

# **What Makes Gas Micro Flows So Complicated: Non-classical Physical Laws and their Morphing into Gas-Surface Interaction**

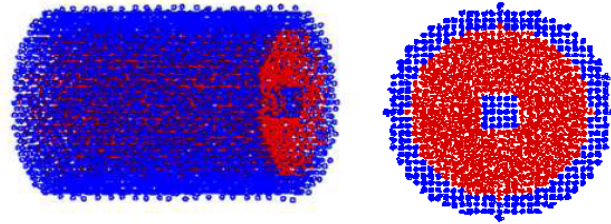
**June 6 Wed, 2012 (8:45-9:30AM)**

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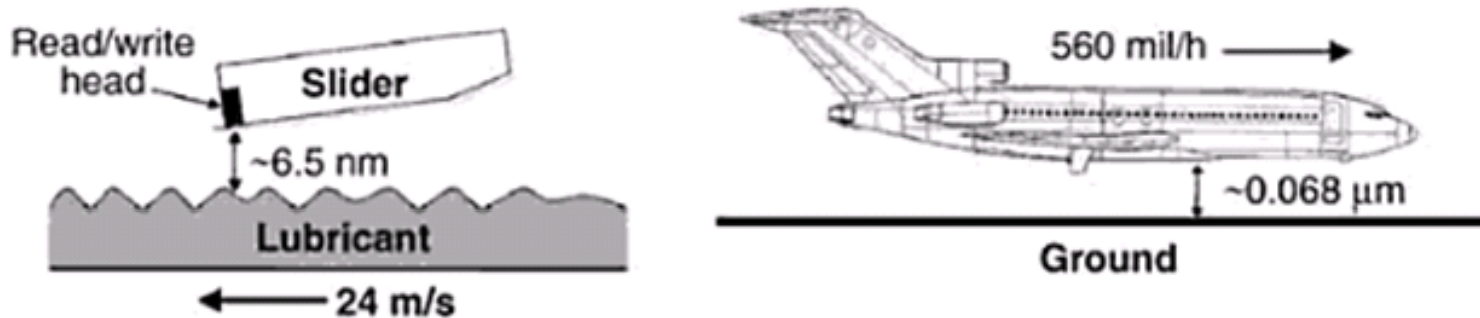
**Presented at 1<sup>st</sup> European Conference on Gas Micro Flows**  
**Skiathos Island, Greece**

**Many thanks to  
organizers of this conference  
(Profs. Colin, Frijns, Valougeorgis)  
for making this opportunity possible.**

# Introduction to gas micro flows



Micro and nanoscale cylindrical flow



Hard disk drive:  $Kn=0.6$ ,  $M=0.7$

## Gas flow in micro/nano devices

Molecular interaction between gas particles and solid atoms  
Velocity shear dominated flows (high  $Kn$ , but relatively low  $M$ )

# Theory and modeling of gas micro flows

## Continuum approach

Chapman-Enskog: Burnett

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

(constitutive equations taking into account  
the microscopic nature of gas  
molecules)

Top-down

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

## Molecular approach

DSMC

Linearized Boltzmann equation

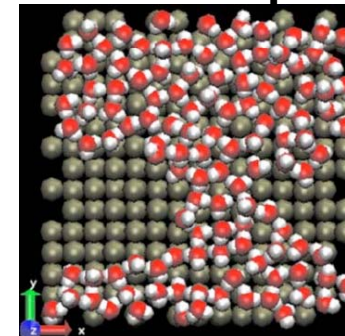
Lattice-Boltzmann method

## Hybrid approach

DSMC-continuum coupling (based on domain decomposition)

Multi-scale method (non-conserved variables calculated by MD)

Bottom-up



# **Research goal of present study**

**Develop a unified computational model for  
rarefied and micro- & nano-scale gases**

**upon which others can build efficient (3-D) CFD  
codes (like state-of-the-art FLUENT package)**

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

# Challenges and emphasis

## Challenges in gas micro flows:

- unknown problem (deviation from classical physics)
- not easily testable (limited information)
- theoretical barrier (G.E. and B.C.)
- cross-disciplines

## Emphasis in this talk:

- clear demonstration of knowns (fully exact analytic approach, focusing on simple problems)
- qualitative over quantitative (putting many abnormal behaviors in proper context, rather than one-time snap-shot agreement)
- sharing failure and struggle (rather than making conclusive)
- verification & validation of computational simulation of gas micro flows

# Scope

**Focusing on (1-D velocity shear dominated) benchmark flows:**

- Couette (generated by moving wall)
- force-driven Poiseuille (pure 1-D)
- pressure-driven Poiseuille (testable)
- verification & validation (V & V)

**Based on published journal papers**

- *Physics of Fluids* (2011)
- *Computers & Fluids* (2011)
- *Int. J. Heat Mass Transfer* (2006; with Lockerby & Reese)
- *Physics of Fluids* (2004)
- *Physics of Fluids* (1999)

**and on-going work** on Couette and pressure-driven Poiseuille flows

## **Part I.**

# **Governing equations and boundary conditions**



# Governing equations

**Assumption:** Non-classical phenomena are related to what happens in bulk flow region and what happens near the solid wall and to their combination.

## Boltzmann equation (1844-1906)

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

$\mathbf{a}$  : force

collision integral

*Differentiating* the statistical definition

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

*with time*

*and then combining*

*with the Boltzmann equation*

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

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

## Moment equation

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

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

shear stress  
tensor

heat flux  
vector

# Derivation of continuum model

Conservation laws (exact) in vector form

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

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

$$\boldsymbol{\psi}^{(\Pi)} \equiv \langle m[\mathbf{cc}]^{(2)} \mathbf{cf} \rangle$$

Constitutive equation (exact) in vector form

$$\boldsymbol{\Lambda}^{(\Pi)} \equiv \langle m[\mathbf{cc}]^{(2)} C[f, f_2] \rangle = -\frac{\mathbf{\Pi}}{\eta/p} q(\mathbf{\Pi}, \mathbf{Q}, \dots)$$

$\frac{\partial \mathbf{\Pi}}{\partial t} + \mathbf{u} \cdot \nabla \mathbf{\Pi} = -\nabla \cdot \boldsymbol{\psi}^{(\Pi)} - 2[\mathbf{\Pi} \cdot \nabla \mathbf{u}]^{(2)} - 2p[\nabla \mathbf{u}]^{(2)} + \boldsymbol{\Lambda}^{(\Pi)}$					
<b>Unsteady</b>	<b>Convection</b>	<b>Higher-order</b>	<b>Kinematic</b>	<b>Thermo. driving</b>	<b>Dissipation</b>

Key observations:

- NSF limit dictated by  $\frac{2[\mathbf{\Pi} \cdot \nabla \mathbf{u}]^{(2)}}{2p[\nabla \mathbf{u}]^{(2)}} \sim \frac{\mathbf{\Pi}}{p} \sim Kn \cdot M \sim \frac{M^2}{Re}$ ; Euler if  $|\nabla \cdot \mathbf{\Pi}| < |\nabla \cdot p\mathbf{I}|$  or  $|\nabla \cdot \rho\mathbf{u}\mathbf{u}|$
- NSF limit recovered from the last two terms and a relaxation (BGK) approximation  $q(\mathbf{\Pi}, \mathbf{Q}, \dots) \approx 1$

$$0 = \text{small} - 2p[\nabla \mathbf{u}]^{(2)} - \frac{\mathbf{\Pi}}{\eta/p} 1 \Rightarrow \mathbf{\Pi} = -2\eta[\nabla \mathbf{u}]^{(2)}$$

# Derivation of algebraic constitutive relations

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

Original Grad closure  $\langle mccc \rangle = \frac{2}{5} \left( \left\langle \frac{1}{2} mc^2 \mathbf{c} \right\rangle_i \delta_{jk} + \left\langle \frac{1}{2} mc^2 \mathbf{c} \right\rangle_j \delta_{ik} + \left\langle \frac{1}{2} mc^2 \mathbf{c} \right\rangle_k \delta_{ij} \right)$  and  $q(\Pi, \mathbf{Q}, \dots) \approx 1$

$$\frac{\partial \Pi}{\partial t} + \mathbf{u} \cdot \nabla \Pi = -\frac{2}{5} [\nabla \mathbf{Q}]^{(2)} - 2[\Pi \cdot \nabla \mathbf{u}]^{(2)} - 2p[\nabla \mathbf{u}]^{(2)} - \frac{\Pi}{\eta/p} 1$$

~~$\frac{\partial \Pi}{\partial t}$~~   ~~$\mathbf{u} \cdot \nabla \Pi$~~   ~~$\frac{2}{5} [\nabla \mathbf{Q}]^{(2)}$~~   ~~$2[\Pi \cdot \nabla \mathbf{u}]^{(2)}$~~   ~~$2p[\nabla \mathbf{u}]^{(2)}$~~   ~~$\frac{\Pi}{\eta/p} 1$~~

steady no convective in velocity-shear yielding partial differential type!

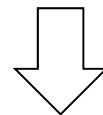
$$u \frac{\partial}{\partial x} + \frac{\partial}{\partial y}$$

New closure  $|\nabla \cdot \Psi^{(\Pi)}| < 2|[\Pi \cdot \nabla \mathbf{u}]^{(2)}|$  and  $q(\Pi, \mathbf{Q}, \dots) = \frac{\sinh \kappa}{\kappa}$  where  $\kappa \sim \left( \frac{\Pi : \Pi}{2\eta} + \frac{\mathbf{Q} \cdot \mathbf{Q}}{kT} \right)^{1/2}$

$$\frac{\partial \Pi}{\partial t} + \mathbf{u} \cdot \nabla \Pi = \text{small} - 2[\Pi \cdot \nabla \mathbf{u}]^{(2)} - 2p[\nabla \mathbf{u}]^{(2)} - \frac{\Pi}{\eta/p} q(\Pi, \mathbf{Q}, \dots)$$

~~$\frac{\partial \Pi}{\partial t}$~~   ~~$\mathbf{u} \cdot \nabla \Pi$~~  ~~small~~  ~~$2[\Pi \cdot \nabla \mathbf{u}]^{(2)}$~~   ~~$2p[\nabla \mathbf{u}]^{(2)}$~~   ~~$\frac{\Pi}{\eta/p} q(\Pi, \mathbf{Q}, \dots)$~~

yielding algebraic type!



Interesting non-classical physical laws

can be identified!

# Linear uncoupled Navier-Fourier equations: classical physical laws

**Navier (1822)**      $\Pi = -\eta[\nabla\mathbf{u}]^{(2)}$

**Fourier (1822)**      $\mathbf{Q} = -k\nabla T$

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

$u_x$  case (compression and expansion)

$$-2\eta(T) \begin{bmatrix} 2u_x/3 & 0 \\ 0 & -u_x/3 \end{bmatrix} \quad \text{Newtonian or linear}$$

Not like  $(u_x)^2$

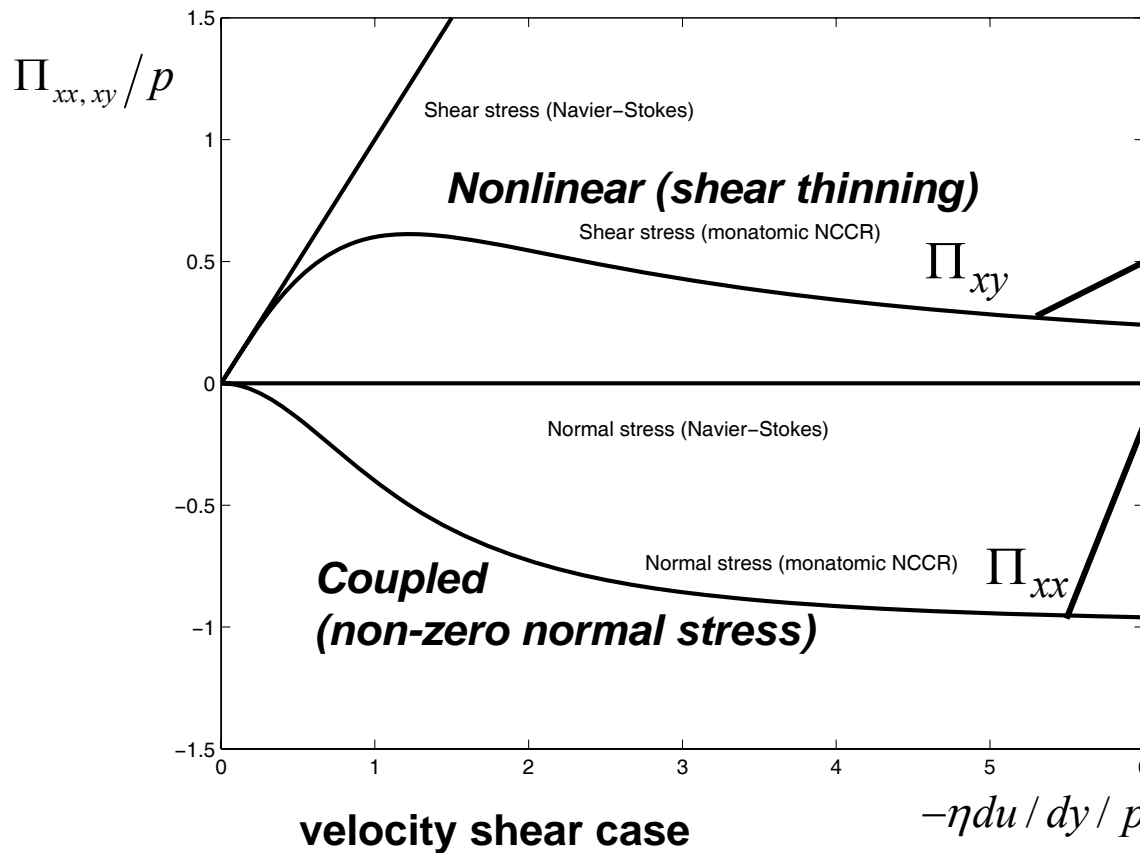
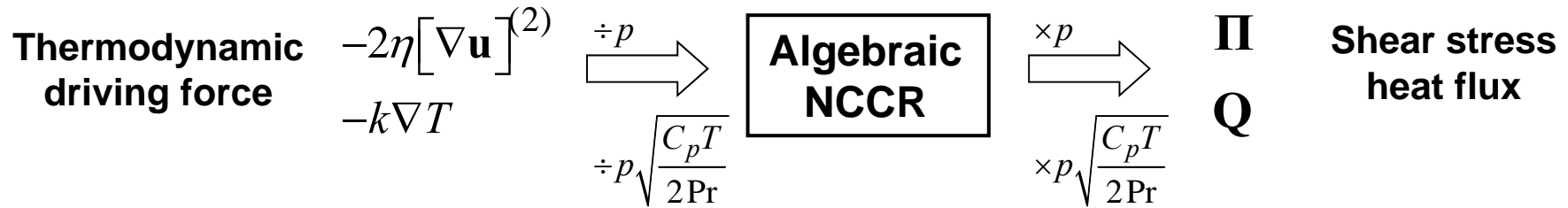
$u_y$  case (velocity shear only)

$$-2\eta(T) \begin{bmatrix} 0 & u_y/2 \\ u_y/2 & 0 \end{bmatrix} \quad \text{Uncoupled}$$

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

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

# Non-classical laws embodied in nonlinear coupled constitutive relations (NCCR)



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

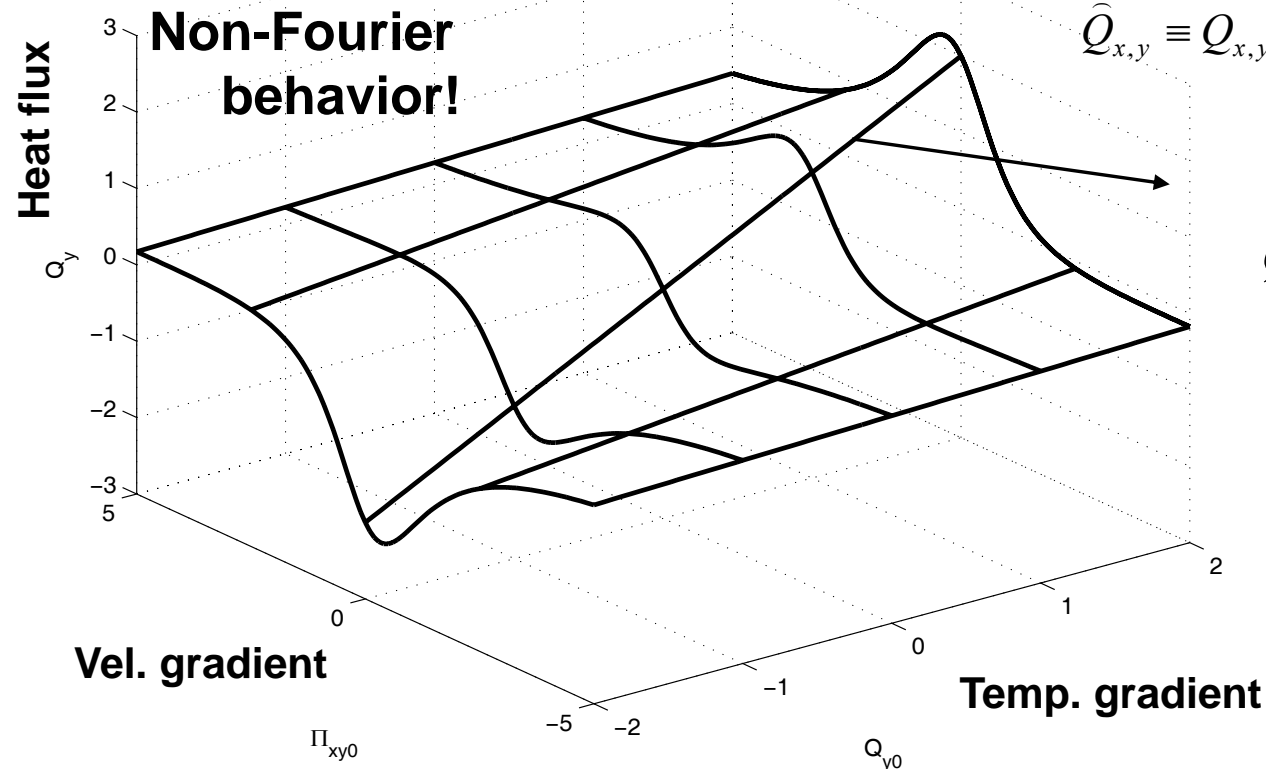
**kinematic stress constraint!**

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

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

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

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

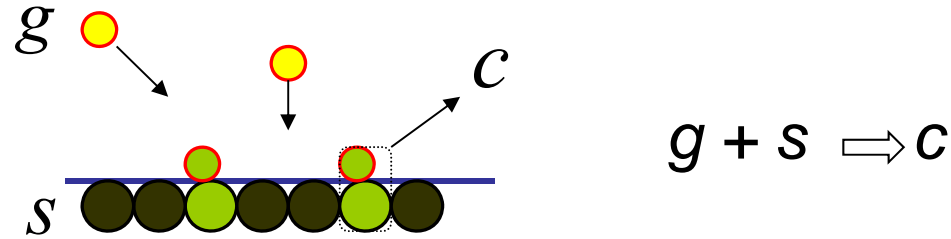


# Slip/jump models (boundary conditions)

General comments:

- B.C. should describe the molecular interaction of the gas particles with the solid surface atoms, involving the kinetic theory of gases and solid state physics.
- Boltzmann equation based on collision of gas particles only may not be valid.
- Concept based on gaseous adsorption may give a hint for parameters governing the gas-surface atom molecular interaction. Also, surface diffusion can be built from adsorption.
- We may have to live with simple B.C. such as Maxwell model in case of continuum-based computational models.

# Langmuir slip model based on gaseous adsorption isotherm (*PoF 2004*)



Condense on the surface, being held by the field of force of the surface atoms, and subsequently evaporate from the surface  
 $\Rightarrow$  time lag  $\Rightarrow$  adsorption  $\Rightarrow$  slip and jump

$N$  : number of sites ( $s$ ) interacting with gas molecules ( $m$ )

$N\alpha$  : number of sites which are covered

Then the equilibrium constant  $K$  becomes

$$K = \frac{C_c}{C_m C_s} = \frac{N\alpha}{[p / k_B T_w] N(1-\alpha)}, \quad \text{that is, } \alpha = \frac{\beta p}{1 + \beta p} \quad \text{where } \beta = \frac{K}{k_B T_w}.$$



# Heat of adsorption vs accommodation coeff.

## Langmuir model (Dirichlet type)

$$u = \alpha u_w + (1 - \alpha)u_r, \alpha = \frac{p/4\omega Kn}{1 + p/4\omega Kn}$$

$$\omega = \omega_0(\nu) \left( \frac{T_w}{T_r} \right)^{1+2/(\nu-1)} \exp\left( -\frac{D_e}{k_B T_w} \right) = fn(\nu, T_w, D_e)$$

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

## Maxwell model (Neumann type)

$$u = u_w + \omega_M \ell \left( \frac{\partial u}{\partial n} \right)_w, \omega_M \equiv \frac{2 - \sigma_v}{\sigma_v}; \text{slip (accommodation) coeff.}$$

## Assignment of physical meaning to accommodation coeff.

An equivalence relation can be proved by solving pressure-driven gas flow in a microchannel with two slip models

$$\frac{2 - \sigma_v}{\sigma_v} \sim \omega = \omega_0(\nu) \left( \frac{T_w}{T_r} \right)^{1+2/(\nu-1)} \exp\left( -\frac{D_e}{k_B T_{wr}} \right)$$

## **Morphing of NCCR into B.C.**

### **Troubles found during the implementation**

- how to determine reference velocity in the Langmuir model

$$u = \alpha u_w + (1 - \alpha) u_r$$

- not successful in showing the velocity gradient singularity (identified by Lilley *PRE 2007*) in Couette flow by NCCR and B.C. (Maxwell & Langmuir)

### **Morphing of nonlinearity and coupling (of NCCR) into B.C.**

- back to the original concept of Maxwell model (degree of slip proportional to the degree of non-equilibrium near the wall)

# Morphing of NCCR into B.C.: Nonlinear coupled Maxwell model

## Conventional linear velocity slip and temperature jump models

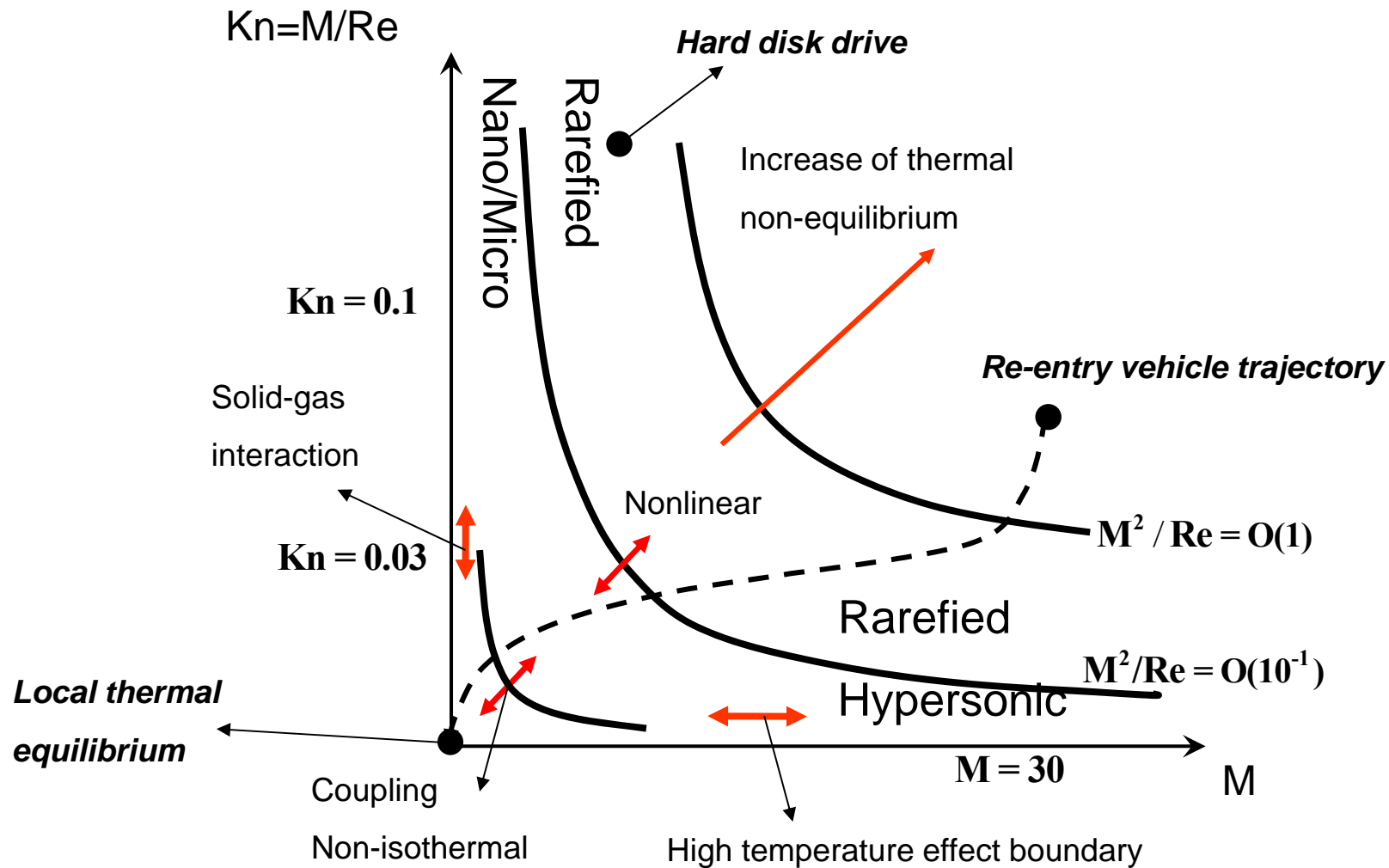
$$u(h/2) = V + \sigma_V l \cdot \left. \left( - \frac{\partial u}{\partial y} \right) \right]_{h/2} - \frac{3}{4} \frac{\eta}{\rho T} \left. \frac{\partial T}{\partial x} \right]_{h/2}, \quad T(h/2) = T_w + \sigma_T l \cdot \left. \left( - \frac{\partial T}{\partial y} \right) \right]_{h/2}$$

## Nonlinear coupled velocity slip and temperature jump models

$$u(h/2) = V + \sigma_V l \left. \frac{\Pi}{\eta} \right]_{h/2} + \frac{3}{4} \frac{(\gamma - 1)}{\gamma / \text{Pr}} \left. \frac{Q_x}{p} \right]_{h/2}, \quad T(h/2) = T_w + \sigma_T l \left. \frac{Q_y}{k} \right]_{h/2}$$

- Non-Navier-Stokes shear thinning behavior morphs into shear stress
- Non-Fourier law morphs into heat flux
- Morphing of NCCR (tangential heat flux generated by velocity shear) into velocity slip
- Capable of describing the velocity gradient singularity

# Summary of G.E. and B.C. (I)



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

Two terms: Kn

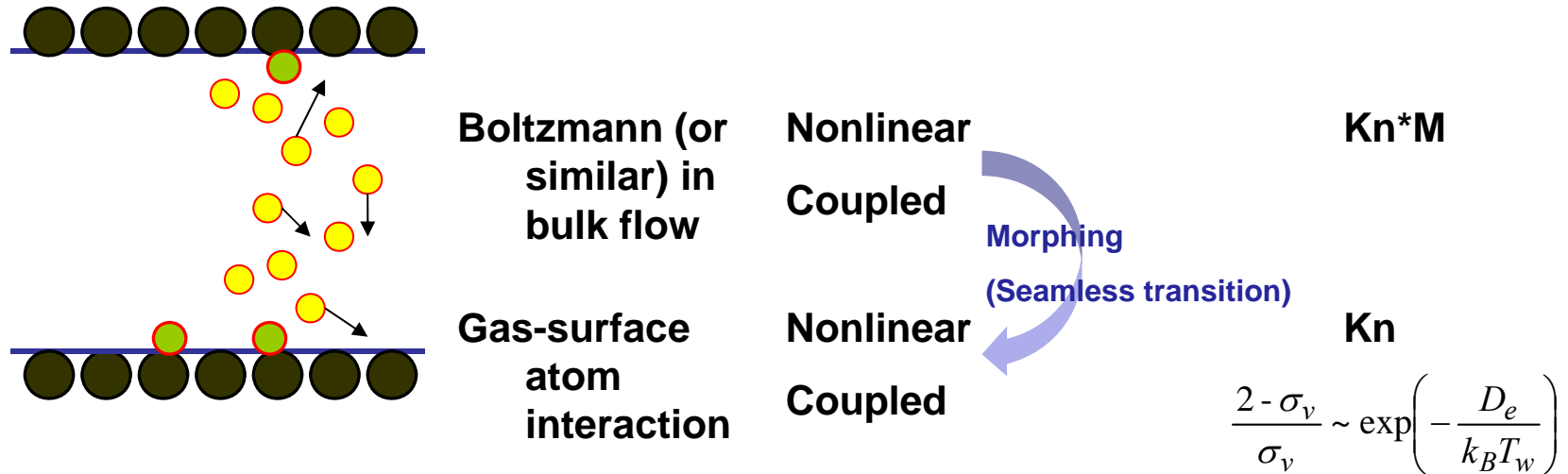
$$\rho \mathbf{u} \cdot \nabla \mathbf{u} + \nabla \cdot p \mathbf{I} + \nabla \cdot \Pi = 0$$

Three terms: M, Kn



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

## Summary of G.E. and B.C. (II)



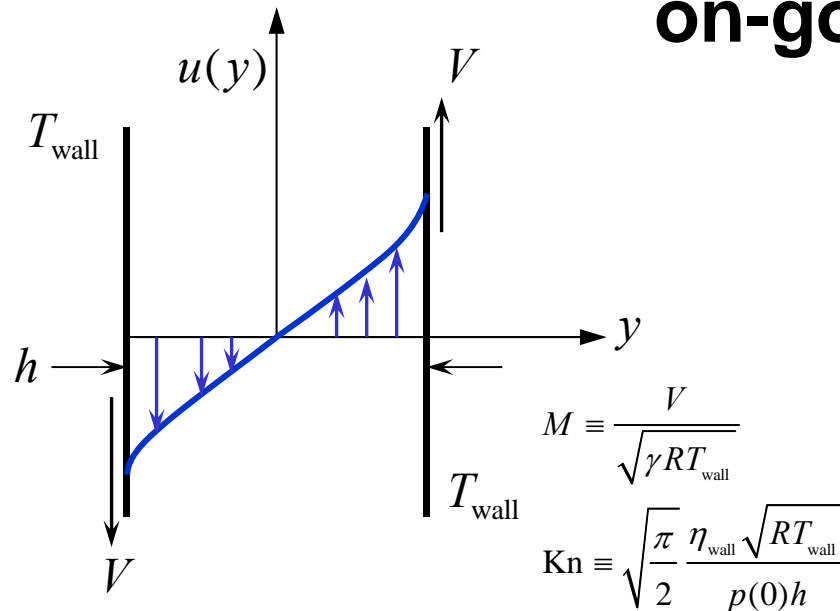
Combination of two nonlinearities and two couplings—nonlinear coupled constitutive relation for bulk flow and nonlinear coupled boundary conditions at the wall—may be critical within the continuum framework.

There may exist many cases in how to combine them, making qualitative & many-facets agreement more difficult.

**Part II.**

**Couette flow**

# Gaseous Couette flow (*Comp. Fluids 2011* and on-going)



$$\frac{d}{dy} \begin{bmatrix} \Pi_{xy} \\ p + \Pi_{yy} \\ \Pi_{xy}u + Q_y \end{bmatrix} = \begin{bmatrix} 0 \\ 0 \\ 0 \end{bmatrix}$$

with

$$(\Pi_{xy,xx}, Q_{x,y}) = \text{fn} \left( -\eta \frac{du}{dy}, -k \frac{dT}{dy} \right)$$

nonlinear & coupled

## Non-classical behaviors (well-understood parts)

- nonlinear velocity profile (non-isothermal)
- non-zero tangential heat flux and normal shear stress (coupling)
- small shear stress (shear thinning)

## However, unsolved problems persist (within continuum framework)

- velocity gradient singularity (power law identified from DSMC)
- smaller slip (or larger velocity slope)
- exact role of non-isothermal physics

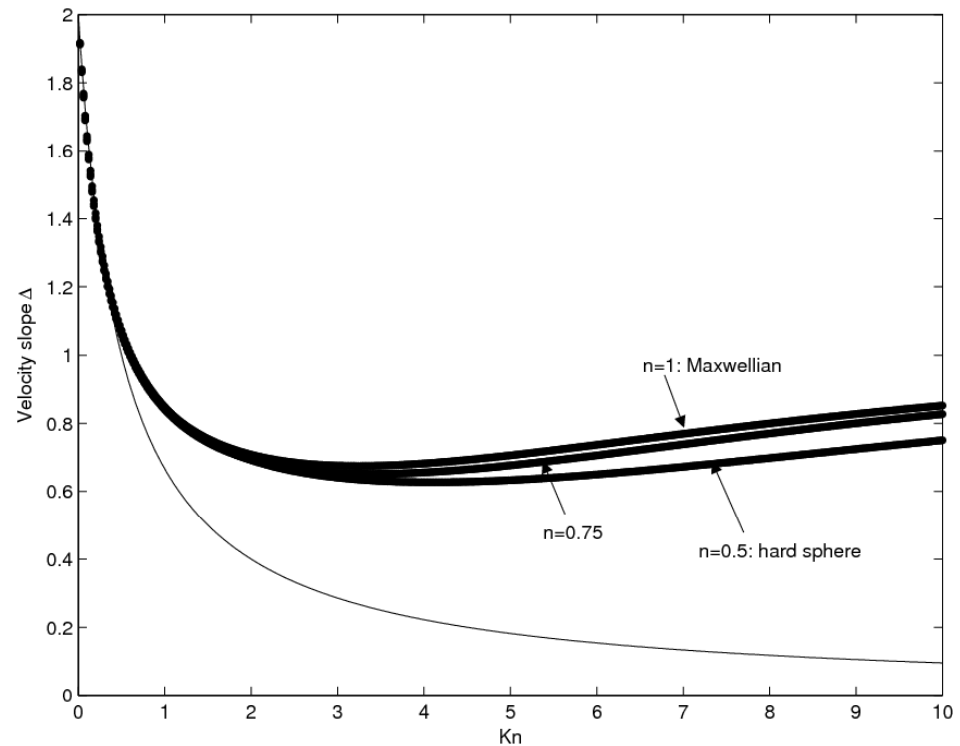
# NCCR + nonlinear Maxwell

## With NCCR + linear Maxwell

- capable of describing non-zero tangential heat flux and normal shear stress
- but not able to describe the velocity gradient singularity in the Knudsen layer

## With NCCR + nonlinear (coupled) Maxwell

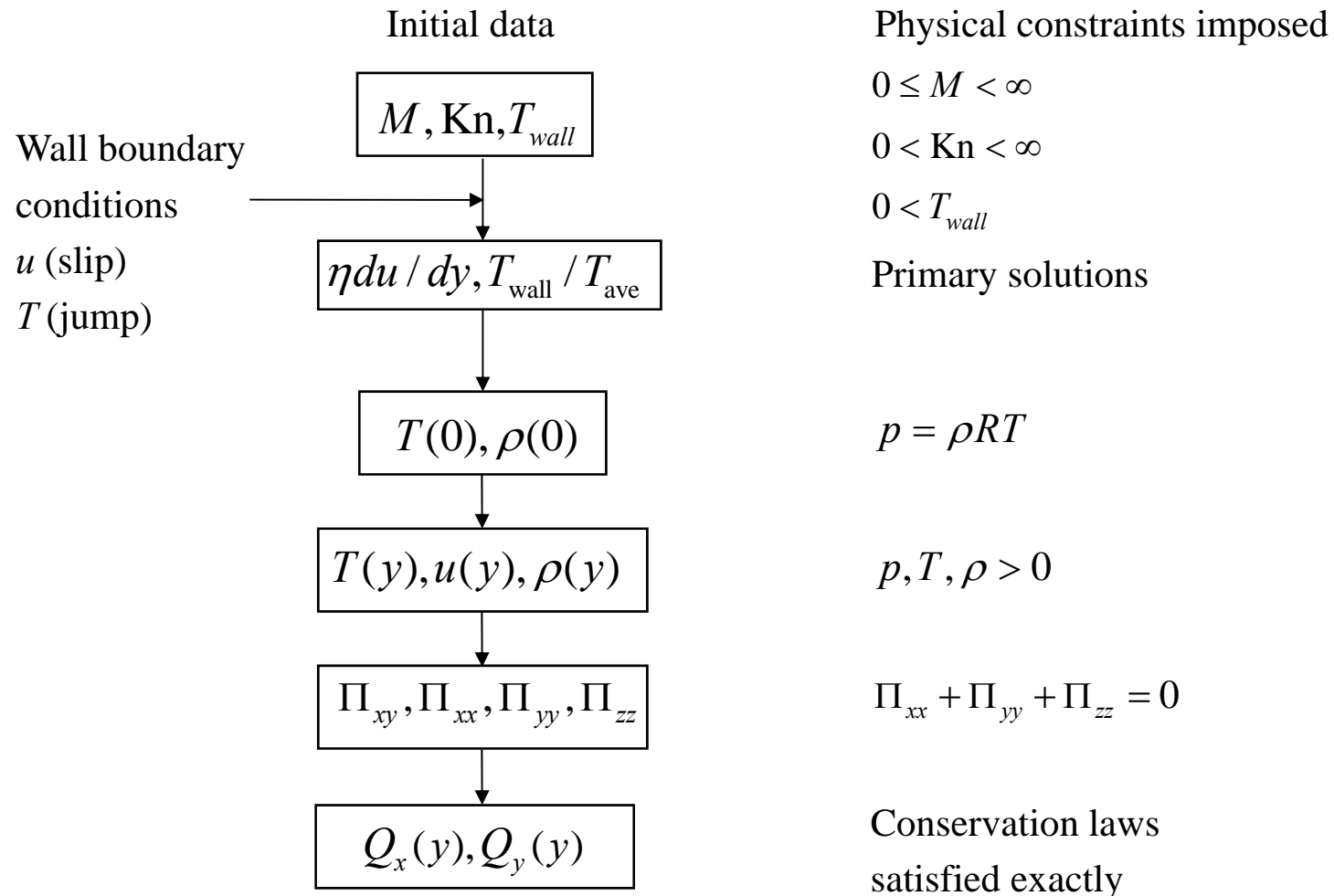
- capable of explaining the origin of the velocity gradient singularity
- at the same time being able to describe all other abnormal behaviors in qualitative agreement with DSMC



$$u(h/2) = V + \sigma_v l \cdot \left[ \frac{\Pi}{\eta} \right]_{h/2} + \frac{3(\gamma-1)}{4} \left[ \frac{Q_x}{\gamma/Pr \cdot p} \right]_{h/2}$$



# Summary of Part II: Well-posedness of Couette flow

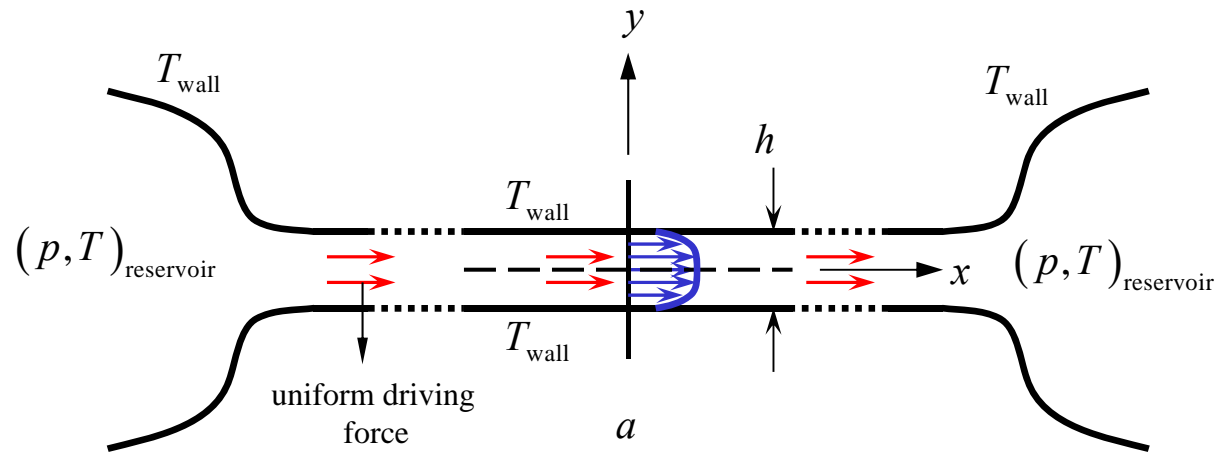


**Note:**  $T(0)$  itself is the part of solution. Without it, the analysis remains incomplete. (For example, Marques et al. 2001 in *Contin. Mech. Thermo.*)

## **Part III.**

**Force-driven and  
pressure-driven  
Poiseuille  
(monatomic)  
gas flows**

# 1-D force-driven compressible Poiseuille gas flow



$$\frac{d}{dy} \begin{bmatrix} \Pi_{xy} \\ p + \Pi_{yy} \\ \Pi_{xy}u + Q_y \end{bmatrix} = \begin{bmatrix} \rho a \\ 0 \\ \rho au \end{bmatrix}$$

with

$$(\Pi_{xy,xx}, Q_{x,y}) = \text{fn} \left( -\eta \frac{du}{dy}, -k \frac{dT}{dy} \right)$$

nonlinear & coupled

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

## Non-classical behaviors (easy parts)

- central temperature minimum  $\hat{Q}_y = \frac{3}{(3 + 2\hat{\Pi}_{xy,NSF}^2)} (\hat{Q}_{y_0} + \hat{a}\hat{\Pi}_{xy,NSF})$
- non-zero tangential heat flux and normal shear stress

## However, difficult parts (within continuum framework)

- concave cross-stream pressure distribution with central temp. minimum
- correct cross-stream density distribution
- exact role of non-isothermal physics (for example, Knudsen minimum in mass flow rate)

# Exact analytic solutions (with only one assumption $|\nabla \cdot \psi^{(\Pi)}| < 2|[\Pi \cdot \nabla \mathbf{u}]^{(2)}|$ : *PoF 2011*)

## Rigorous treatment of thermal property through

$$\text{Average quantities } u_r = \frac{2}{h} \int_0^{h/2} u dy, \quad T_r = \frac{h/2}{\int_0^{h/2} T^{-1} dy}$$

A new (temperature scaled) variable  $T^* ds^* = dy^*$  and auxiliary relations

$$s^* \left( y^* = \frac{1}{2} \right) = \frac{1}{2}, \quad \int_0^{1/2} u^* T^* ds^* = \frac{1}{2}, \quad \int_0^{1/2} T^* ds^* = \frac{1}{2}$$

## Analytic form of concave pressure distribution

$$\frac{d}{dy} (p + \Pi_{yy}) = 0, \quad \frac{d\Pi_{xy}}{dy} = \rho a, \quad p = \rho RT \quad \text{and} \quad \Pi_{xy}^2 = -\frac{3}{2} (p + \Pi_{yy}) \Pi_{yy}$$

$$\Rightarrow p^* = 1 + \tan^2 \left( \sqrt{\frac{2}{3}} \varepsilon_{h_w} T_w^* s^* \right), \quad \Pi_{yy}^* = -\frac{1}{N_\delta} \tan^2 \left( \sqrt{\frac{2}{3}} \varepsilon_{h_w} T_w^* s^* \right),$$

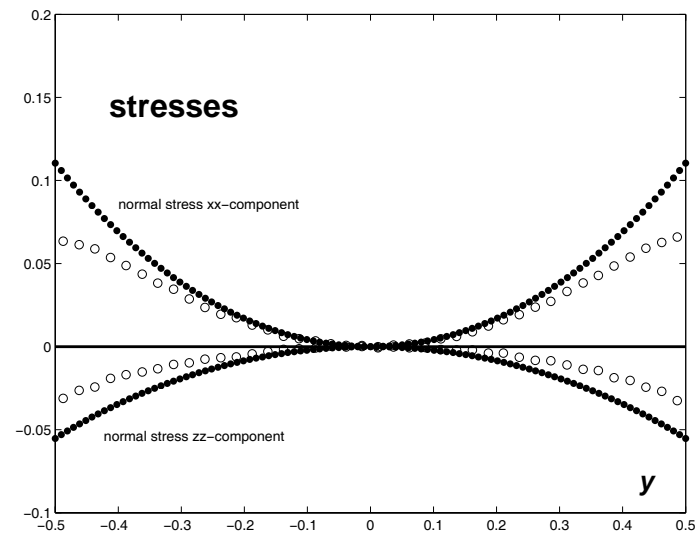
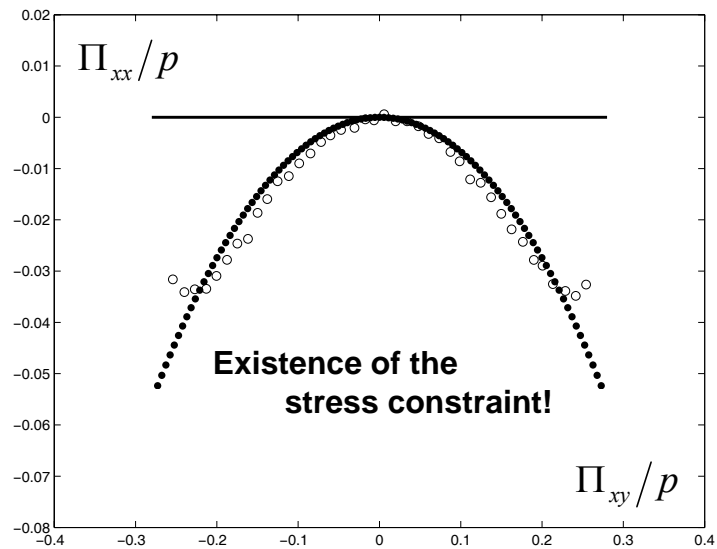
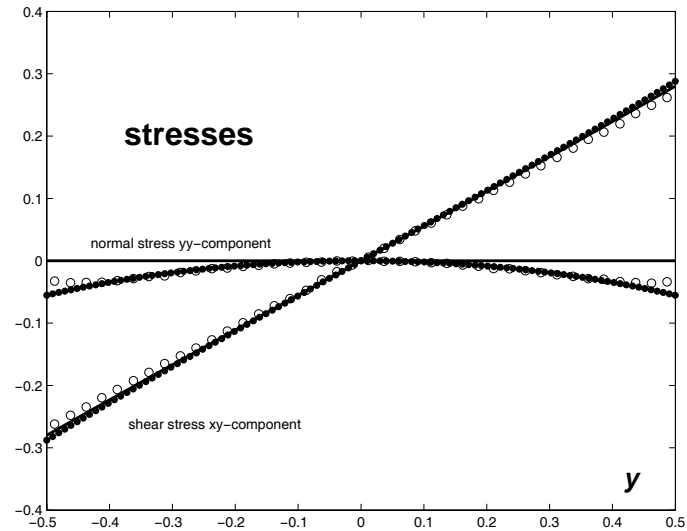
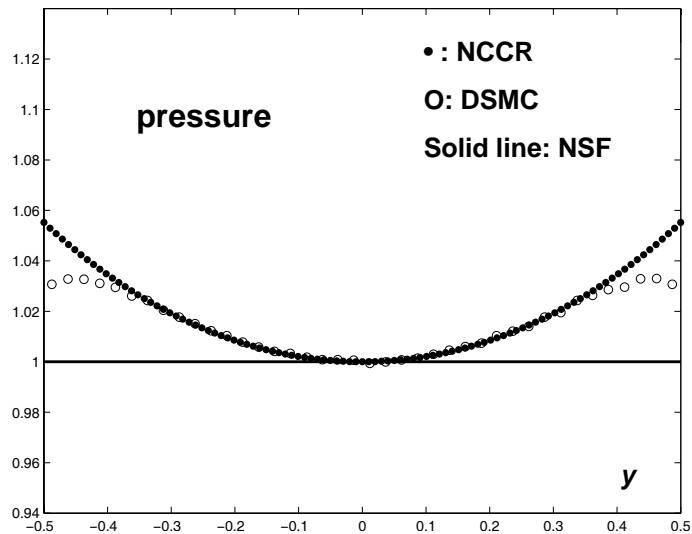
$$\Pi_{xy}^* = \frac{1}{N_\delta} \sqrt{\frac{3}{2}} \tan \left( \sqrt{\frac{2}{3}} \varepsilon_{h_w} T_w^* s^* \right)$$

**Very surprising *tangent* profile!**

**Pressure *more fundamental* (than velocity, temperature)!**

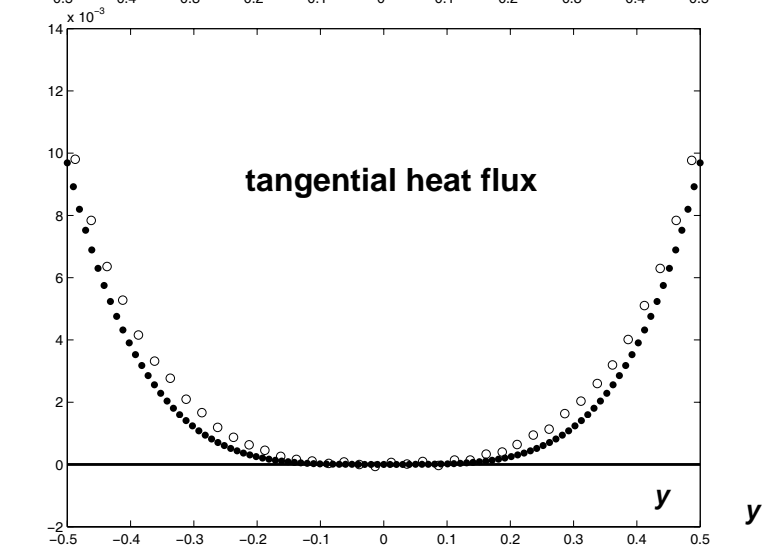
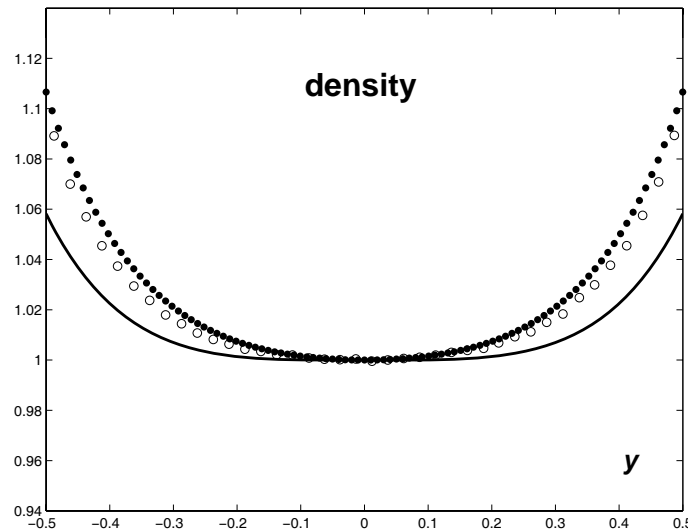
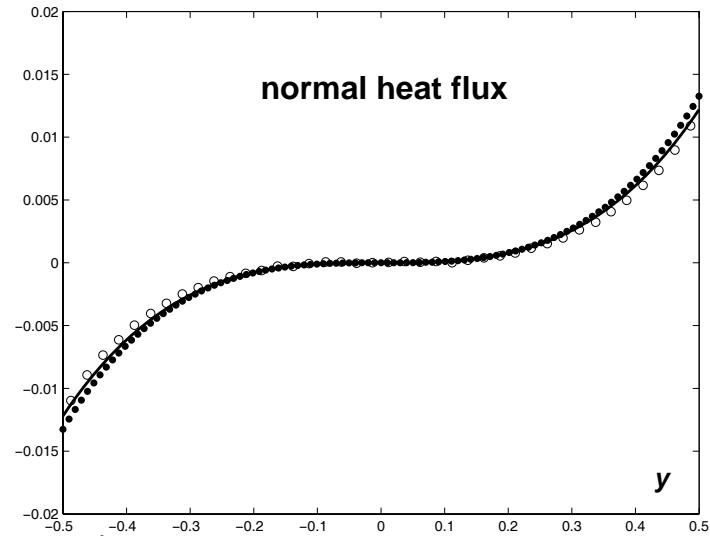
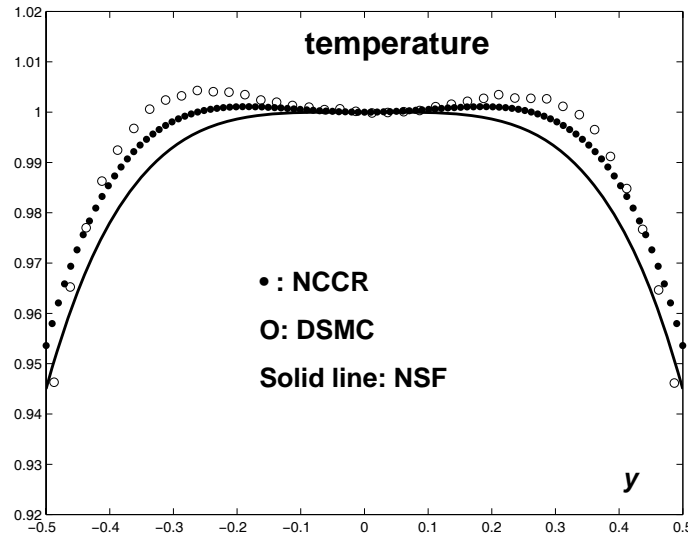
# Exact analytic solutions: stresses

Qualitative agreement with DSMC ( $\varepsilon_{h_{\text{wall}}} = 0.6$ ,  $\text{Kn}=0.1$ )



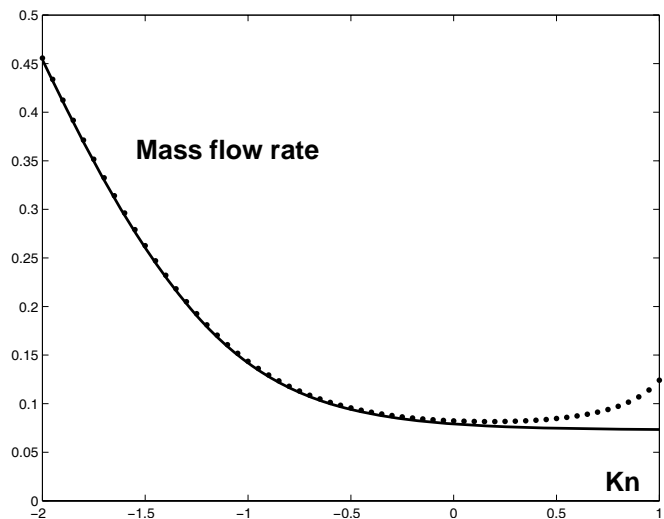
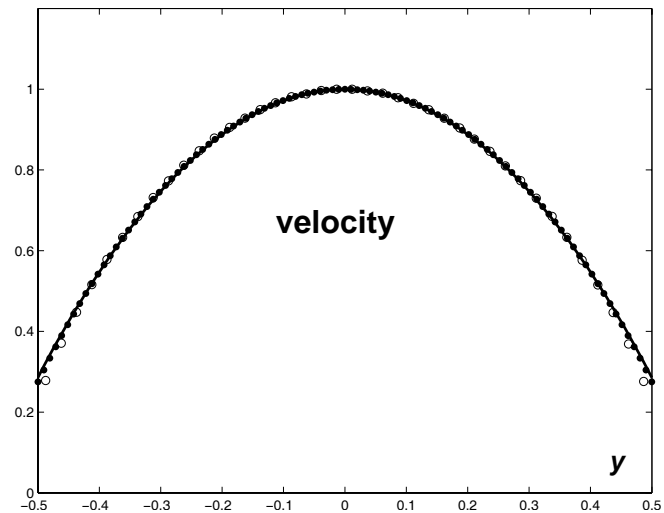
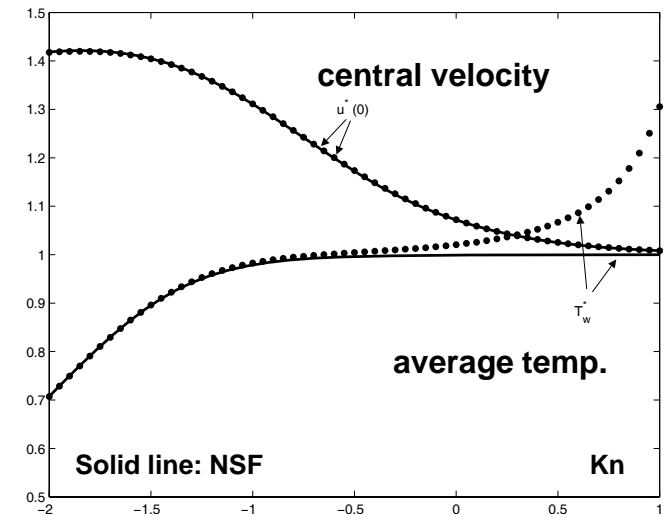
# Exact analytic solutions: temp., density, heat fluxes

After applying the Langmuir slip/jump model



# Exact analytic solutions: Knudsen minimum

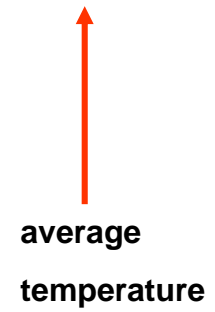
Capturing all the qualitative features predicted by the DSMC and providing insights DSMC can not !



$$\frac{\dot{m}/2h}{\rho_r \sqrt{\gamma RT_w}} \equiv \frac{\int_0^{h/2} \rho u dy}{2\sqrt{\gamma RT_w} \int_0^{h/2} \rho dy}$$

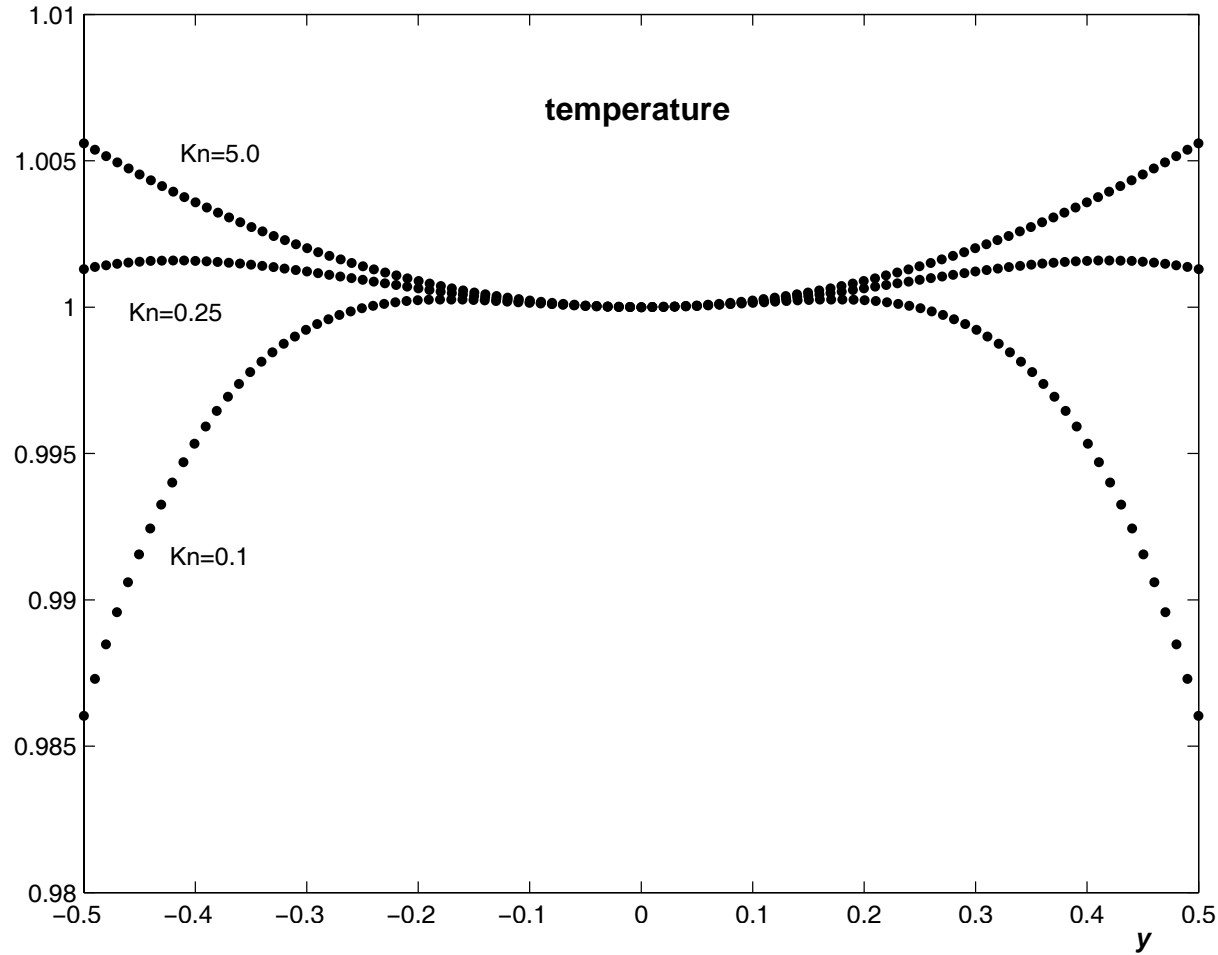
$$= \frac{\sqrt{\pi}}{16\sqrt{2\gamma}} \frac{\varepsilon_{h_w}}{\text{Kn}} \left( \frac{1 - \frac{1/4\omega\text{Kn}}{3(1+1/4\omega\text{Kn})}}{1 + 1/4\omega\text{Kn}} \right) \frac{1}{u^*(0)} \left( \frac{\tan S_{1/2}^*}{2S_{1/2}^*} \right)^2 \left( \frac{T_w}{T_{ave}} \right)^2$$

Responsible for Knudsen minimum !



slip      central velocity      Stress constraint

# What happened here: Knudsen minimum



$$\frac{\dot{m}/2h}{\rho_r \sqrt{\gamma R T_w}} \sim \left( \frac{T_w}{T_{ave}} \right)^2$$

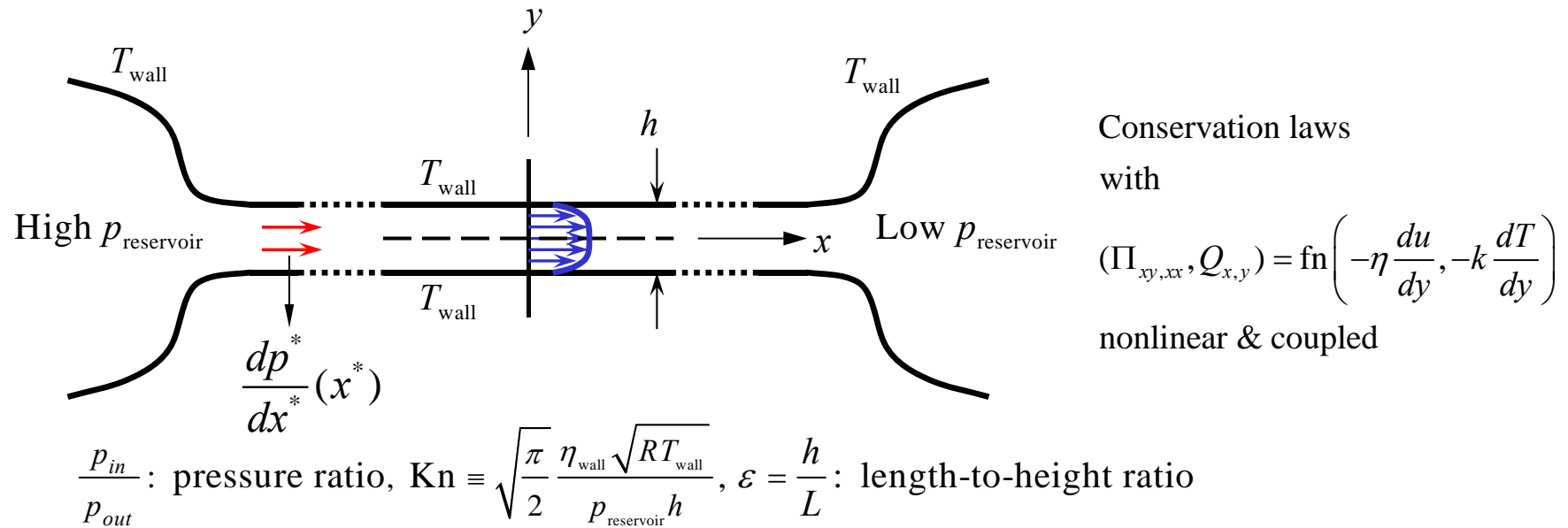
average  
temperature



Responsible for  
Knudsen  
minimum !



# Pressure-driven compressible Poiseuille gas flow



## Easy (or already-done) parts

- the benchmark problem most studied in the past
- experimental data available (but, mass flow rate and stream-wise pressure distribution only)

## Difficult parts

- overall flowfields physics remain illusive (for example, concave or convex cross-stream pressure distribution)
- how subtle the effect of channel length-to-height ratio is
- exact role of non-isothermal physics (in particular, high Knudsen flows)

# Exact analytic solutions (on-going work)

Analytic form of sectional pressure distribution and effect of length-to-height ratio on the mass flow rate

$$\frac{p^*(y^*)}{p_m^*} = 1 + \tan^2 \left( \sqrt{\frac{2}{3}} \frac{h}{L} \frac{d(-\ln p_m^*)}{dx^*} y^* \right) \quad \text{concave (tangent-type)}$$

$$\dot{m} \frac{24\eta LRT}{H^3 p_{m_L}^2} = \frac{d(-\ln p_m^*)}{dx^*} \left( \frac{\tan S_{1/2_L}^*}{S_{1/2_L}^*} \right)^3 = \frac{d(-\ln p_m^*)}{dx^*} \left( 1 + S_{1/2_L}^{*2} + \dots \right)$$

$$\text{where } S_{1/2_L}^* \equiv \sqrt{\frac{2}{3}} \frac{h}{L} \frac{d(-\ln p_m^*)}{dx^*} \frac{1}{2}$$

**Non-classical term  
related to the stress  
constraint**

## Summary of Part III

In contrast with Couette flow, the boundary condition seems to remain secondary in case of the force (or pressure) driven Poiseuille flows.

In the force-driven flow, non-isothermal effect has a definite role in high Knudsen flows. For example, the change of temperature profile (measured by the average temperature) is responsible for the Knudsen minimum.

The concave cross-stream pressure distribution is due to the non-classical stress constraint.

Further experimental study on cross-stream pressure distribution and temperature flowfield is strongly recommended.

## **Part IV.**

**Diatomic gas  
and  
verification  
and validation  
(V & V)**

# Diatomic gas case

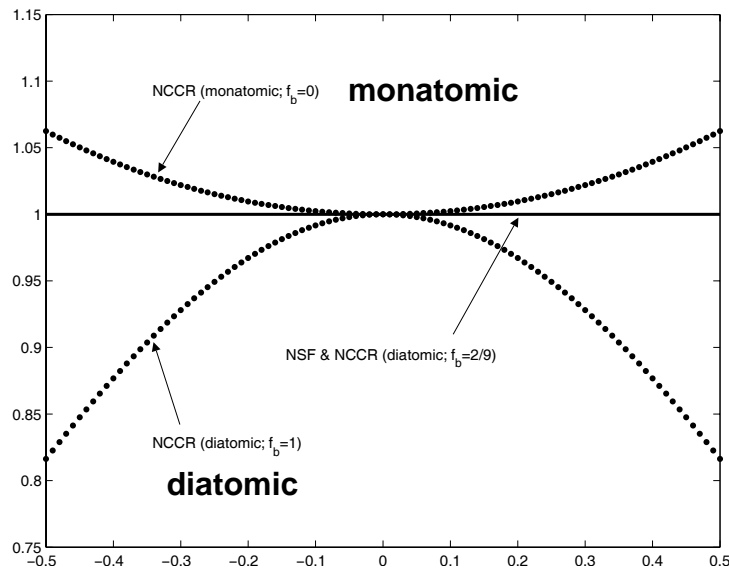
Surprisingly, there is even **no consensus** what the proper master kinetic equations would be for describing **diatomic gases** like nitrogen in thermal non-equilibrium.

A proposed master equation: **Boltzmann-Curtiss equation** with a moment of inertia  $I$  and an angular momentum  $\mathbf{j}$

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

$\Delta$ : excess normal stress

$$\frac{\partial \mathbf{\Pi}}{\partial t} + \mathbf{u} \cdot \nabla \mathbf{\Pi} = \text{small} - 2[\mathbf{\Pi} \cdot \nabla \mathbf{u}]^{(2)} - 2(p + \Delta)[\nabla \mathbf{u}]^{(2)} - \frac{\mathbf{\Pi}}{\eta/p} q(\mathbf{\Pi}, \mathbf{Q}, \Delta, \dots)$$



Pressure profile across channel

$$p^* = 1 - \tanh^2 \left( \sqrt{\frac{7}{2}} \varepsilon_{h_w} T_w^* s^* \right)$$

**Convex hyperbolic tangent profile! (PoF 2011)**

# Why $V$ & $V$ in gas micro flows are difficult?

Too many computational models (governing equation, boundary condition)

Cf. Only one in near-equilibrium: Linear uncoupled NSF + no-slip

DSMC is not immune since it is also highly subject to the boundary condition and post-processing employed.

Lack of experimental data (how to measure exotic properties such as temperature jump?)

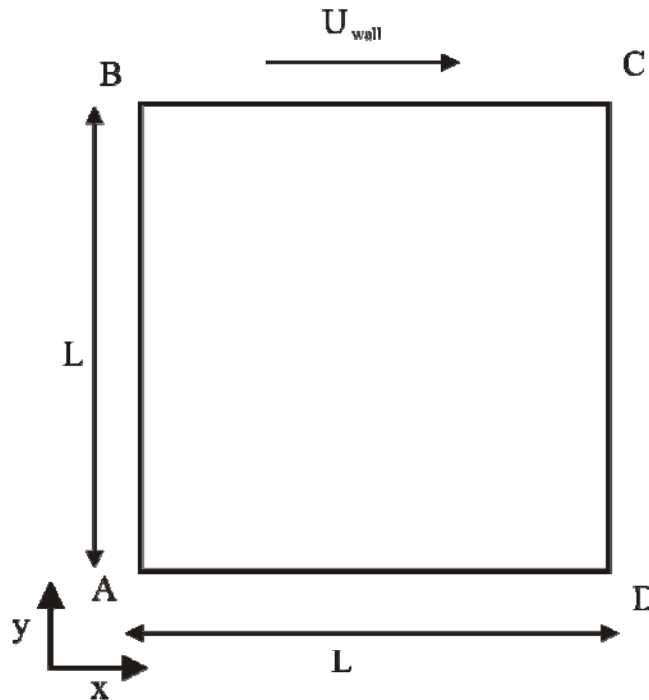
Lack of theories:

- no consensus what the proper master kinetic equations would be for describing diatomic gases like simple nitrogen in thermal non-equilibrium
- no rigorous gas-surface molecular interaction theory

# Microscopic sampling vs macroscopic

DSMC solutions of the two-dimensional *lid-driven cavity* gas flow are considered ( $Kn=0.1$ ).

The exact values of slip velocity and temperature jump in the DSMC method are *prone* to how these properties are obtained from the simulation results.

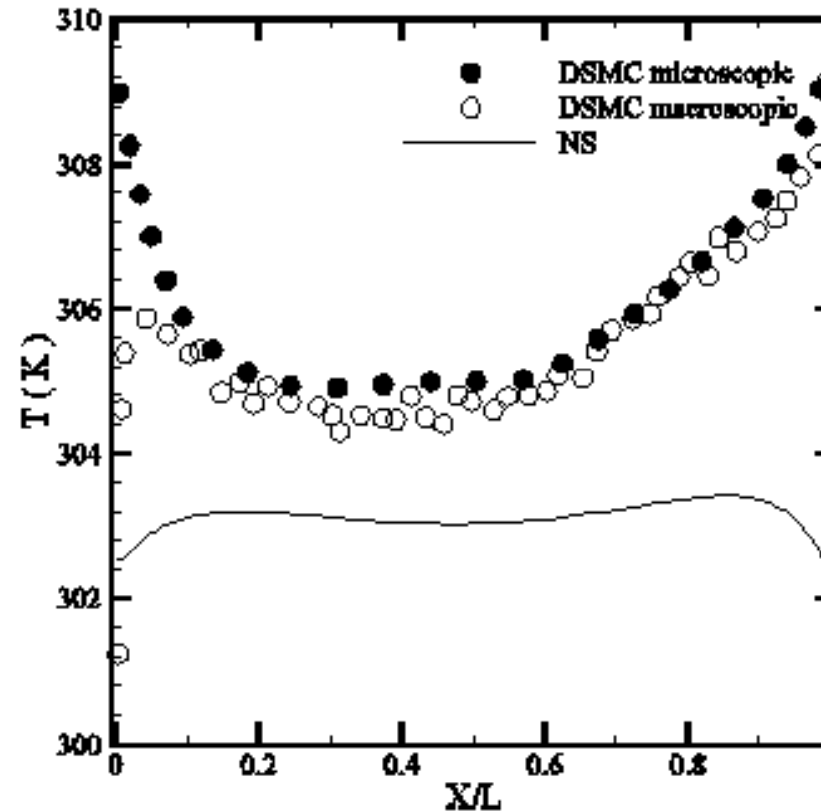


# Microscopic sampling vs macroscopic (courtesy of Dr. Roohi)

Direct microscopic  
sampling of the  
molecular  
properties of  
particles that strike  
the wall surface

VS

macroscopic  
approach that  
accounts for all  
molecules in the  
adjacent cell

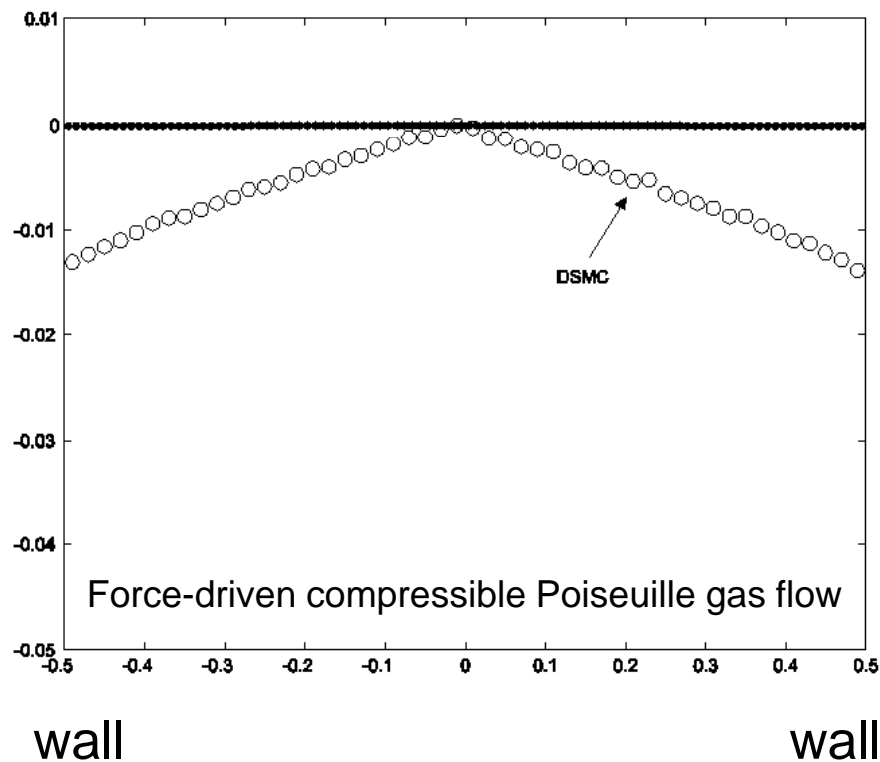




# Assessment of internal errors in DSMC

**Key observation: The conservation laws must be satisfied irrespective of computational models.**

The relative internal error of numerical solutions for one-dimensional gas flow can be checked (*Comp. Fluids* 2011).

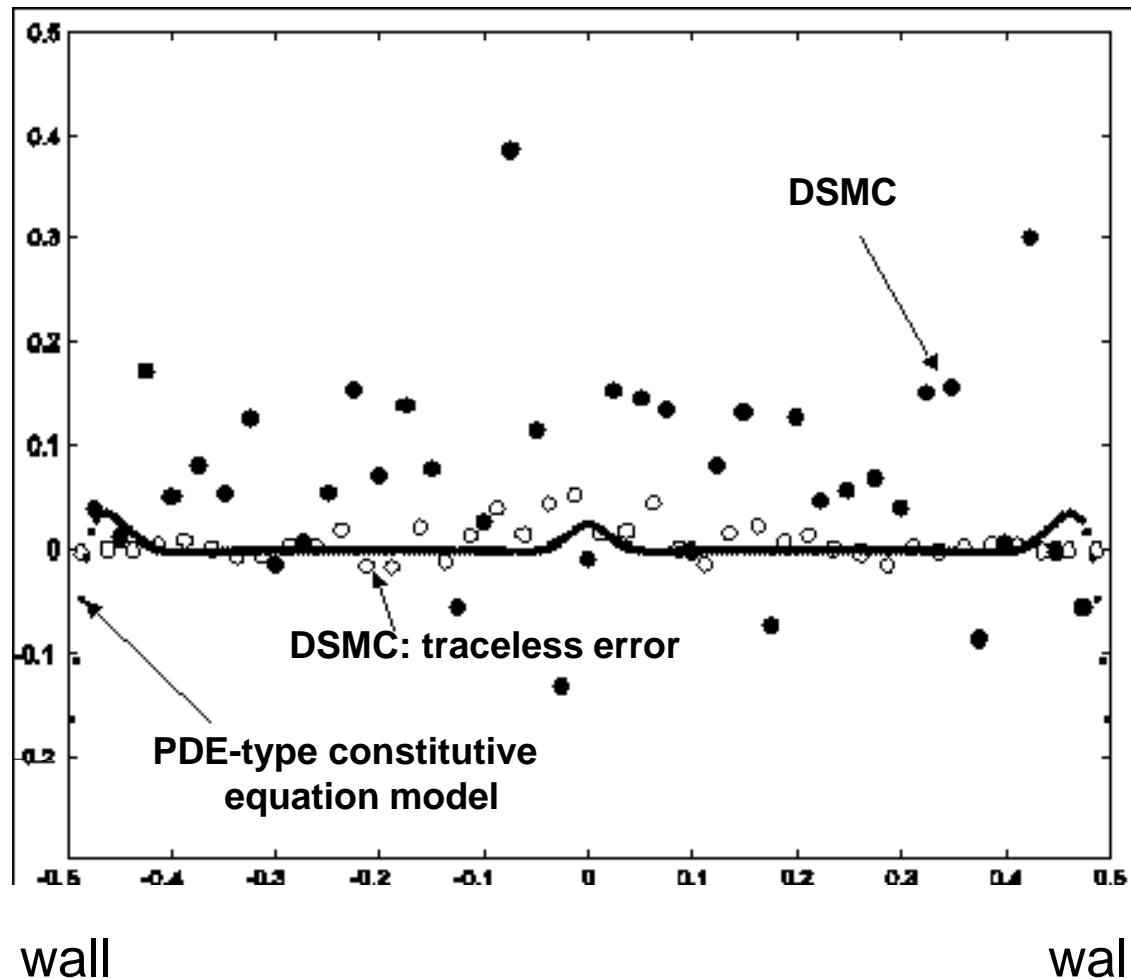


$$\text{error}_{x\text{-momentum}} \equiv \frac{\Pi_{xy}(y) - \int_0^y \rho(y)ady}{\rho(0)ah}$$

$$\text{error}_{\text{energy}} \equiv \frac{\Pi_{xy}(y)u(y) + Q_y(y) - \int_0^y \rho(y)u(y)ady}{\rho(0)ahu(0)}$$

The relative error of the DSMC increases from the center to the solid wall and reaches non-negligible value near the solid wall ( $\text{Kn}=0.1$ ).

# Assessment of internal errors: Another examples



The relative errors of the DSMC is not negligible.

In case of a PDE-type higher-order model, large errors are found in the center as well as near the wall.

# **Concluding remarks: What makes gas micro flows so complicated—and difficult?**

Complicated physics coming from non-classical physics (nonlinearity and couplings in G. E. and B. C.).

Lack of theories in some problems; in particular, rotational non-equilibrium and gas-surface molecular interaction.

Presence of exotic properties such as tangential heat flux (extremely difficult to measure experimentally).

Need of theoretical and experimental investigation on the whole flowfields, including diatomic gases, beyond a reduced quantity such as the mass flow rate. Showing a snap-shot agreement one thing, but describing many features simultaneously quite another.