

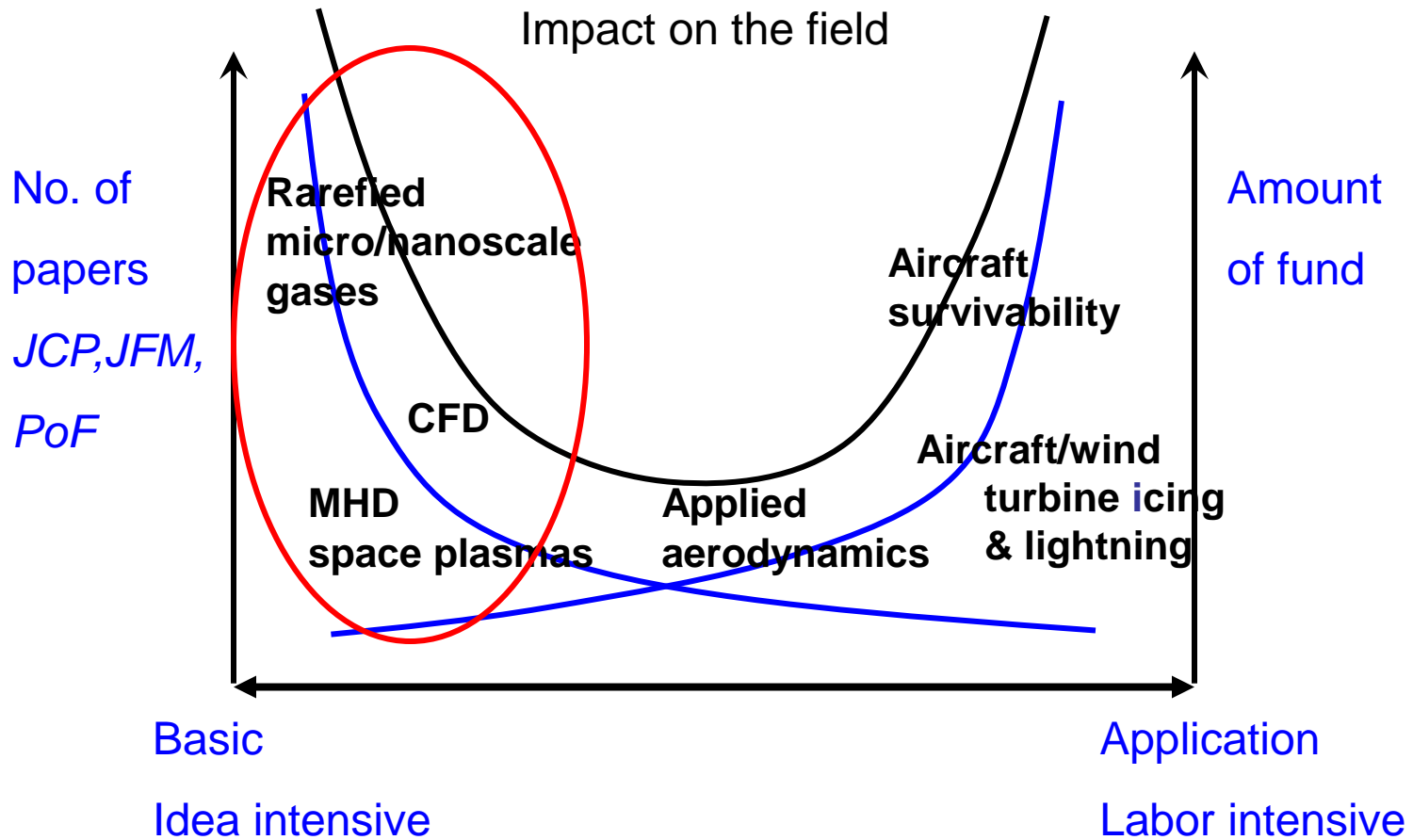
**Contributions to Fundamentals of
MHD and Gases
in Thermal Nonequilibrium**

via

**Mathematical Equations
and
Figures**

December 20, 2013

Basic Research

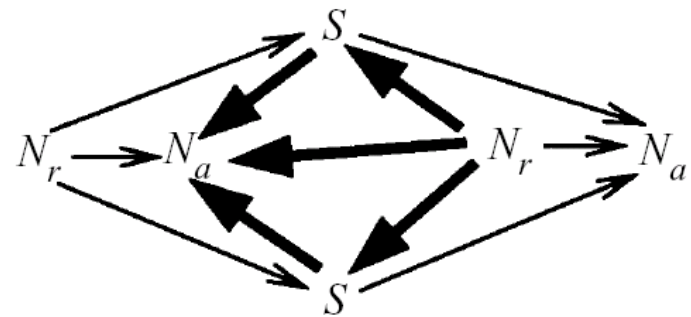
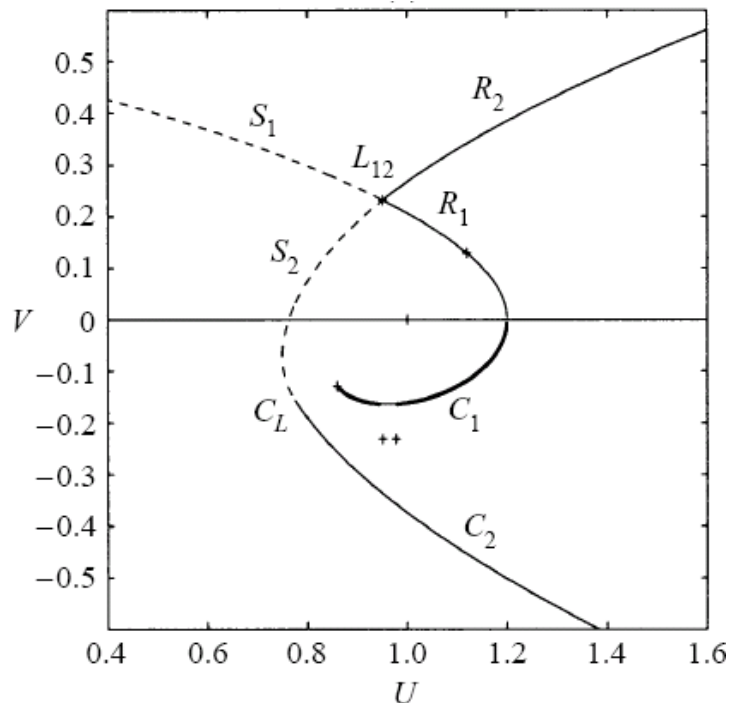


MHD: Shocks and Riemann Problem I

Planar Riemann problem is well-posed when intermediate shocks are included.

$$([U] + \gamma \bar{V}[V]) \left\{ \gamma(\gamma - 1)[V]^3 + 4\gamma \bar{U}[V] - 4\bar{V}[U] \right\} - 4\gamma[U][V] = 0$$

$U \equiv \gamma p / B_x^2$, $V \equiv B_y / B_x$: MHD Rankine-Hugoniot

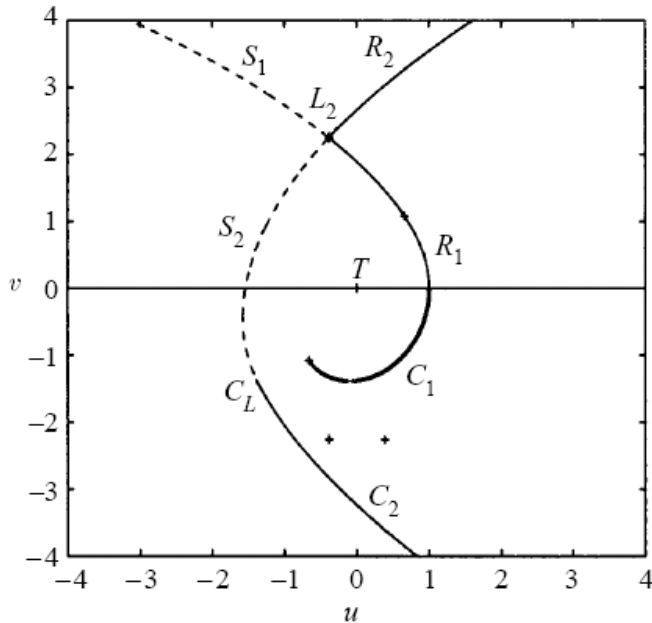


MHD: Shocks and Riemann Problem II

A 3*3 model problem exactly preserving the MHD hyperbolic singularities

$$\begin{bmatrix} u \\ v \\ w \end{bmatrix}_t + \begin{bmatrix} (\gamma + 1)u^2 + v^2 + w^2 \\ 2uv \\ 2uw \end{bmatrix}_x = \begin{bmatrix} \mu & 0 & 0 \\ 0 & \eta & -\chi \\ 0 & \chi & \eta \end{bmatrix} \begin{bmatrix} u \\ v \\ w \end{bmatrix}_{xx}$$

$$u \equiv \gamma p / B_x^2 - 1, \quad v \equiv B_y / B_x, \quad w \equiv B_z / B_x$$



An overcompressive shock structure

$$u(x) = -u_0 \tanh(2u_0 x / \mu),$$

$$v(x) = -v_0 \tanh(2u_0 x / \mu) + Cw_0 \operatorname{sech}(2u_0 x / \mu),$$

$$w(x) = -w_0 \tanh(2u_0 x / \mu) - Cv_0 \operatorname{sech}(2u_0 x / \mu),$$

$$C^2 \equiv 1 + (\gamma - 1)u_0^2 / (v_0^2 + w_0^2)$$

Thermodynamically-Consistent Algebraic Constitutive Relation for Rarefied and Microscale Gases beyond Navier-Stokes-Fourier

$$0 = - \left[\begin{array}{c} 2[\mathbf{\Pi} \cdot \nabla \mathbf{u}]^{(2)} \\ C_p \mathbf{\Pi} \cdot \nabla T + \mathbf{Q} \cdot \nabla \mathbf{u} + \frac{D\mathbf{u}}{Dt} \cdot \mathbf{\Pi} \end{array} \right] + \left[\begin{array}{c} 0 \\ \mathbf{a} \cdot \mathbf{\Pi} \end{array} \right] - \left[\begin{array}{c} 2p[\nabla \mathbf{u}]^{(2)} \\ C_p p \nabla T \end{array} \right] + \left[\begin{array}{c} \Lambda^{(\Pi)} \\ \Lambda^{(Q)} \end{array} \right]$$

Kinematic
Force
Thermo. driving
Dissipation

$$\Lambda^{(\Pi)} = -\frac{\mathbf{\Pi}}{\eta/p} q(\kappa), \quad \Lambda^{(Q)} = -\frac{\mathbf{Q}}{k/pC_p} q(\kappa),$$

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

$$\sigma_{\text{entropy production}} = -k_B \langle \ln FC[F, F_2] \rangle = k_B \frac{(m/2k_B T)^{1/2}}{n^2 d^2} \kappa \sinh \kappa \geq 0$$

A Computational Framework Based on NCCR

Thermodynamic driving force

$$\begin{aligned} -2\eta[\nabla\mathbf{u}]^{(2)} \\ -k\nabla T \end{aligned}$$

$$\begin{aligned} \xrightarrow{\div p} \\ \xrightarrow{\div p \sqrt{\frac{C_p T}{2\text{Pr}}}} \end{aligned}$$

Nonlinear Coupled Constitutive Relation
 f_{Π}, f_Q

$$\begin{aligned} \xrightarrow{\times p} \\ \xrightarrow{\times p \sqrt{\frac{C_p T}{2\text{Pr}}}} \end{aligned}$$

Shear stress
Heat flux

$$\begin{aligned} \Pi \\ Q \end{aligned}$$

$$\begin{array}{ccc} \bullet & | & \bullet \\ i & i+1/2 & i+1 \end{array}$$

$$\Pi_{i+1/2_{NSF}} = -2\eta_{i+1/2}[\nabla\mathbf{u}]_{i+1/2}^{(2)}$$

$$Q_{i+1/2_{NSF}} = -k_{i+1/2}(\nabla T)_{i+1/2}$$

$$\Pi_{i+1/2_{NCCR}} = f_{\Pi}(\Pi_{i+1/2_{NSF}}, Q_{i+1/2_{NSF}}, P_{i+1/2}, T_{i+1/2})$$

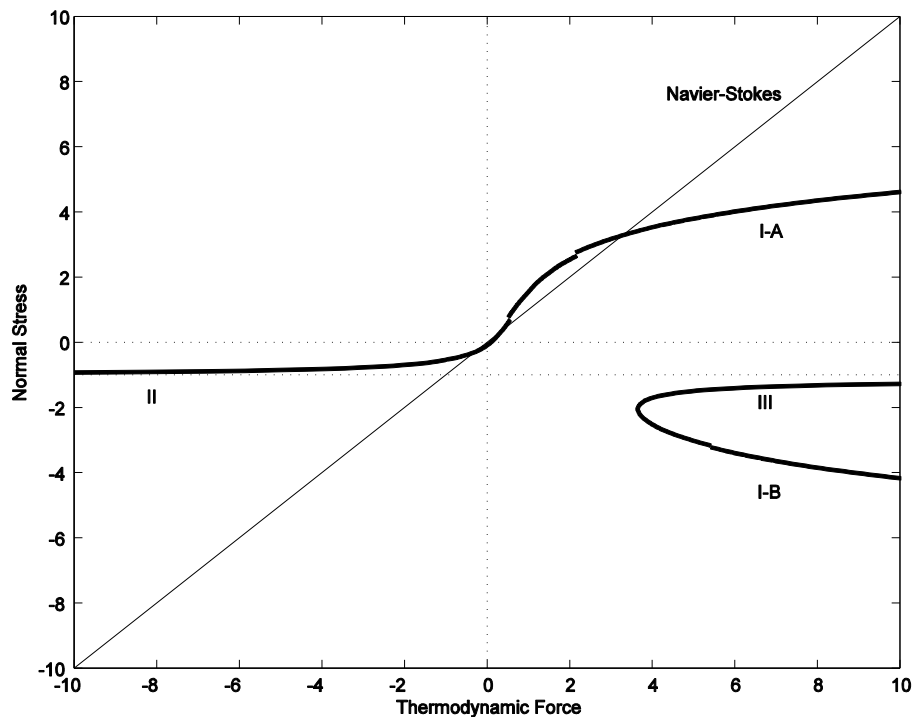
$$Q_{i+1/2_{NCCR}} = f_Q(\Pi_{i+1/2_{NSF}}, Q_{i+1/2_{NSF}}, P_{i+1/2}, T_{i+1/2})$$

A Model Exactly Preserving NCCR

Nonlinearity: NCCR-Burgers

$$\frac{\partial u}{\partial t} + \frac{\partial(u^2 / 2)}{\partial x} = -\frac{\partial \hat{\Pi}}{\partial x}, \quad a \leq x \leq b, \quad t \geq 0,$$

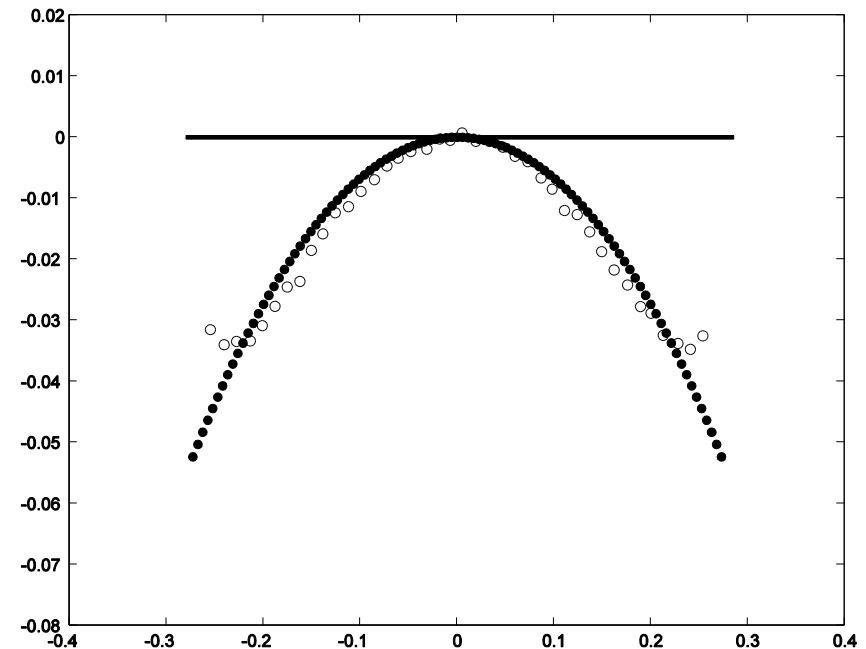
$$\hat{\Pi} q(\hat{\Pi}) = (1 + \hat{\Pi}) \hat{\Pi}_{NS}, \quad \text{where } q(\hat{\Pi}) \equiv \frac{\sinh \hat{\Pi}}{\hat{\Pi}}, \quad \hat{\Pi}_{NS} \equiv -\mu \frac{\partial u}{\partial x}$$



Kinematic Stress Constraint and Cross-Stream Pressure Variation in Nonequilibrium Gases

$$\left(\frac{\Pi_{xy}}{p}\right)^2 = -\frac{3}{2}\left(1 + \frac{\Pi_{yy}}{p}\right)\frac{\Pi_{yy}}{p}$$

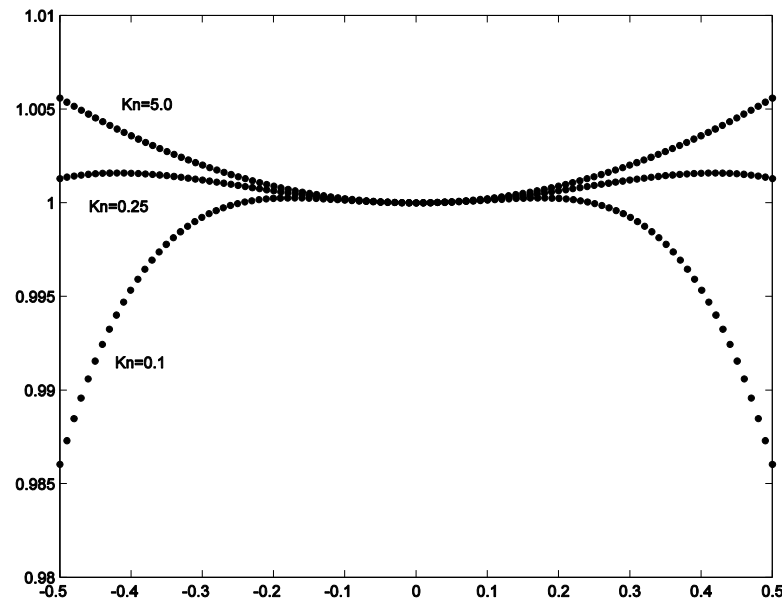
$$\frac{p(S^*)}{p(0)} = 1 + \tan^2 S^*$$



Central Temperature Minimum in Force-Driven Poiseuille Gas Flow

$$T^*(S^*) = \sec^e S^* \left\{ T^*(0) - \left[T^*(0) - \sec^{-e} S^*_{1/2} \left(\alpha_T T^*_{1/2} + (1 - \alpha_T) T^*(0) \right) \right] \frac{F(S^*)}{F(S^*_{1/2})} \right\},$$

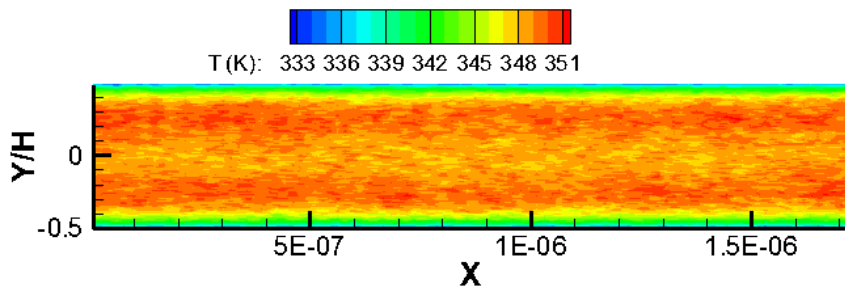
$$F(S^*) \equiv (4 - e) \left[\frac{1}{(4 - e) \cos^{4-e} S^*} - \frac{1}{(2 - e) \cos^{2-e} S^*} - \left(\frac{1}{4 - e} - \frac{1}{2 - e} \right) \right], \quad e = \frac{3(\gamma - 1)}{2\gamma}$$



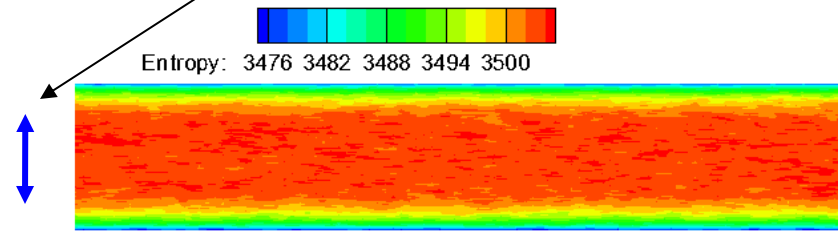
An Exotic Prediction: Heat Conduction from Cold to Hot

Non-Fourier behavior
in NCCR

$$\hat{Q}_y = \frac{3}{(3 + 2\hat{\Pi}_{xyNSF}^2)} \left(\hat{Q}_{yNSF} + a\hat{\Pi}_{xyNSF} \right); \quad a \text{ is force}$$



Temperature contours



Heat transfer from
cold (center) to hot (wall)

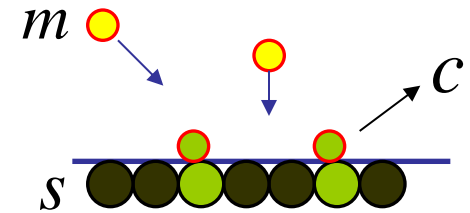
H function contours

Boundary Condition Based on Langmuir Adsorption Isotherm

Fraction of sites in thermal equilibrium α

$$K = \frac{C_c}{C_m C_s} = \frac{N\alpha}{[p / k_B T_w] N(1-\alpha)},$$

$$\alpha = \frac{\beta p}{1 + \beta p} \quad \text{where} \quad \beta = \frac{K}{k_B T_w}.$$

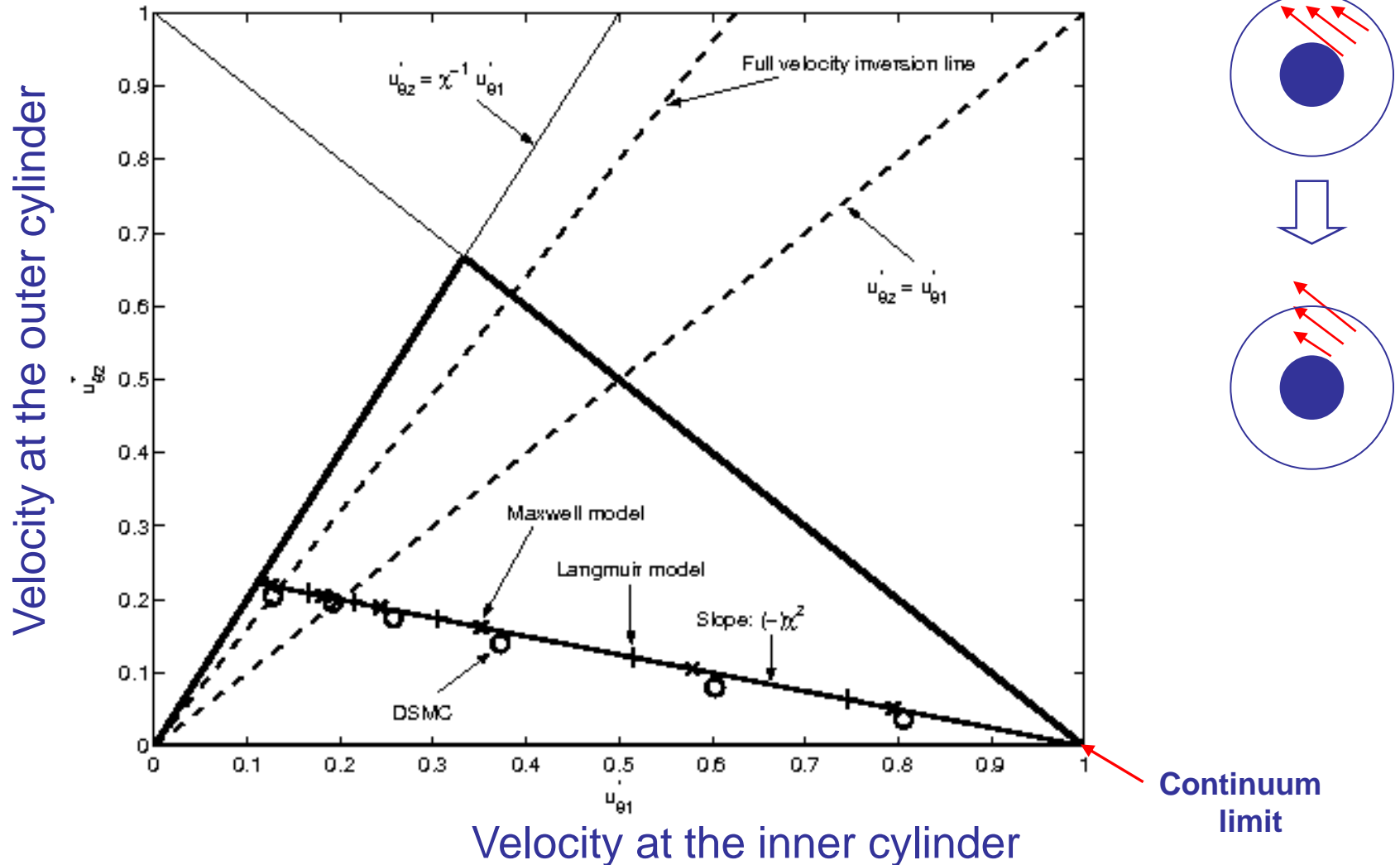


Maxwell accommodation coefficients $\sigma_{v,T}$

$$\sigma_{v,T} \sim \omega_0(\nu) \left(\frac{T_w}{T_r} \right)^{1+2/(\nu-1)} \exp\left(-\frac{D_e}{k_B T_w} \right)$$

D_e : Heat of adsorption [$O(10^{-1} \sim 10)$ kcal/mol]

Microscale Cylindrical Couette Gas Flow



Microscale Cylindrical Couette Gas Flow

If the radius ratio is equal to the golden ratio $(3 - \sqrt{5})/2$, Maxwell and Langmuir models coincide.

Gaseous Slip on Microscale Heat Transfer (An Extended Graetz Problem)

$$(1-r^2) \frac{\partial \theta}{\partial z} = \frac{1}{r} \frac{\partial}{\partial r} \left(r \frac{\partial \theta}{\partial r} \right) + \frac{\alpha(2-\alpha)^2}{Pe^2} \frac{\partial^2 \theta}{\partial z^2}$$

(Confluent hypergeometric function of the first kind and finite integral transform technique)

The Reynolds analogy between heat transfer and momentum transfer is preserved in slip - flow regimes with low Mach numbers.

Analytical Solutions of Shock Structure Thickness and Asymmetry in Navier-Stokes-Fourier Framework (Pr=3/4)

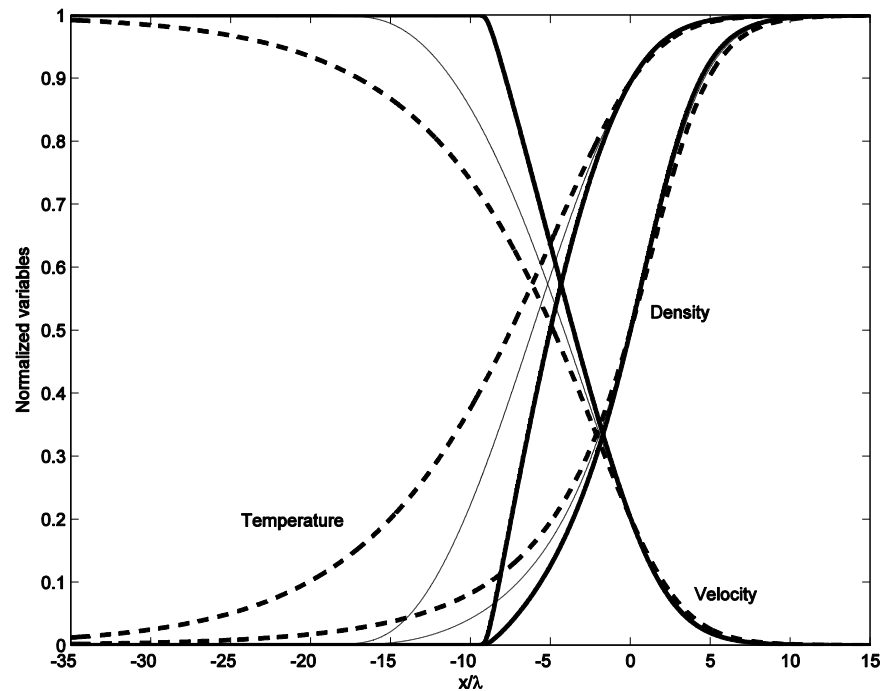
Asymmetry of Maxwellian molecule

$$Q_s = \frac{\int_{-\infty}^0 (r(x) - r_1) dx}{\int_0^{\infty} (r_2 - r(x)) dx} = \frac{\int_{r_a}^{r_1} x(r) dr}{\int_{r_a}^{r_2} x(r) dr} =$$

$$\frac{-\frac{\mu}{4} \left[\frac{5}{4} \ln \frac{r_1}{r_a} - \frac{1}{2} \left(\frac{1}{r_1} - \frac{1}{r_a} \right) - \frac{1}{r_a} \left(\frac{5}{4} + \frac{1}{2r_a} \right) (r_1 - r_a) \right] - \frac{5}{4} \left(\frac{1}{r_2} - \frac{1}{r_1} \right) \ln \frac{r_1}{r_a} - \left(2\alpha - \frac{1}{r_2^2} \right) \left(1 - \frac{r_1}{r_2} \right) \ln \left(\frac{r_a^{-1} - r_2^{-1}}{r_1^{-1} - r_2^{-1}} \right)}{-\frac{\mu}{4} \left[\frac{5}{4} \ln \frac{r_2}{r_a} - \frac{1}{2} \left(\frac{1}{r_2} - \frac{1}{r_a} \right) - \frac{1}{r_a} \left(\frac{5}{4} + \frac{1}{2r_a} \right) (r_2 - r_a) \right] - \frac{5}{4} \left(\frac{1}{r_2} - \frac{1}{r_1} \right) \ln \frac{r_2}{r_a} - \left(2\alpha - \frac{1}{r_1^2} \right) \left(\frac{r_2}{r_1} - 1 \right) \ln \left(\frac{r_1^{-1} - r_a^{-1}}{r_1^{-1} - r_2^{-1}} \right)}$$

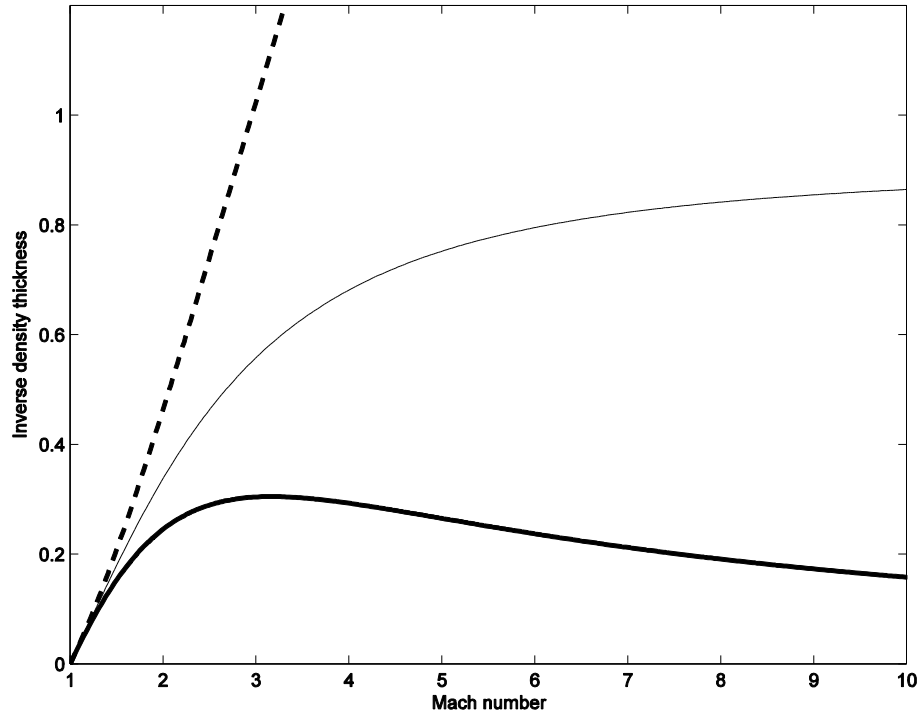
$$Q_{s_{M \rightarrow 1}} = 1, \quad Q_{s_{M \rightarrow \infty}} = \frac{125}{106} \ln 5 - \frac{38}{53} \doteq 1.181.$$

Analytical Solutions of Shock Structure Thickness and Asymmetry in Navier-Stokes-Fourier Framework ($Pr=3/4$)



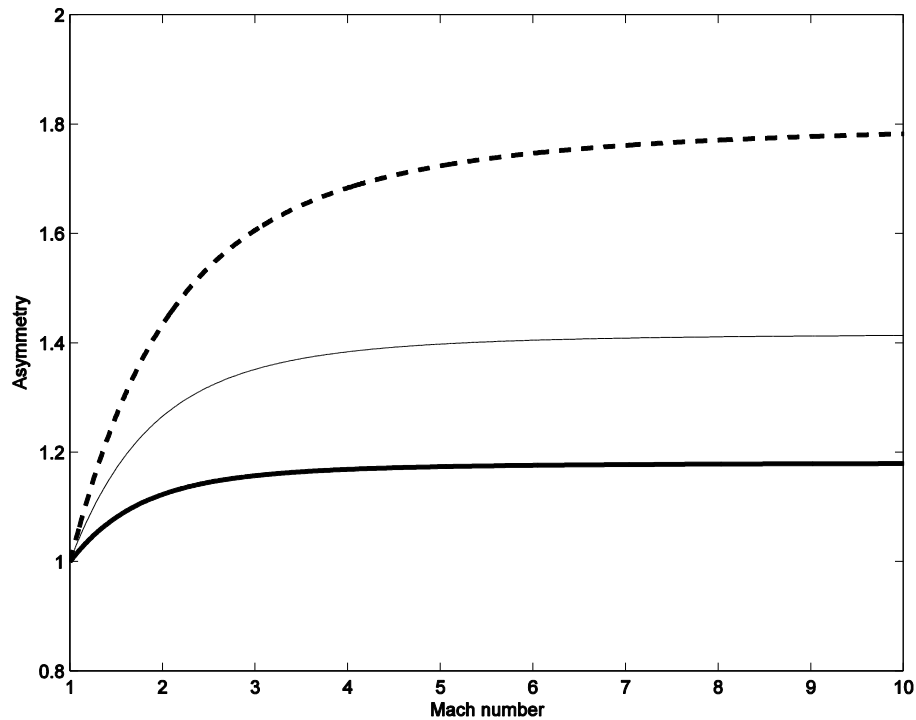
Shock structure profiles ($M=15$). Maxwellian molecule ($s=1$) for the thick solid curve; hard sphere ($s=1/2$) for the thin solid curve; constant case ($s=0$) for the broken curve

Analytical Solutions of Shock Structure Thickness and Asymmetry in Navier-Stokes-Fourier Framework ($Pr=3/4$)



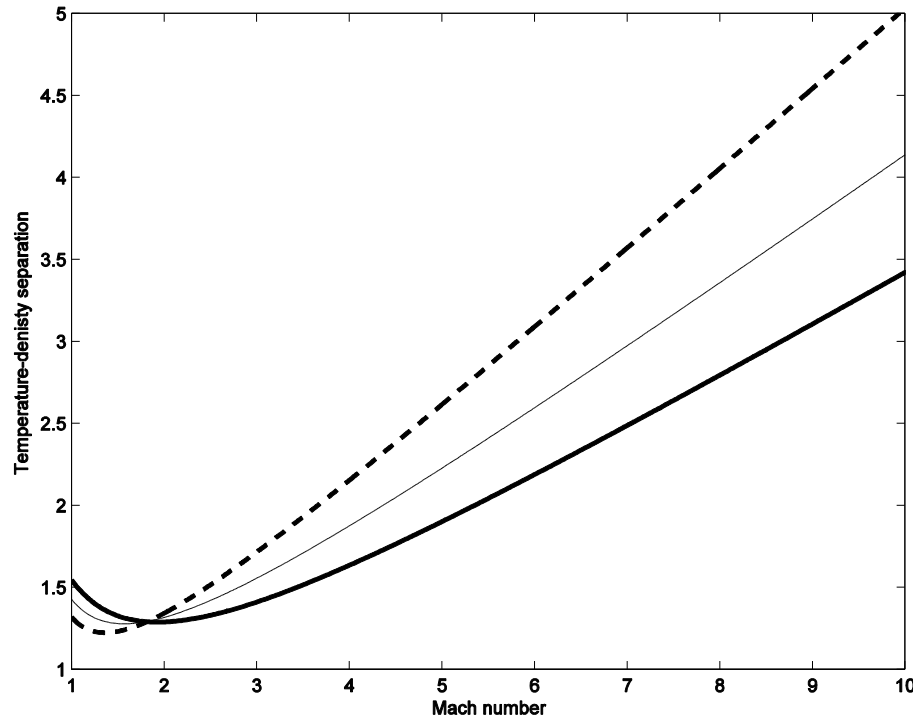
Inverse shock density thickness

Analytical Solutions of Shock Structure Thickness and Asymmetry in Navier-Stokes-Fourier Framework ($Pr=3/4$)



Shock asymmetry

Analytical Solutions of Shock Structure Thickness and Asymmetry in Navier-Stokes-Fourier Framework (Pr=3/4)



Shock temperature–density separation

$$\Delta_{M \rightarrow 1} = \frac{4}{5} \sqrt{\frac{10}{\pi}} \doteq 1.427, \quad \Delta_{M \rightarrow \infty} \rightarrow \infty \text{ for hard sphere}$$