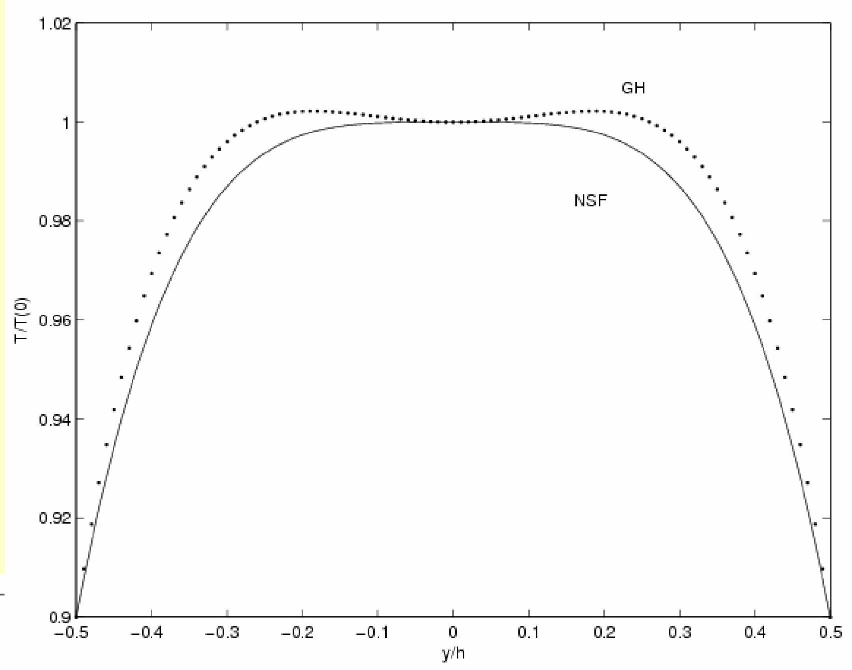
$$\frac{T(y)}{T_{y=0}} = \sec^c\left(\sqrt{\tfrac{2}{3}}\varepsilon_h \frac{y}{h}\right)\left\{1 - \left[1 - \frac{T_w}{T_{y=0}}\sec^{-c}\left(\sqrt{\tfrac{2}{3}}\varepsilon_h \frac{0.5}{h}\right)\right]\frac{F\left(\sqrt{\tfrac{2}{3}}\varepsilon_h \frac{y}{h}\right)}{F\left(\sqrt{\tfrac{2}{3}}\varepsilon_h \frac{0.5}{h}\right)}\right\}$$

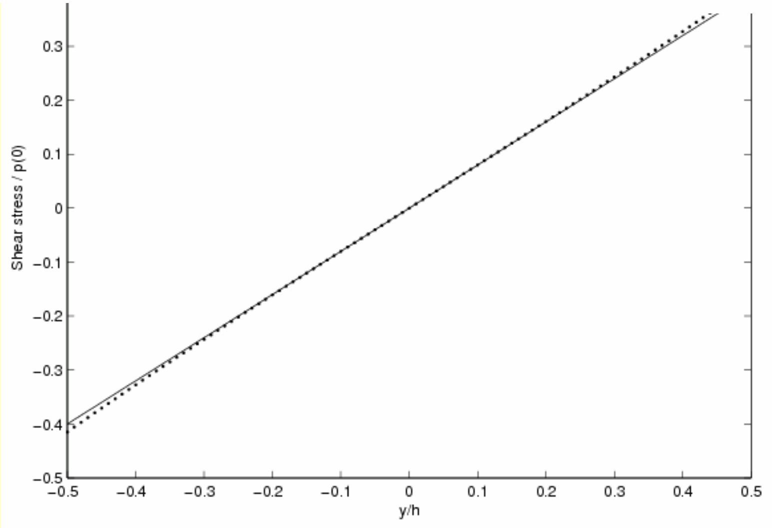
where $c = \dfrac{3(\gamma - 1)}{2\gamma}$, $F(y) \equiv \dfrac{\sin^2(y)}{\cos^{4-c}(y)} + \dfrac{2}{2-c}\left(1 - \dfrac{1}{\cos^{2-c}(y)}\right)$

and $\varepsilon_h \equiv \dfrac{ah}{RT_w}$ (**Rayleigh no.** in case of gravitational force).

Force-driven Poiseuille 1-d gas flow: An analytical solution (IV)







$$\varepsilon_h = 0.8$$

$$T_w = 0.9 T_{y=0}$$

Summary

- Constitutive equations: Multi-axial, viscoelastic flow in stress/pressure domain (rheology)
- Subtle interplay of terms in the constitutive equations

  1) Nonlinearity (dissipation) and asymmetry (kinematics) in 1-d compression and expansion flow

  2) Stress coupling and constraint (kinematics) in 1-d shear flow; minor role of the dissipative term
- Solved the force-driven Poiseuille flow by a hydrodynamic model

Acknowledgements

- Supported by Korea Research Foundation

A missing component in the moment method

Molecular (Probabilistic)

Thermodynamics (Reduction of Information)

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

Continuum (Hydrodynamic)

Phase Space

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

?

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

Thermodynamic Space

Boltzmann

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

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

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

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

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

Conservation Laws Moment Equation

Not far from LTE

Navier-Stokes-Fourier