

# **Pushing the Limits of Continuum Fluid Mechanics and Going beyond the Navier-Stokes-Fourier**

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**Presented at Mechanical Engineering Colloquium in McGill  
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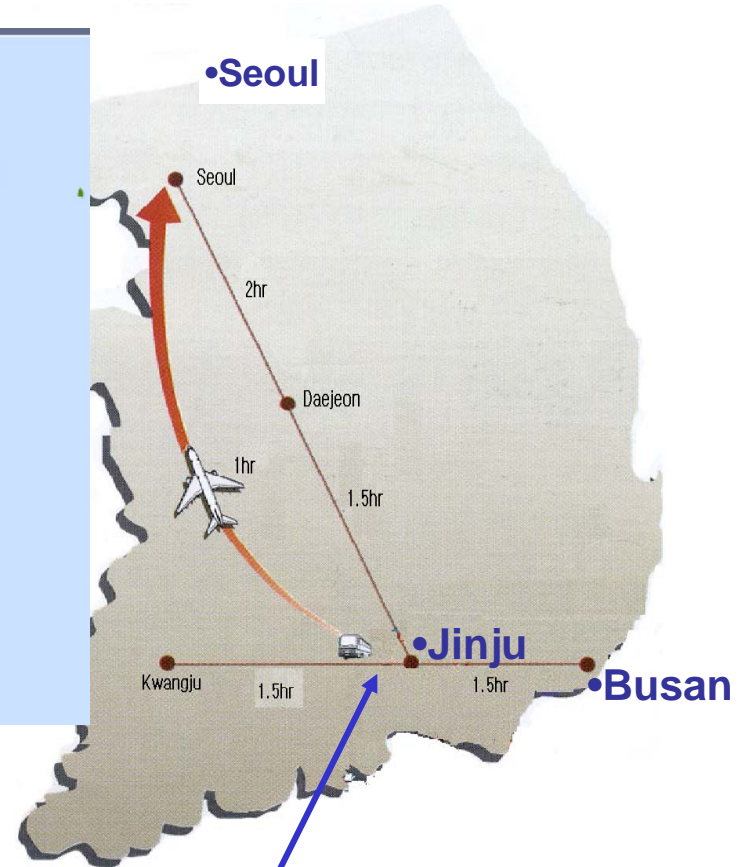
**Many thanks to**

**Prof. W. G. Habashi  
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**and**

**Prof. Damiano Pasini, Antonella Fratino  
for all the arrangements.**

# Introduction to Gyeongsang National University

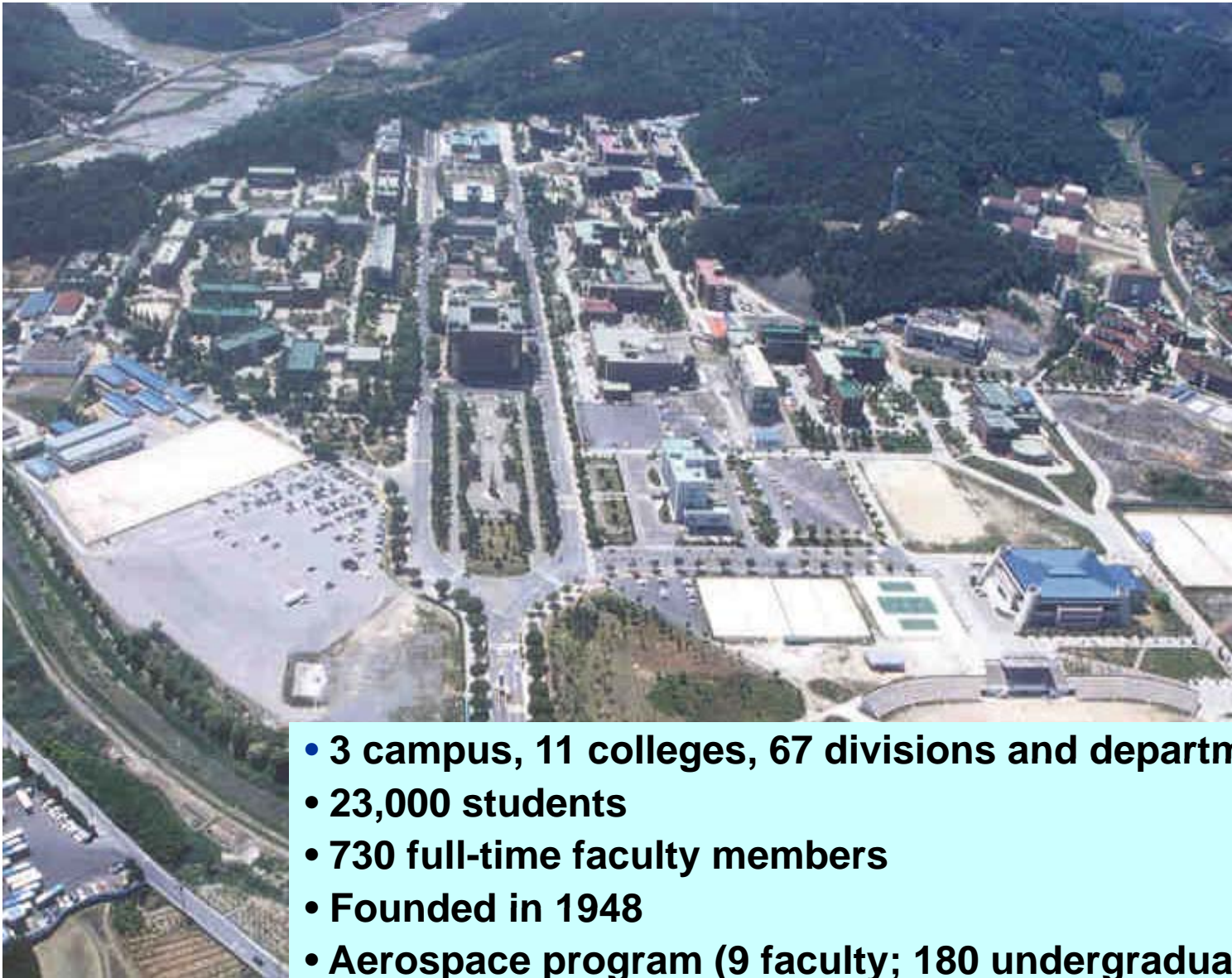


**9 Provinces in South Korea**

**One of the major national universities**

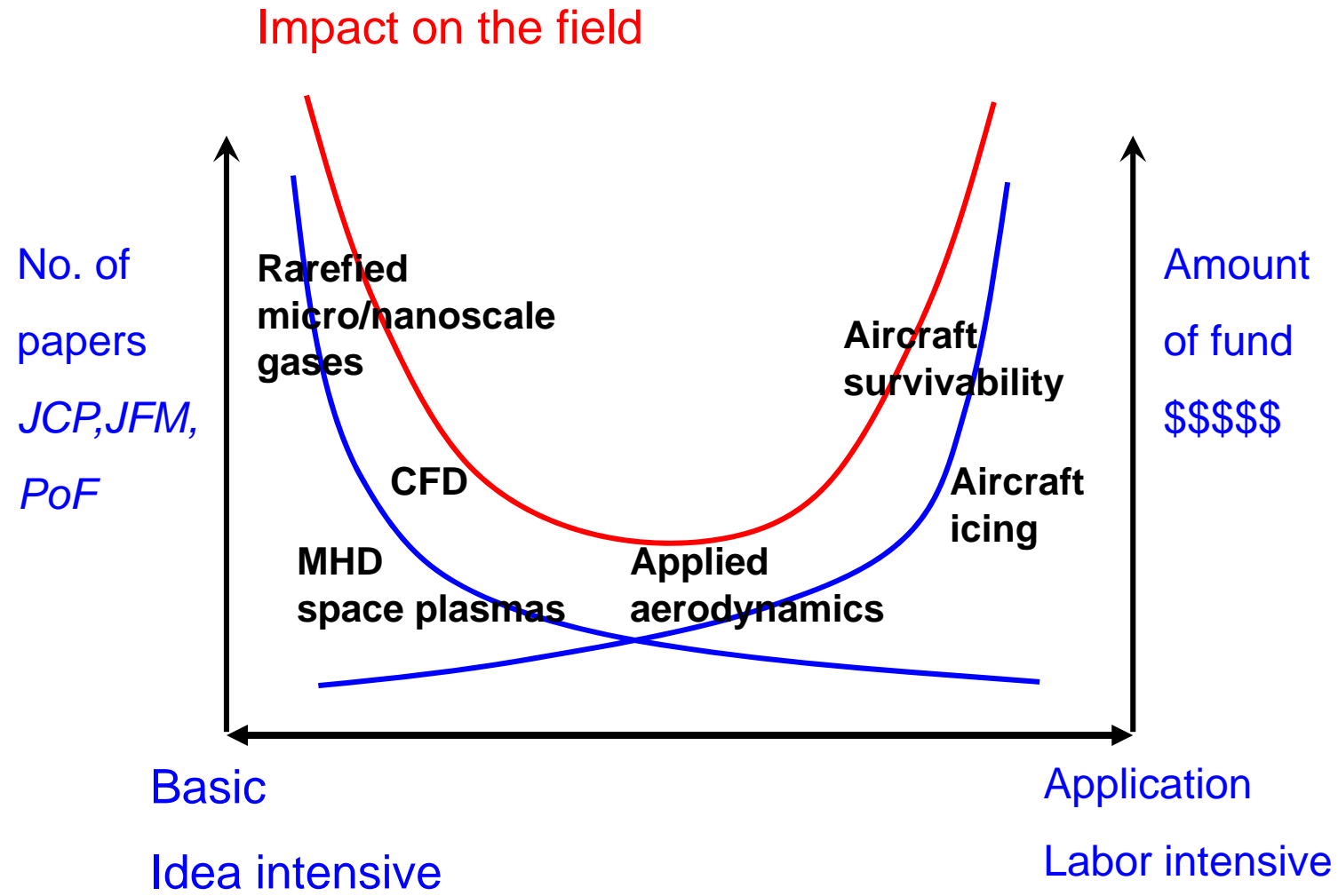
**Located in Gyeongnam province  
(manufacturing industrial belt)**

# Overview of GNU



- **3 campus, 11 colleges, 67 divisions and departments**
- **23,000 students**
- **730 full-time faculty members**
- **Founded in 1948**
- **Aerospace program (9 faculty; 180 undergraduates; 120 graduates)**

# Research areas of Aerospace Comp. Modeling Lab



## **Research goal:**

**Develop a unified computational model for rarefied and micro- & nano-scale gases upon which others can build efficient CFD codes**

<http://acml.gnu.ac.kr>  **<Open knowledge>**

**Part I.**

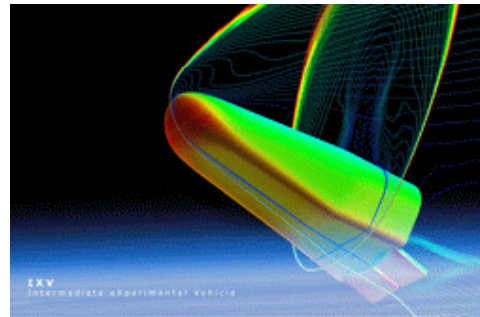
**Fundamentals**



# Introduction to rarefied and micro/nanoscale gases

Compression-dominated  
High  $M$ , low  $Kn$

Intermediate Experimental Vehicle



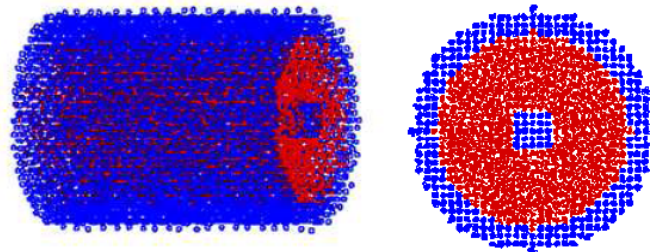
**Gas flows around hypersonic vehicles and plume flows**

Continuous shift of continuum, transition, and free-molecular regimes  
Coexistence of various regimes

Need of unified framework



Shear-dominated  
Low  $M$ , high  $Kn$



Micro and nanoscale cylinder

**Gas (liquid) flow + MN solid devices**

Molecular interaction between gas (liquid) particles and solid atoms  
Gas (liquid) flows in thermal (trans., rot.) nonequilibrium regimes  
Electrokinetics, surface tension etc.



# Approaches for modeling rarefied and micro/nanoscale gases

## Molecular approach

DSMC (Direct Simulation Monte Carlo) (Bird)

Linearized Boltzmann equation (Cercignani, Sone)

Lattice-Boltzmann method

## Continuum approach

Chapman-Enskog: Burnett (1935) etc.

**Moment method:** Grad (1949), Eu (1992), regularized-13 (2005)

**Constitutive equations:** the only ingredient in the conservation laws in which the microscopic nature of gas molecules is taken into account.

## Hybrid approach

DSMC-continuum coupling (Nie 2004, Schwartzenuber 2007)

Seamless multi-scale method: viscous stress calculated by MD (Weinan 2009)

# 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).

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

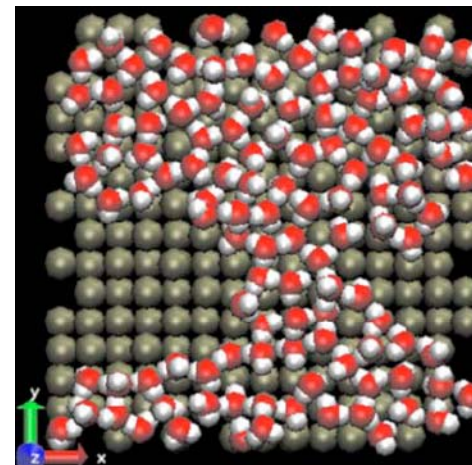
$$\mathbf{\Pi} = -\eta [\nabla \mathbf{u}]^{(2)}, \quad \mathbf{Q} = -k \nabla T$$

**Navier**

**Fourier**

**Linear uncoupled**  
constitutive relations

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



**A critical observation: an efficient way of including the molecular nature of gases is to develop **nonlinear coupled** constitutive relations but to retain the conservation laws.**

# Linear uncoupled Navier-Fourier equations

**Navier (1822)**  $\rho \frac{D\mathbf{u}}{Dt} + \nabla p + \nabla \cdot \mathbf{\Pi} = \mathbf{0}, \quad \rho \frac{DE_t}{Dt} + \nabla \cdot p\mathbf{u} + \nabla \cdot [\mathbf{\Pi} \cdot \mathbf{u} + \mathbf{Q}] = 0$

**Fourier (1822)**

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

$$\begin{bmatrix} \Pi_{xx} & \Pi_{xy} \\ \Pi_{yx} & \Pi_{yy} \end{bmatrix} \leftarrow -2\eta \begin{bmatrix} u_x - (u_x + v_y)/3 & (u_y + v_x)/2 \\ (v_x + u_y)/2 & v_y - (u_x + v_y)/3 \end{bmatrix}$$

$u_x$  case (compression and expansion)

$$-2\eta \begin{bmatrix} 2u_x/3 & 0 \\ 0 & -u_x/3 \end{bmatrix}$$

Not like  $(u_x)^2$

**Newtonian or linear**

$u_y$  case (velocity shear only)

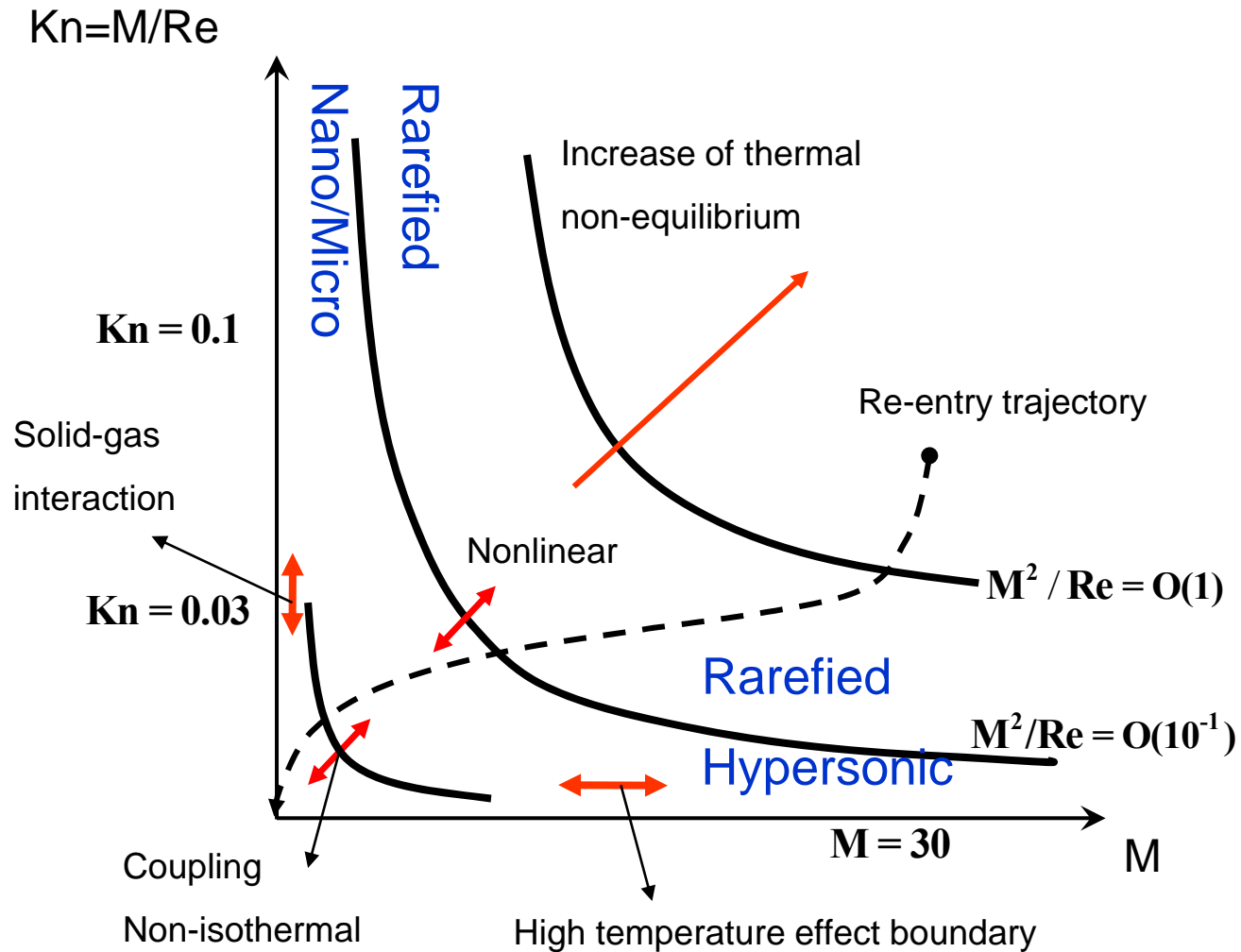
$$-2\eta \begin{bmatrix} 0 & u_y/2 \\ u_y/2 & 0 \end{bmatrix}$$

**Uncoupled**

Always vanishing normal stress  $\Pi_{xx}$  or  $\Pi_{yy}$

$$\begin{bmatrix} Q_x \\ Q_y \end{bmatrix} \leftarrow -k \begin{bmatrix} T_x \\ T_y \end{bmatrix}. \quad \text{Not like } (T_x)^2$$

# Physics of rarefied and micro/nanoscale gases



$$\mathbf{v} \cdot \nabla f(\mathbf{r}, \mathbf{v}) = C[f, f_2]$$

Two terms: Kn

$$\rho \mathbf{u} \cdot \nabla \mathbf{u} + \nabla \cdot p \mathbf{I} + \nabla \cdot \Pi = 0$$

Three terms: M, Kn



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

# Modelling of nonequilibrium gas system

Molecular (Probabilistic)

Phase Space

Boltzmann (1844-1906)

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

Thermodynamics  
(Reduction of  
Information)

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

Statistical average

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

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

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

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

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

Continuum

(Hydrodynamic)

Thermodynamic

Space

Conservation Laws

Moment Equation

(Constitutive Relation)

Not far from LTE

Navier-Stokes-Fourier

# A modified moment method [Eu, 1992]

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

*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 modified moment method (continued)

Moment equations in vector form

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

**Unsteady**

**Convection**

**Higher-order**

$$(\partial_t + \mathbf{v} \cdot \nabla + \mathbf{a} \cdot \nabla_v) f(t, \mathbf{r}; \mathbf{v}) = C[f, f_2]$$

$$\frac{\partial}{\partial t} \begin{bmatrix} \mathbf{\Pi} \\ \mathbf{Q} \end{bmatrix} + \mathbf{u} \cdot \nabla \begin{bmatrix} \mathbf{\Pi} \\ \mathbf{Q} \end{bmatrix} = - \begin{bmatrix} \nabla \cdot \psi^{(\Pi)} \\ \nabla \cdot \psi^{(Q)} + \psi^{(P)} : \nabla \mathbf{u} \end{bmatrix}$$

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

**Kinematic                      Force      Thermo. driving      Dissipation**

$$\mathbf{\Pi} \equiv \langle m[\mathbf{cc}]^{(2)} f \rangle, \quad \mathbf{Q} \equiv \langle mc^2 \mathbf{c} f / 2 \rangle,$$

$$\psi^{(\Pi)} \equiv \langle m[\mathbf{cc}]^{(2)} \mathbf{c} f \rangle, \quad \psi^{(P)} \equiv \langle m \mathbf{c} \mathbf{c} \mathbf{c} f \rangle, \quad \psi^{(Q)} \equiv \langle mc^2 \mathbf{c} \mathbf{c} f / 2 \rangle$$

$$\mathbf{\Lambda}^{(\Pi)} \equiv \langle m[\mathbf{cc}]^{(2)} C[f, f_2] \rangle, \quad \mathbf{\Lambda}^{(Q)} \equiv \langle mc^2 \mathbf{c} / 2 C[f, f_2] \rangle$$



# A physically motivated closure

By noting the **relative** importance of various terms, for example,

**Higher-order**

$$\left| \nabla \cdot \boldsymbol{\Psi}^{(\Pi)} \right| < \left| \left[ \boldsymbol{\Pi} \cdot \nabla \mathbf{u} \right]^{(2)} \right|, \left| p \left[ \nabla \mathbf{u} \right]^{(2)} \right|$$

**Kinematic**                      **Thermo. driving**

one may neglect the higher-order term **as an approximation**.

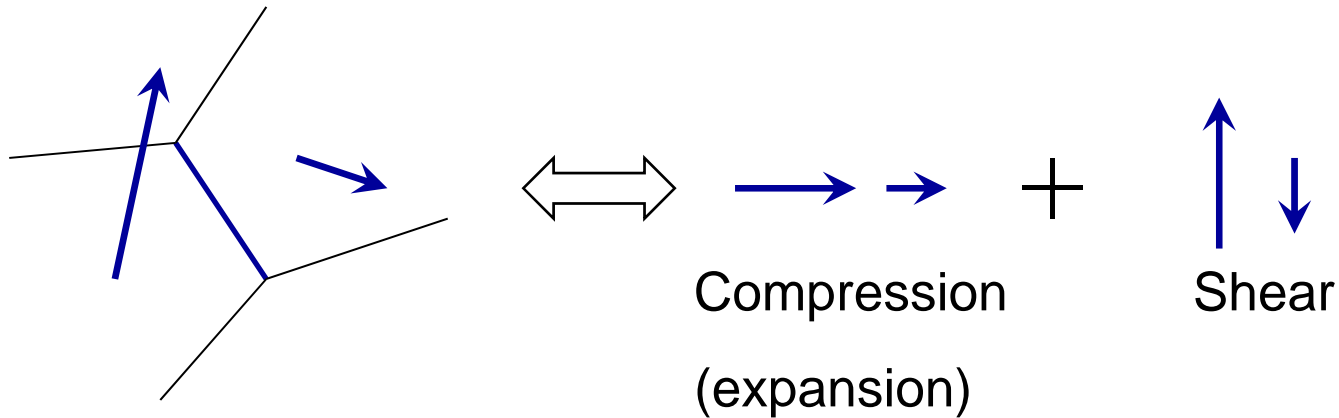
$$\begin{aligned} \nabla \cdot \boldsymbol{\Psi}^{(\Pi)} &\approx 0, \\ \nabla \cdot \boldsymbol{\Psi}^{(Q)} + \boldsymbol{\Psi}^{(P)} : \nabla \mathbf{u} &\approx 0 \end{aligned}$$

Then we have a **nonlinear coupled algebraic constitutive relation (NCCR)**

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

**Kinematic**                      **Force**    **Thermo. driving**    **Dissipation**

# A computational framework based on NCCR



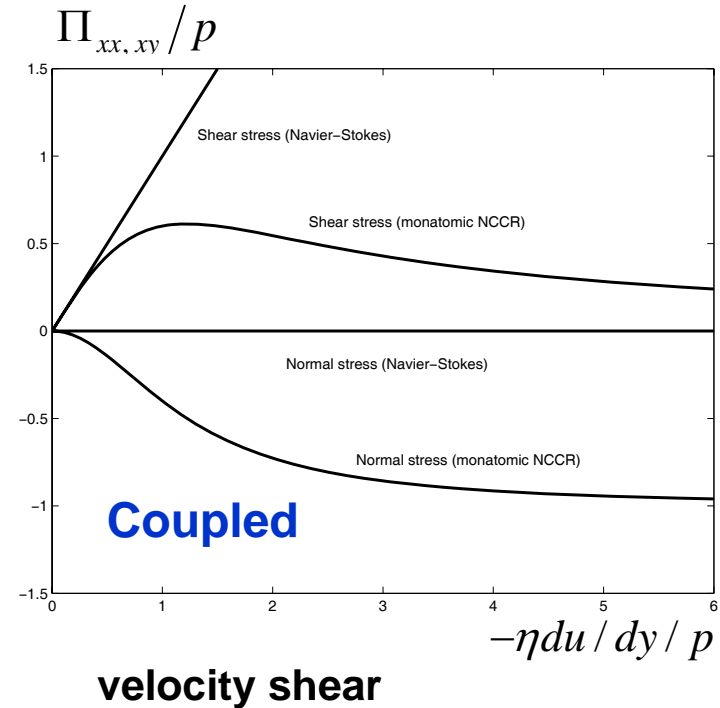
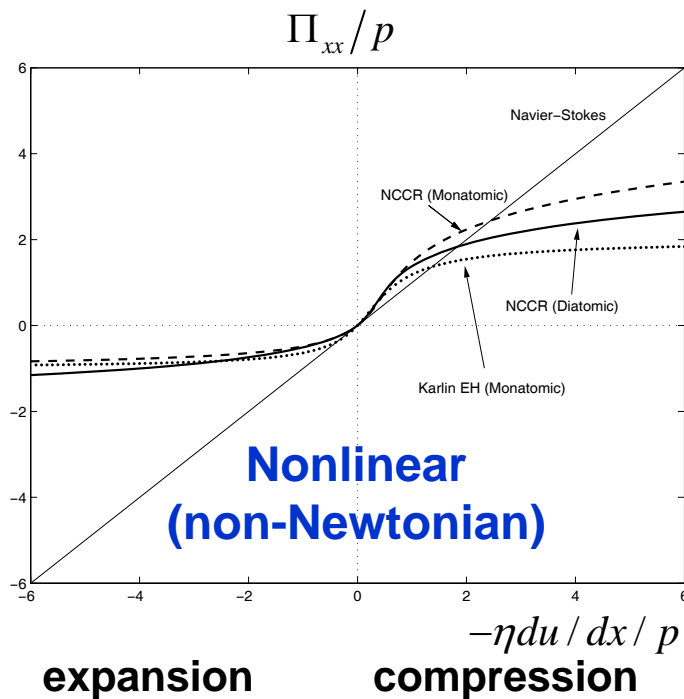
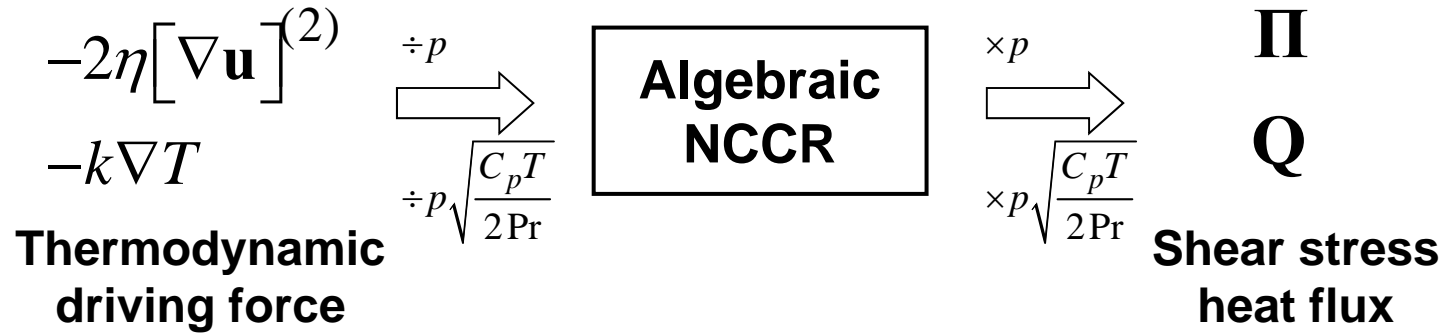
Edge based finite volume formulation in general coordinates (*JCP* 2004)

$$\frac{\partial}{\partial t} \int_V \mathbf{U} dV + \int_S \mathbf{F} \cdot \mathbf{n} dS = 0$$

$$\mathbf{U}_{i,j}^{n+1} = \mathbf{U}_{i,j}^n - \frac{\Delta t}{A_{i,j}} \sum_{k=1}^N \mathbf{R}_k^{-1} \mathbf{F}_k^n \Delta L_k$$

$$\mathbf{\Pi} = f_{\Pi} (\mathbf{\Pi}_{\text{NSF}}, \mathbf{Q}_{\text{NSF}}, p, T), \quad \mathbf{Q} = f_Q (\mathbf{\Pi}_{\text{NSF}}, \mathbf{Q}_{\text{NSF}}, p, T)$$

# NCCR property in compression-expansion and velocity shear case

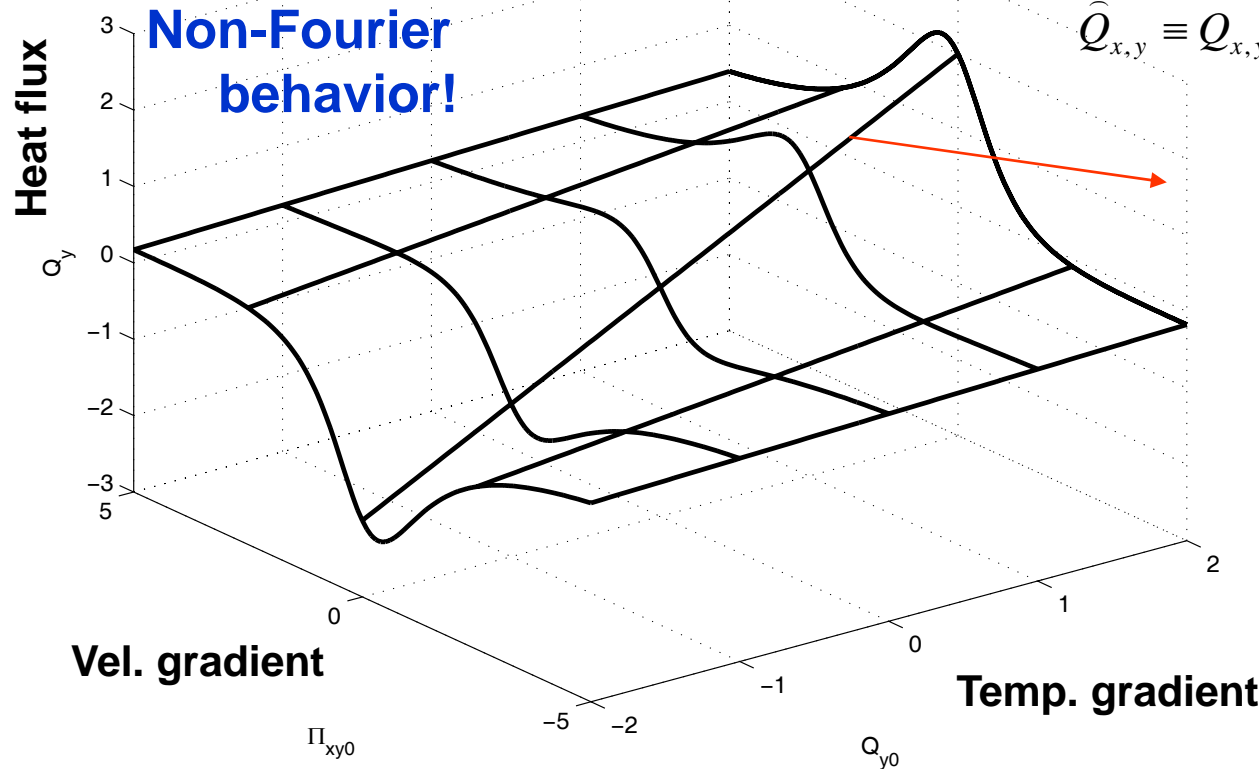


# Non-Fourier law by the coupling of force and shear stress

$$\hat{Q}_y = \frac{3}{(3 + 2\hat{\Pi}_{xy_0}^2)} (\hat{Q}_{y_0} + a\hat{\Pi}_{xy_0}); \quad a \text{ is force}$$

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

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



**Part II.**

**Validation**

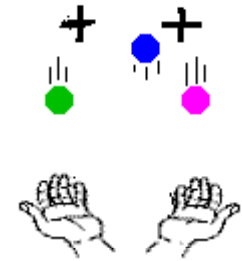


# Validation I (continued)

Unsteady Convection Higher-order

$$\frac{\partial \Pi}{\partial t} + (\mathbf{u} \cdot \nabla) \Pi = -\nabla \cdot \psi^{(\Pi)} - 2[\Pi \cdot \nabla \mathbf{u}]^{(2)} - 2p[\nabla \mathbf{u}]^{(2)} + \Lambda^{(\Pi)}$$

Kinematic      Thermo. driving      Dissipation



**Comment:** In steady-state case, one has to deal with 5 terms, which is really difficult juggling. Even in simple 3 ball juggling, there can be as many as 17 methods.

**Key finding:** Gases are **compressed rapidly** across the shock wave and so accurate treatment of **dissipation** term will be critical.

**What B. C. Eu did:** Assume the distribution function  $f$  in exponential form (not in usual polynomial form) and then apply the cumulant expansion method: the celebrated Eu's **hyperbolic sine** factor.



# Validation I (continued)

Essential terms are three in the right-hand side

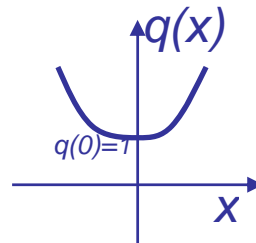
$$0 + 0 = 0 - 2[\mathbf{\Pi} \cdot \nabla \mathbf{u}]^{(2)} - 2p[\nabla \mathbf{u}]^{(2)} + \mathbf{\Lambda}^{(\mathbf{\Pi})}$$

Kinematic      Thermo. driving      **Dissipation**

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

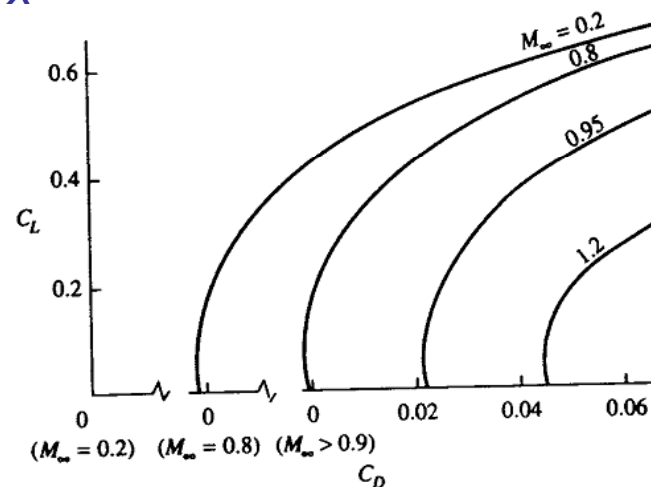
Cf.  $q(\kappa)=1$ ; **BGK** or **relaxation** approx.

$$C[f, f_2] \approx \frac{f^{equil} - f}{\tau}$$



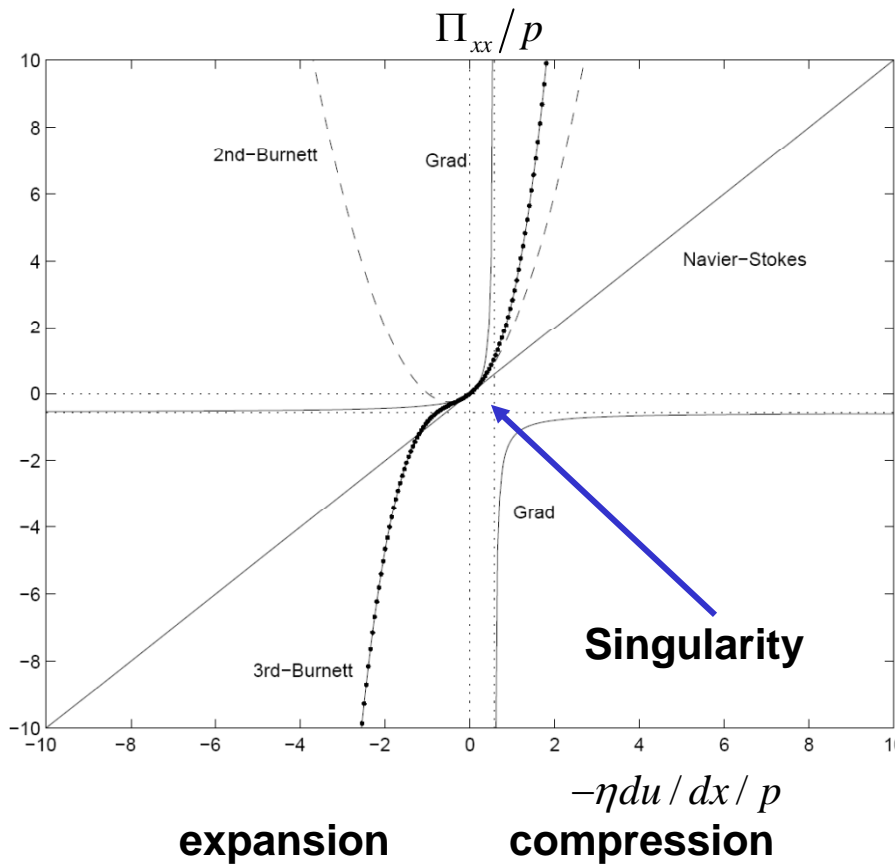
**Comment: No 1st-order term in the series expansion of  $q(\kappa)$  explains why the NSF approximation is so successful.**

Cf. Drag polar in aerodynamics



# Validation I (continued)

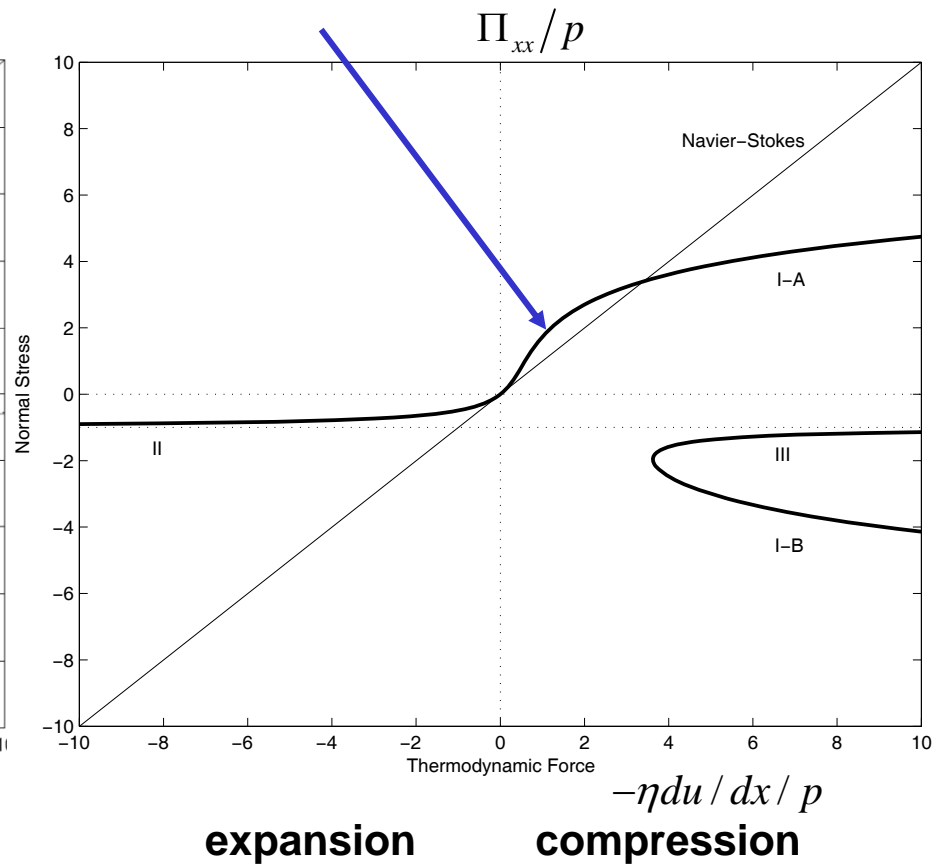
**Before**



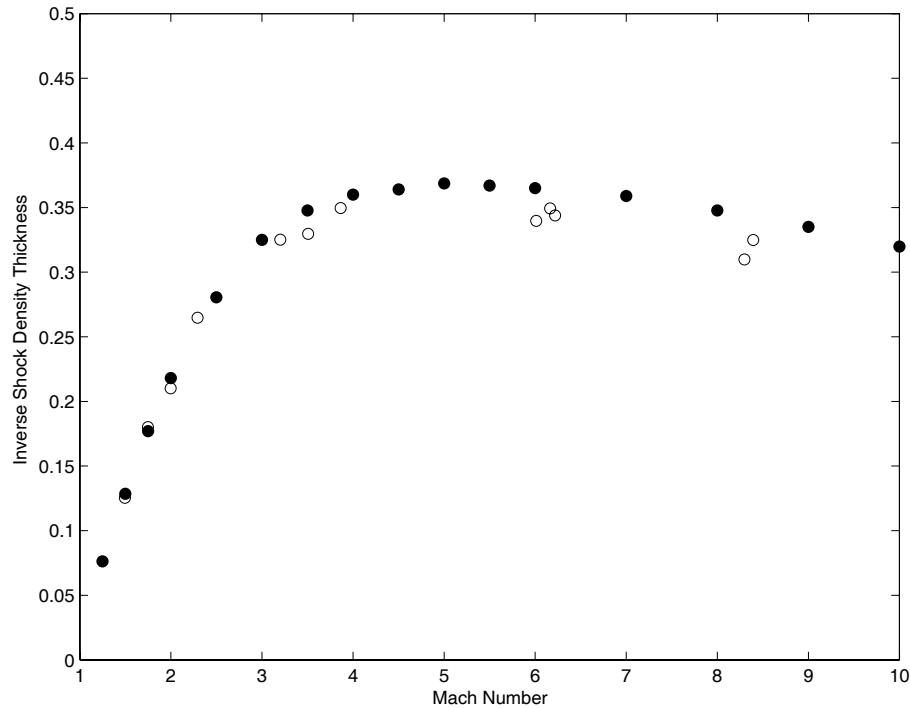
With  $q(\kappa) \equiv \frac{\sinh \kappa}{\kappa}$

**After**

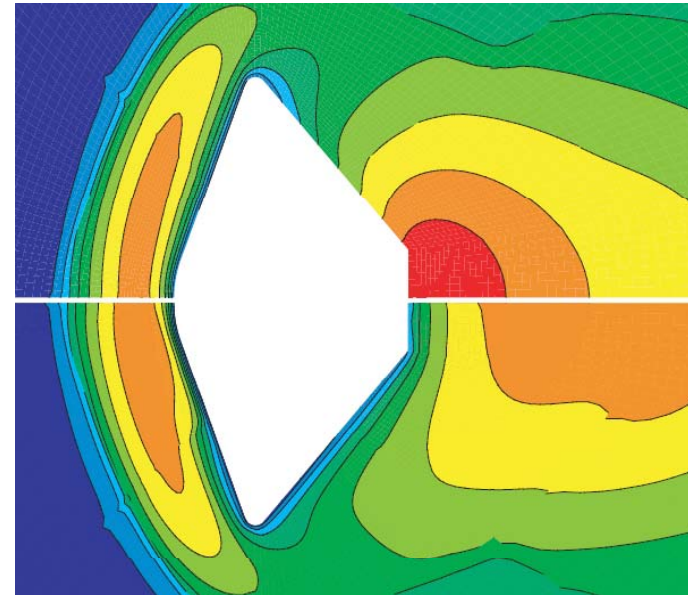
singularity removed!



# Validation I (continued)

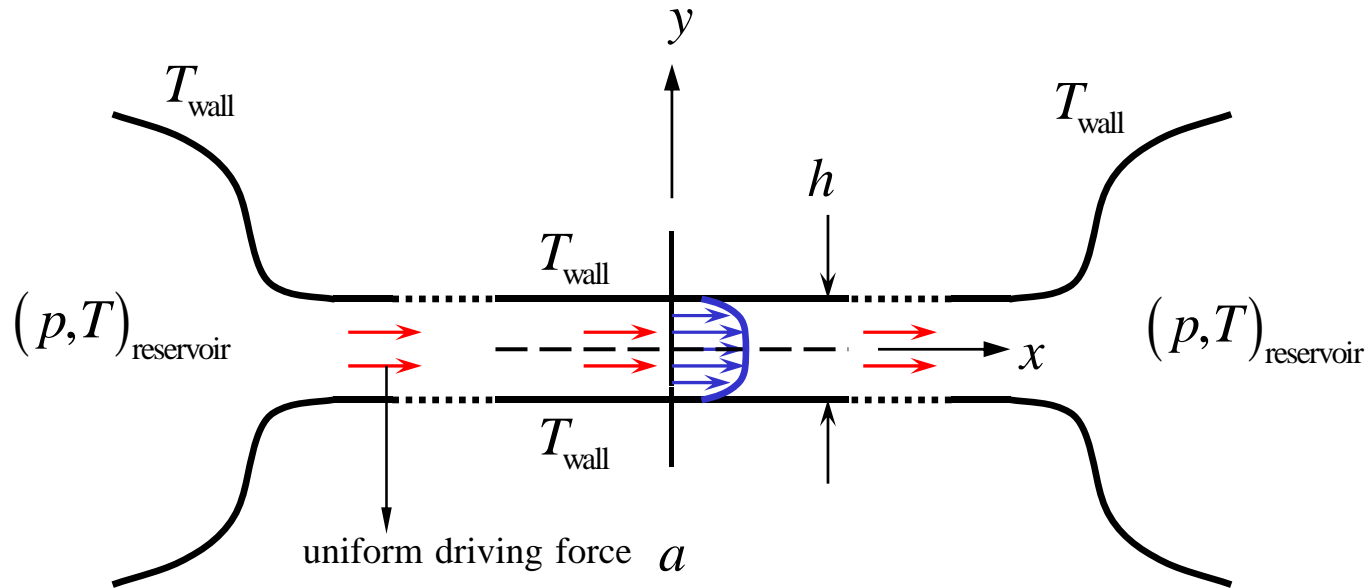


**Shock density thickness for a diatomic gas versus the Mach number (o: experimental data)**



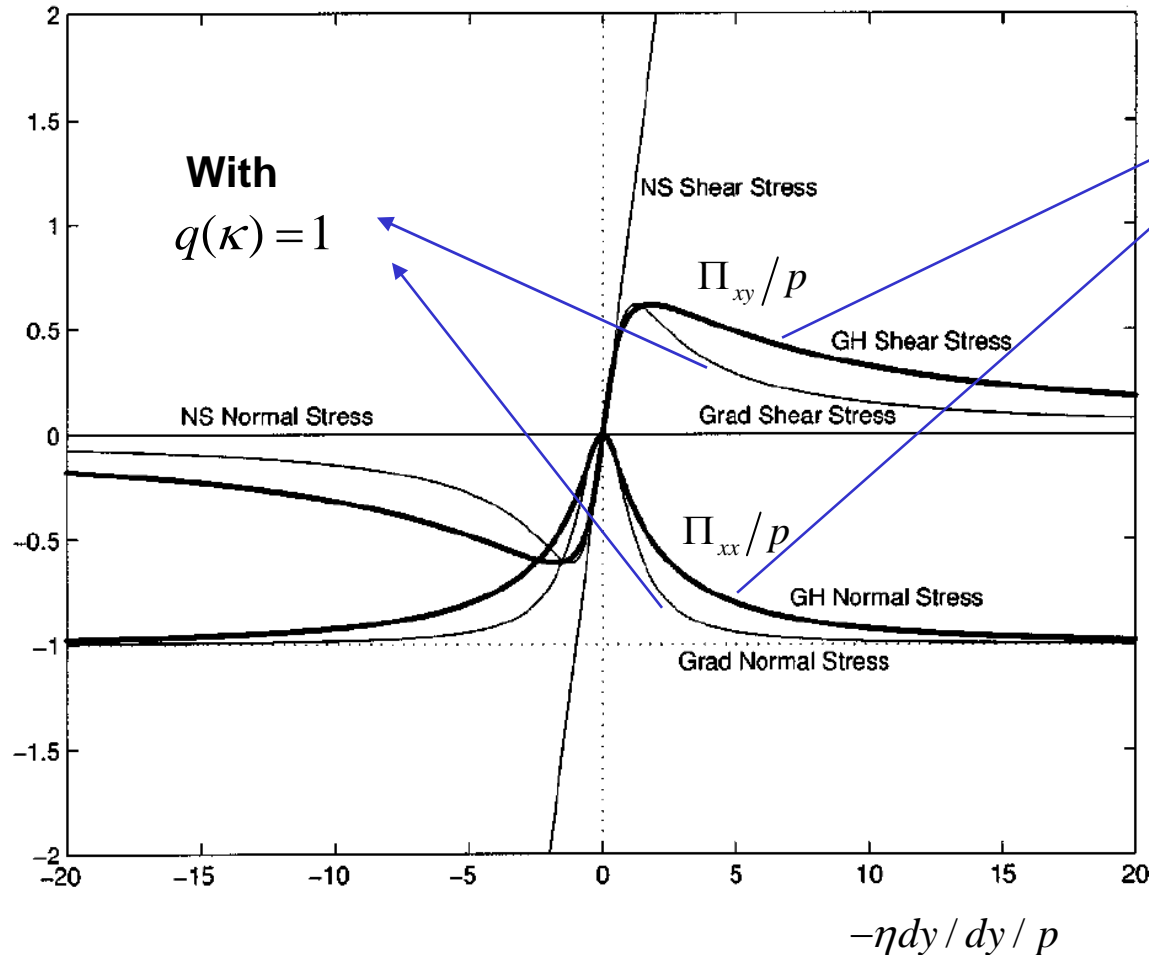
**Normalized temperature contours (NSF vs NCCR) in multi-species flowfield around a reentry vehicle ( $M=23.47$ ,  $Kn=0.2238$ ; courtesy of J. H. Ahn)**

# Validation II: 1-d force-driven compressible Poiseuille gas flow (**velocity shear dominated**; *PoF* 2011)



$$\varepsilon_{h_{\text{wall}}} \equiv \frac{ah}{RT_{\text{wall}}} : \text{Richardson no.}, \quad \text{Kn} \equiv \sqrt{\frac{\pi}{2}} \frac{\eta_{\text{wall}} \sqrt{RT_{\text{wall}}}}{p_{\text{reservoir}} h} : \text{Knudsen no.}$$

# Different role of $q(\kappa)$ term in velocity shear



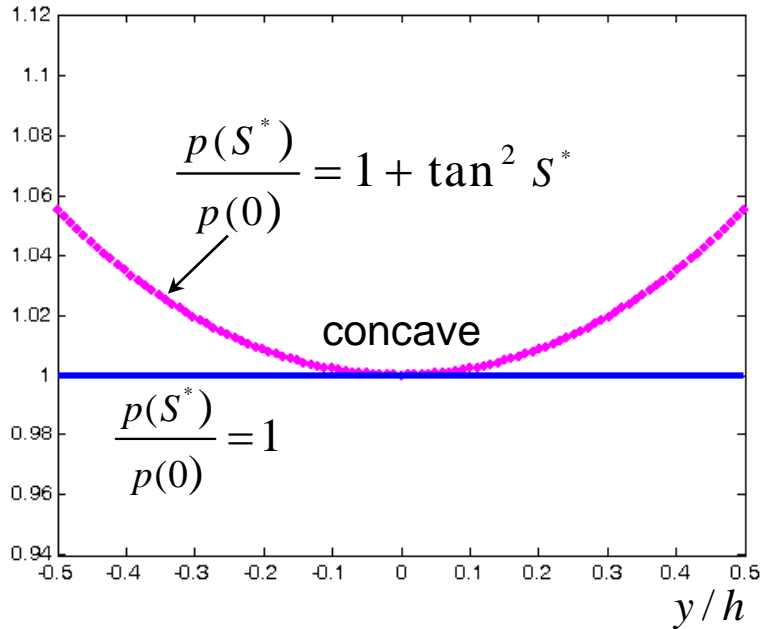
With  $q(\kappa) \equiv \frac{\sinh \kappa}{\kappa}$

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

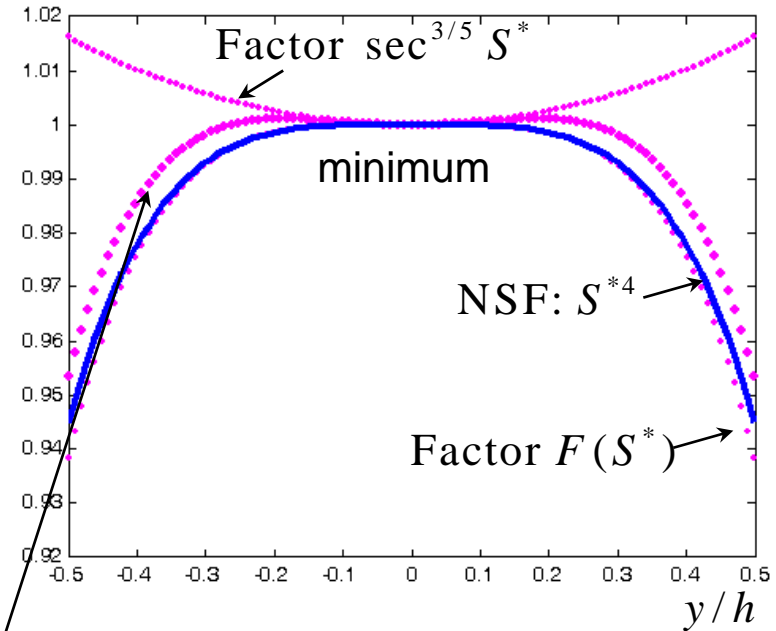
**Local kinematic  
stress constraint**

**BGK or relaxation is fairly good approximation, in stark contrast with the shock structure case!**

# Validation II: Fully analytical solution (Kn=0.1, $\varepsilon_{h_w} = 0.6$ )



Pressure profile across channel  
(NSF: blue, NCCR: cyan)

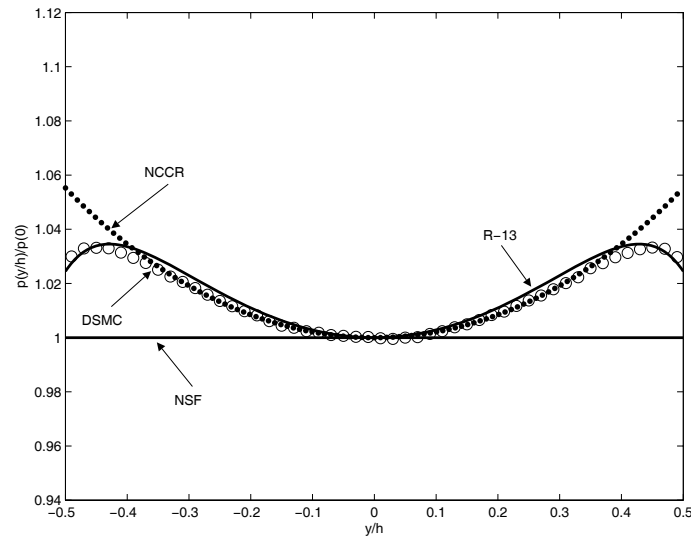


$$\frac{T(S^*)}{T(0)} = \sec^{3/5} S^* \left[ 1 - \frac{\pi \text{Pr}}{816} \frac{T_w^{*5}}{T^*(0)} \frac{\varepsilon_{h_w}^2}{\text{Kn}^2} \frac{F(S^*)}{S_w^{*4}} \right], \quad S^* \equiv \sqrt{\frac{2}{3}} \frac{T_w^* \varepsilon_{h_w} S^*}{T^*(0)}$$

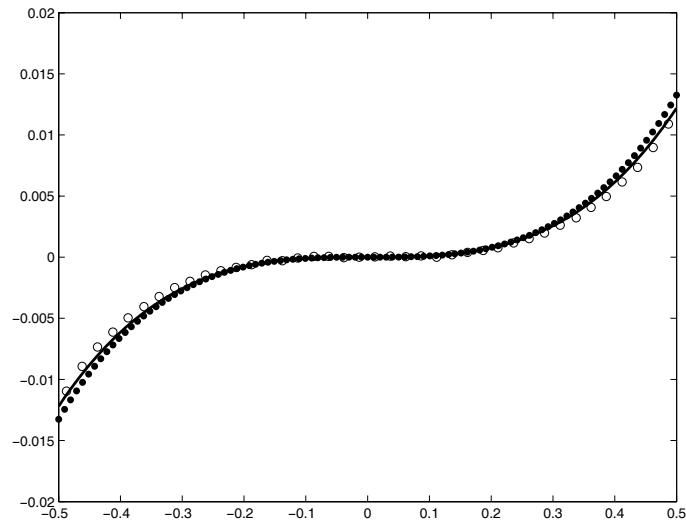
$$F(S^*) \equiv 17 \left[ \frac{1}{17 \cos^{17/5} S^*} - \frac{1}{7 \cos^{7/5} S^*} - \left( \frac{1}{17} - \frac{1}{7} \right) \right]$$

Temperature profile across channel  
(NSF: blue, NCCR: cyan)

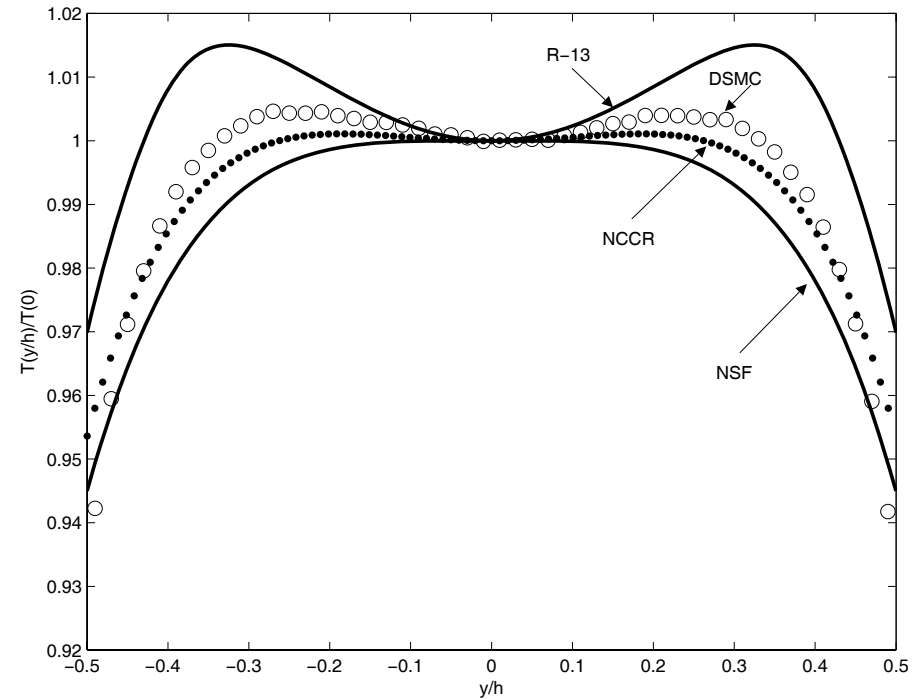
# Validation II: comparison with other solutions



Pressure profile across channel



Normal heat flux profile across channel



Temperature profile across channel

Capturing all the qualitative features predicted by the DSMC

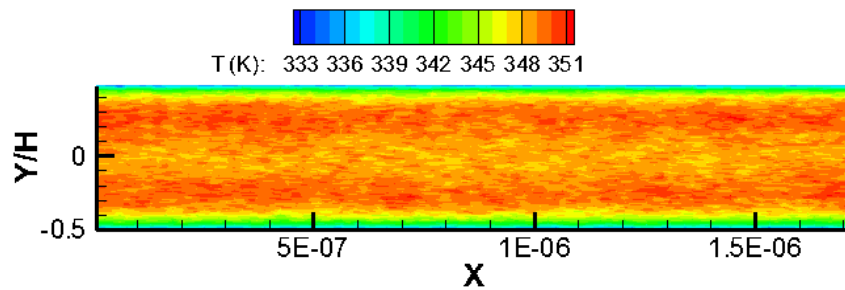
Cf. DSMC (Bird), Regularized-13 (Struchtrup)



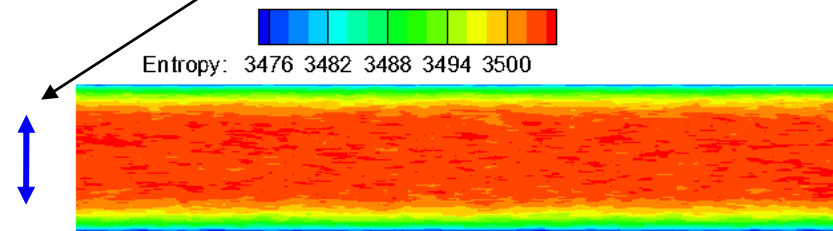
# An exotic prediction: heat conduction from **cold** to **hot**

**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  
(Courtesy of E. Roohi)

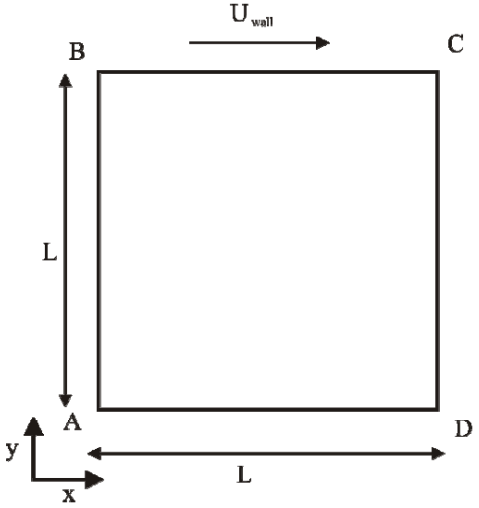


Heat transfer from **Cold** (center) to **hot** *H* function contours

Cf.  $H(t) = \sum_{bins} \Delta v \frac{N_h(v)}{N} \ln \frac{N_h(v)}{N}$  in DSMC

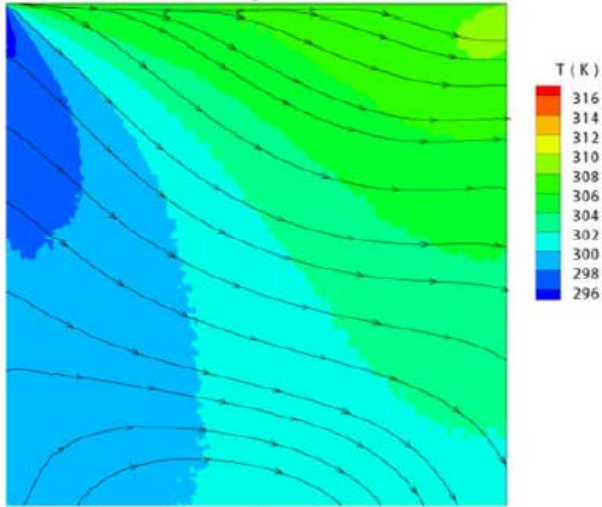
$N_h(v)$ : the number of particles in a histogram bin of width  $\Delta v$

# Another example of exotic prediction: lid-driven cavity 2-D gas flows (no force; DSMC; Kn=0.5)



Lid-driven cavity gases

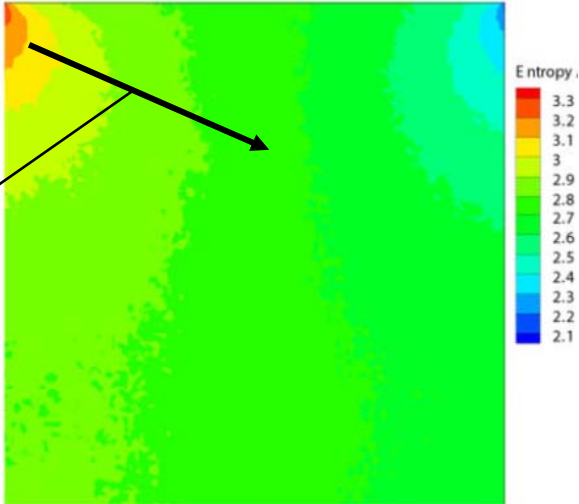
Temperature contours  
(Courtesy of E. Roohi)



**Non-Fourier behavior  
in NCCR**

*H* function contours

Heat transfer from  
**Cold** (center) to **hot**  
in 2-D



## **Part III.**

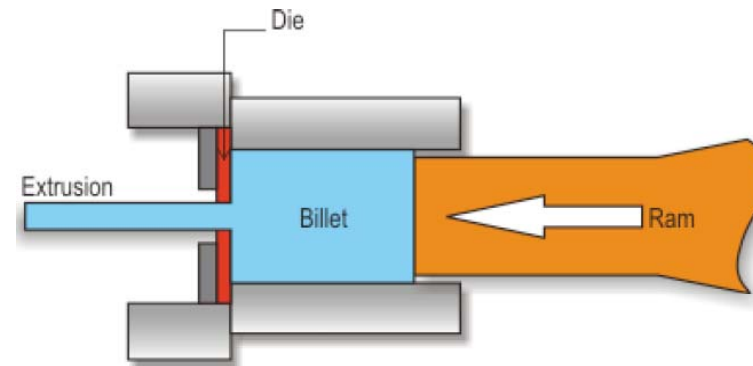
# **New Potential Applications of the Present Framework**

# Loss of convergence of viscoelastic flow solutions in complex fluids (polymer solutions; rheology)

**Viscoelastic** fluids are complex fluids that have “memory” (the state-of-stress depends on the flow history)

**Visco:** friction, irreversibility, loss of memory

**Elastic:** recoil, internal energy storage



**The high-Weissenberg number problem: A 30 year old mystery. ...All methods, without exception, were found to break down at a frustratingly low value of the Weissenberg number around  $We=1$ .**

(R. Fattal, R. Kupferman 2005)

# Analogy of viscoelastic flow and rarefied gases

$$We \equiv \tau / T \sim (l / a) / (L / u) \sim Kn \cdot M \quad \text{vs} \quad N_\delta \equiv \Pi / p \sim Kn \cdot M$$

Upper-convected Maxwell equation  
derived from the stochastic model  
of dumbbells

Nonlinear coupled constitutive  
equation derived from the  
Boltzmann equation

Key observation: almost complete parallel with the gas dynamic  
problem -> on-going topic

# Occurrence of the singularity in the stationary solution of continuum models of carrier transport in semi-conductors

## The mathematic singularity problem in the ballistic regime:

*...Concerning the second effect, the spike is enhanced by a smaller mesh size, which is an indication of the occurrence of some sort of “singularity” in the stationary solution.*

*We remark that such phenomena is not a numerical artifact. Indeed, a similar behavior has been observed with different discretization based on kinetic schemes.*

(A. M. Anile et al. 2000)

## Concluding remarks

- **Pushing the limits of continuum theory:**
  - algebraic nonlinear coupled constitutive relation (NCCR)
  - persistent attack on the key problems—the shock structure problem
  - delicate balancing in juggling terms
- **Going beyond Navier-Stokes-Fourier:**
  - not easy due to no appearance of 1<sup>st</sup> order term
  - nothing taken for granted such as the possibility of heat transfer from cold to hot
- **Applicable to other unsolved issues:** defeating the high Weissenberg number problem in computational rheology and the ballistic transport of carriers in semi-conductors.



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