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

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Many thanks to
organizers of this conference
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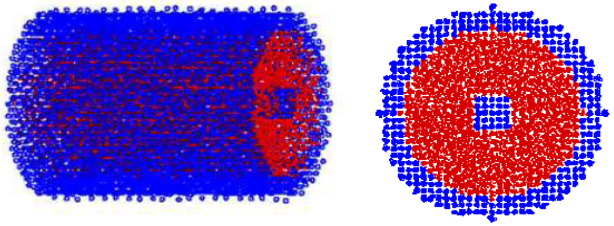
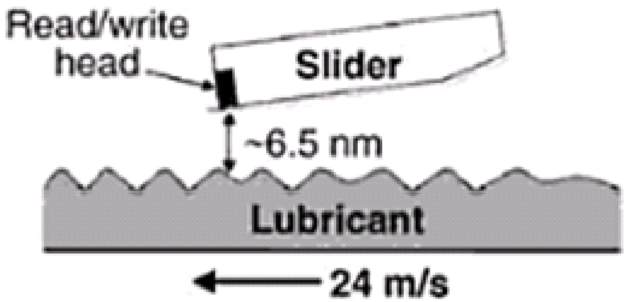
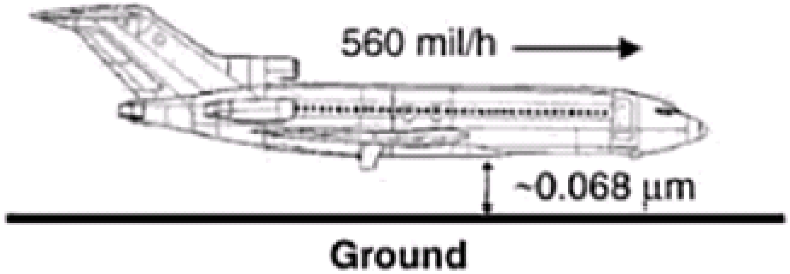
Introduction to gas micro flows



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

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

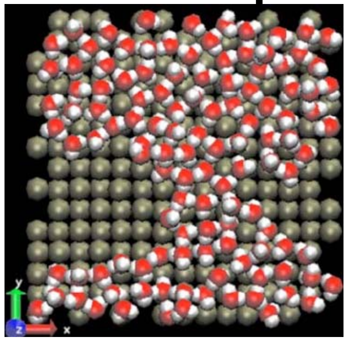
Molecular approach

DSMC

Linearized Boltzmann equation

Lattice-Boltzmann method

Bottom-up



Hybrid approach

DSMC-continuum coupling (based on domain decomposition)

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

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)

collision integral

$$\left(\frac{\partial}{\partial t} + \mathbf{v}\cdot\nabla + \mathbf{a}\cdot\nabla_v\right) f(t,\mathbf{r};\mathbf{v}) = \underbrace{C\left[f, f_2\right]}_{\text{collision integral}}$$

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

$\mathbf{a}$: force

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

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

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

Moment equation

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

$$\left(\rho, \mathbf{u}, T, \underbrace{\mathbf{\Pi}}_{\text{shear stress tensor}}, \underbrace{\mathbf{Q}}_{\text{heat flux vector}}, \cdots\right)(t,\mathbf{r})$$

Derivation of continuum model

Conservation laws (exact) in vector form

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

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

$$\boldsymbol{\psi}^{(\Pi)} \equiv \left\langle m\left[\mathbf{cc}\right]^{(2)}\mathbf{c}f\right\rangle$$

Constitutive equation (exact) in vector form

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

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

Unsteady Convection Higher-order Kinematic Thermo. driving Dissipation

Key observations:

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

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

Derivation of algebraic constitutive relations

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

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

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

steady

no convective in velocity-shear

yielding <u>partial differential</u> type!

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

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

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

yielding <u>algebraic</u> type!

Interesting non-classical physical laws

can be identified!

Linear uncoupled Navier-Fourier equations: classical physical laws

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

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

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

u_x case (compression and expansion)

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

Newtonian or linear

Not like $(u_x)^2$

u_y case (velocity shear only)

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

Uncoupled

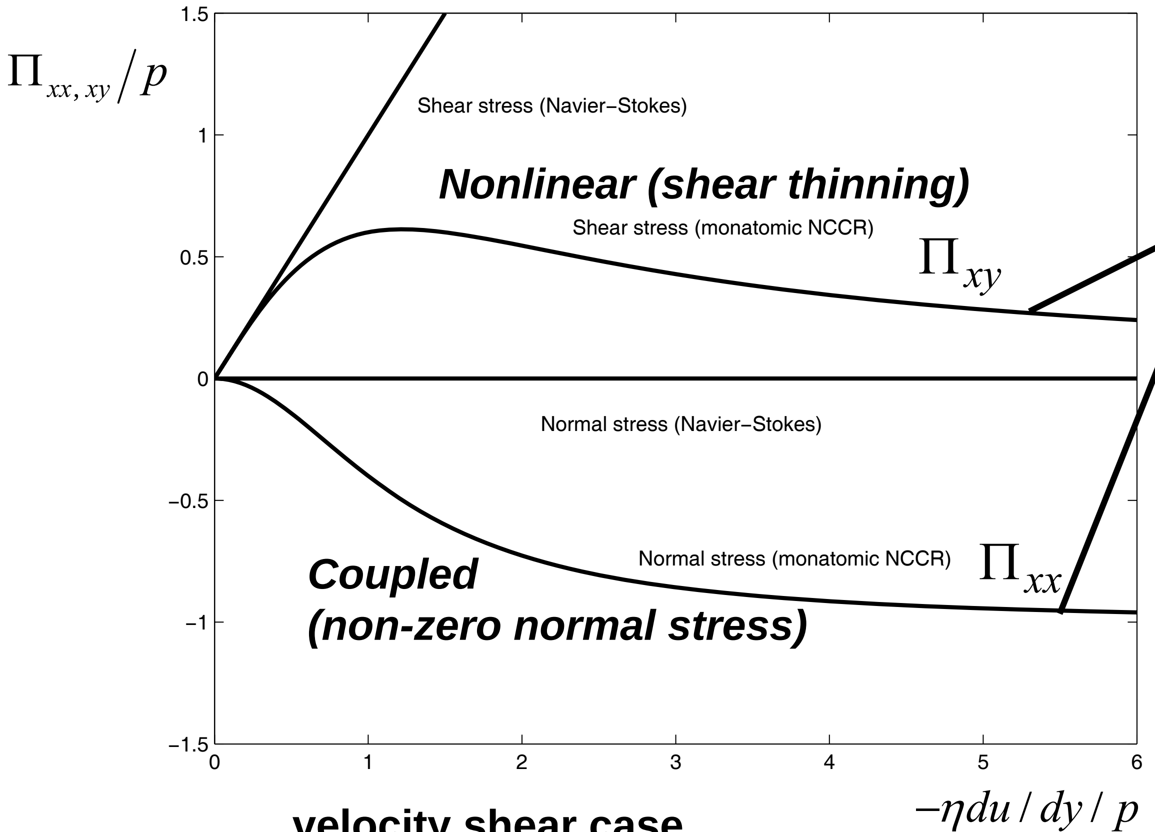
Always vanishing normal stress Π_{xx} or Π_{yy}

$$\begin{bmatrix} Q_x \\ Q_y \end{bmatrix} \leftarrow -k(T)\begin{bmatrix} T_x \\ T_y \end{bmatrix}.$$

Not like $(T_x)^2$

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

Thermodynamic driving force $-2\eta\left[\nabla \mathbf{u}\right]^{(2)}$, $-k\nabla T$ $\xrightarrow{\div p,\ \div p\sqrt{\frac{C_p T}{2\,\mathrm{Pr}}}}$ $\boxed{\textbf{Algebraic NCCR}}$ $\xrightarrow{\times p,\ \times p\sqrt{\frac{C_p T}{2\,\mathrm{Pr}}}}$ $\mathbf{\Pi}$, $\mathbf{Q}$ **Shear stress heat flux**



velocity shear case

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

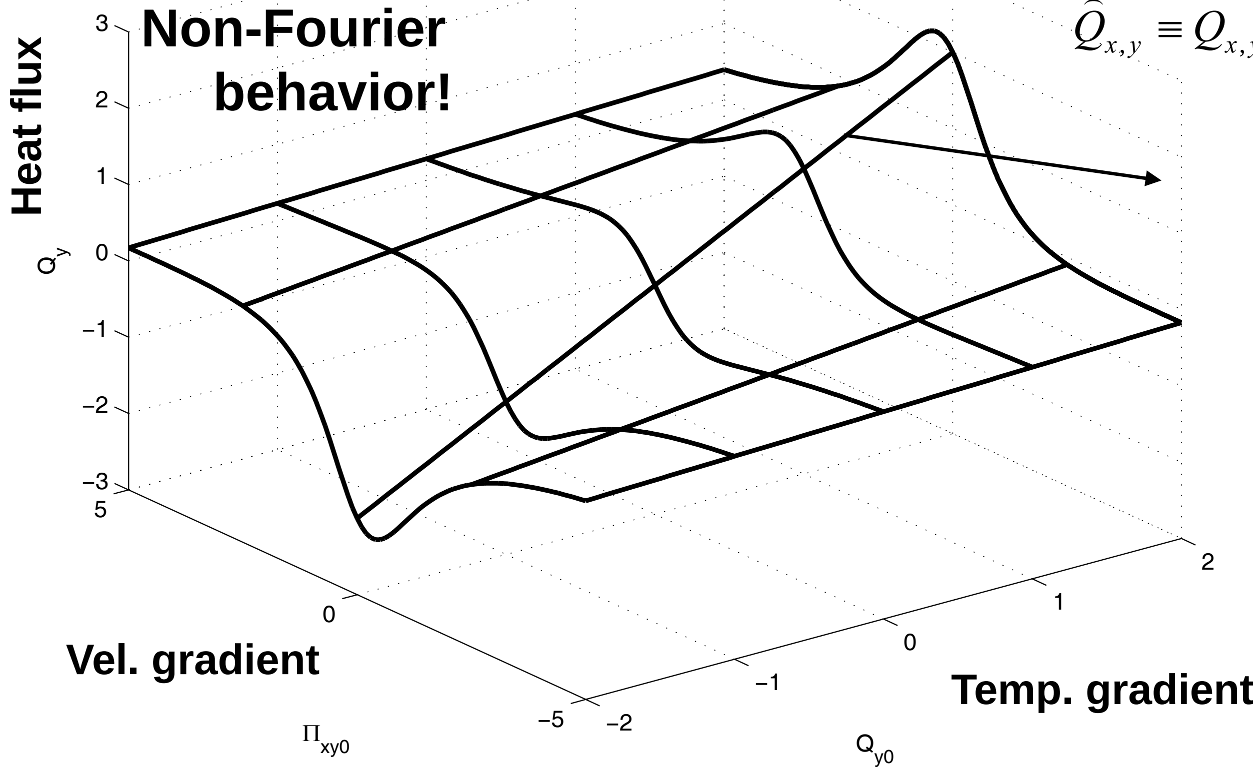
kinematic stress constraint!

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

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

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

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



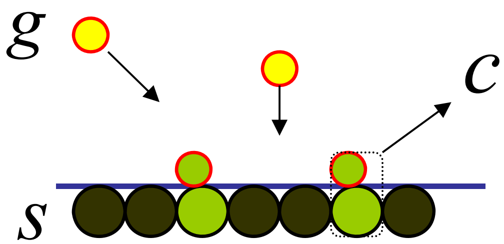
Fourier law
$\hat{Q}_y = \hat{Q}_{y_0}$

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*)



$$g + s \Rightarrow c$$

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

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

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

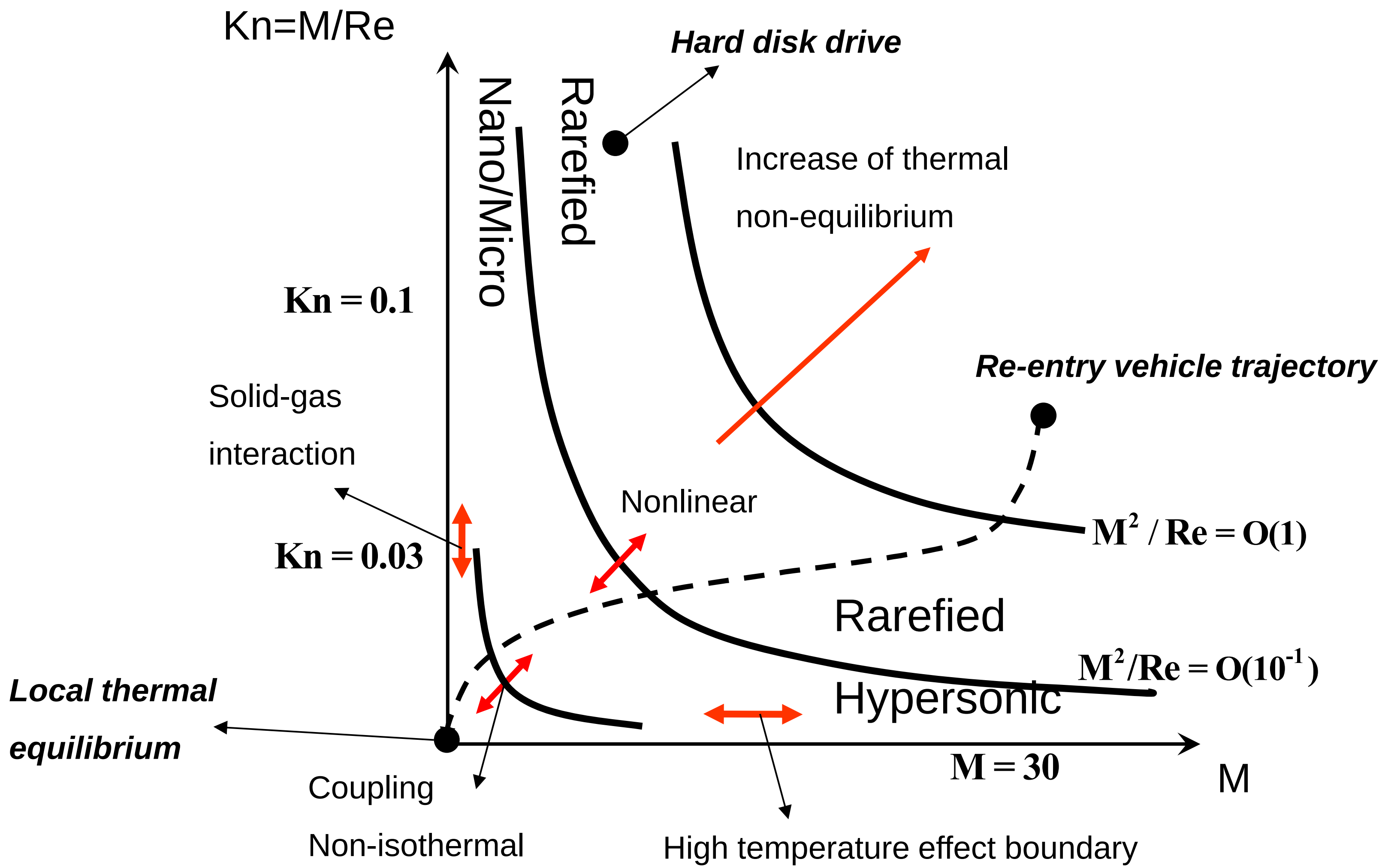
$$u(h/2) = V + \sigma_V l \cdot (-) \left.\frac{\partial u}{\partial y}\right]_{h/2} - \frac{3}{4} \frac{\eta}{\rho T} \left.\frac{\partial T}{\partial x}\right]_{h/2}, \quad T(h/2) = T_w + \sigma_T l \cdot (-) \left.\frac{\partial T}{\partial y}\right]_{h/2}$$

Nonlinear coupled velocity slip and temperature jump models

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

- 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)



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

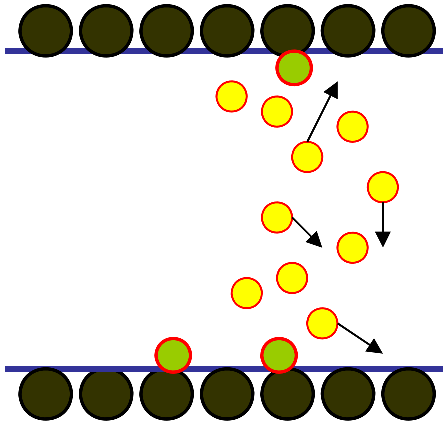
Two terms: Kn

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

Three terms: *M*, Kn

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

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



Boltzmann (or similar) in bulk flow	**Nonlinear** **Coupled**	**Kn*M**
Gas-surface atom interaction	**Nonlinear** **Coupled**	**Kn** $\frac{2-\sigma_v}{\sigma_v} \sim \exp\left(-\frac{D_e}{k_B T_w}\right)$

Morphing

(Seamless transition)

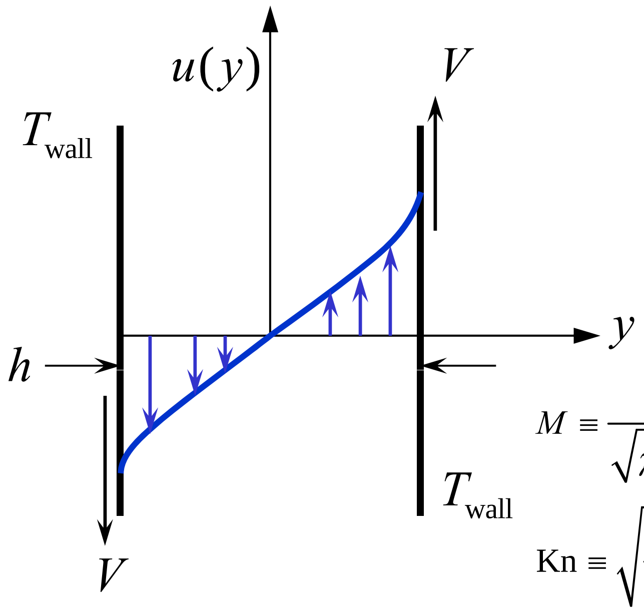
Combination of two nonlinearities and two couplings—nonlinear coupled constitutive relation for bulk flow and nonlinear coupled boundary conditions at the wall—may be critical within the continuum framework.

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)



$$M \equiv \frac{V}{\sqrt{\gamma R T_{\text{wall}}}}$$

$$\text{Kn} \equiv \sqrt{\frac{\pi}{2}}\frac{\eta_{\text{wall}}\sqrt{RT_{\text{wall}}}}{p(0)h}$$

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

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)

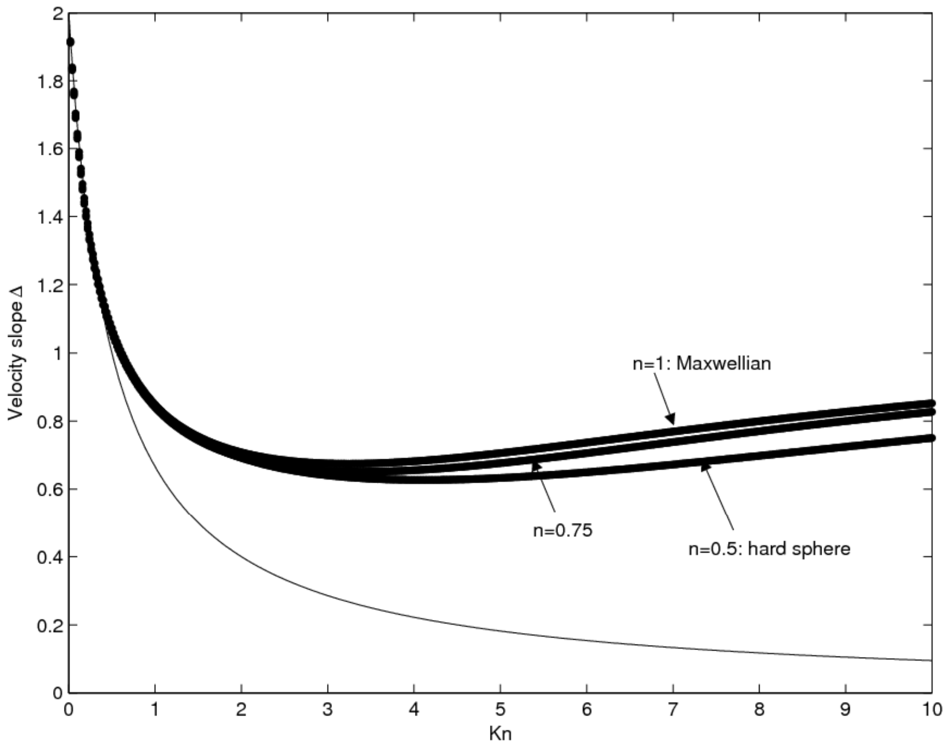
However, unsolved problems persist (within continuum framework)

- 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



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

Summary of Part II: Well-posedness of Couette flow

Initial data	Physical constraints imposed
M, Kn, T_{wall}	$0 \le M < \infty$ $0 < \mathrm{Kn} < \infty$ $0 < T_{wall}$
$\eta du/dy, T_{\mathrm{wall}}/T_{\mathrm{ave}}$	Primary solutions
$T(0), \rho(0)$	$p = \rho RT$
$T(y), u(y), \rho(y)$	$p, T, \rho > 0$
$\Pi_{xy}, \Pi_{xx}, \Pi_{yy}, \Pi_{zz}$	$\Pi_{xx} + \Pi_{yy} + \Pi_{zz} = 0$
$Q_x(y), Q_y(y)$	Conservation laws satisfied exactly

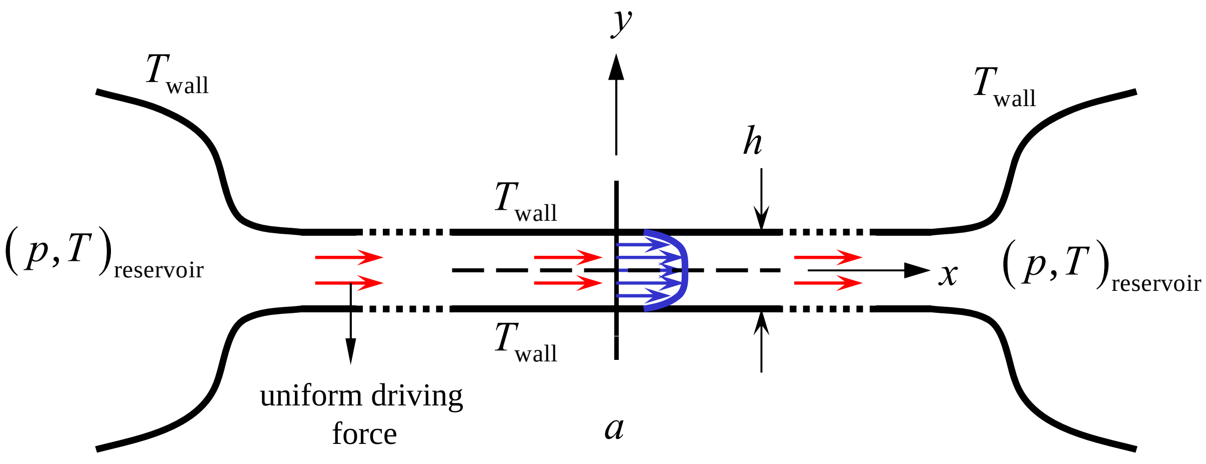
Wall boundary conditions
u (slip)
T (jump)

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



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

with

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

nonlinear & coupled

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

Non-classical behaviors (easy parts)

- central temperature minimum $\hat{Q}_y = \frac{3}{\left(3+2\hat{\Pi}^2_{xy_{NSF}}\right)}\left(\hat{Q}_{y_0} + \boxed{\hat{a}\hat{\Pi}_{xy_{NSF}}}\right)$
- 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 $\left|\nabla\cdot\boldsymbol{\psi}^{(\Pi)}\right| < 2\left|\left[\boldsymbol{\Pi}\cdot\nabla\mathbf{u}\right]^{(2)}\right|$: *PoF* 2011)

Rigorous treatment of thermal property through

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

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

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

Analytic form of concave pressure distribution

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

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

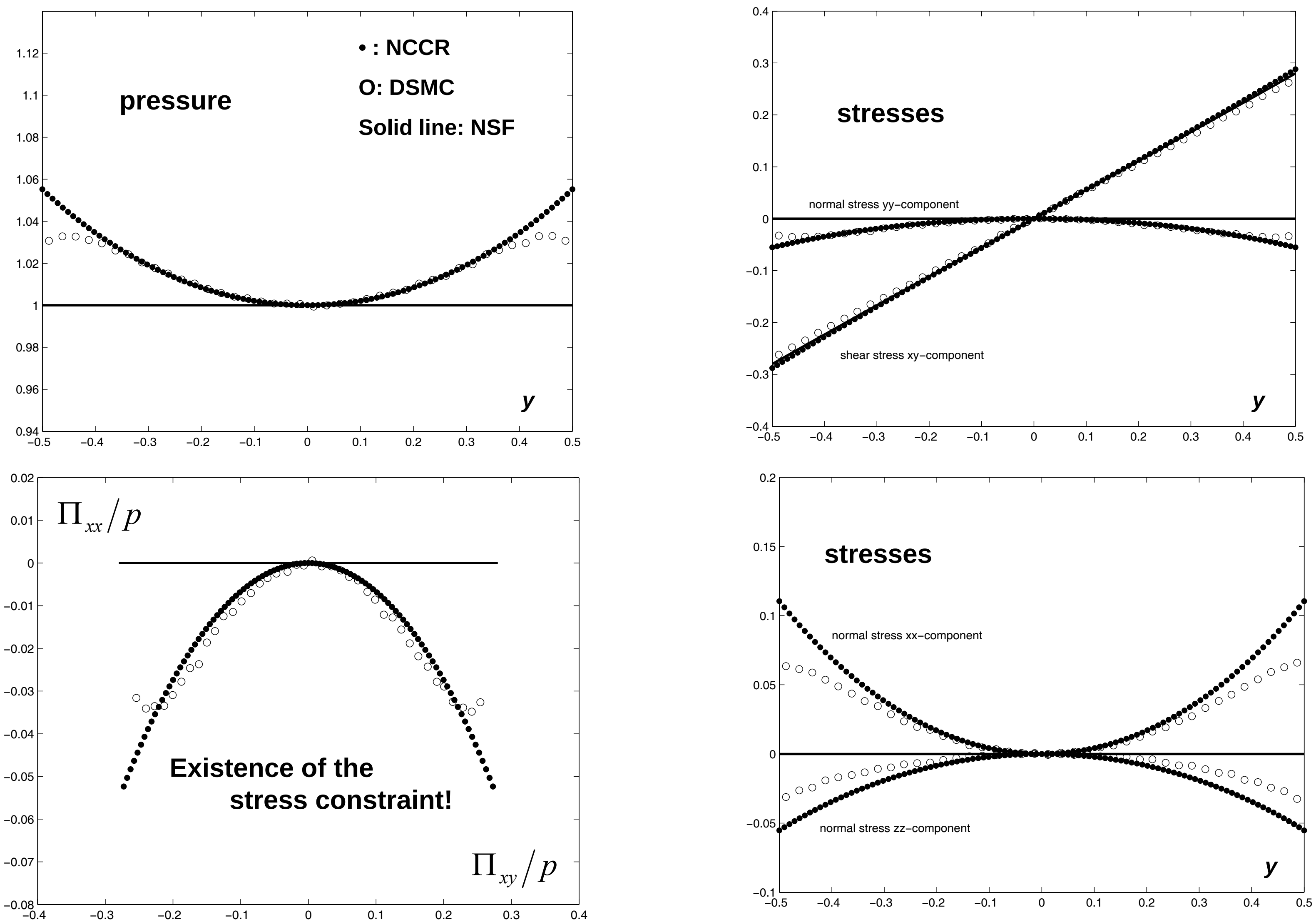
$$\Pi_{xy}^* = \frac{1}{N_\delta}\sqrt{\frac{3}{2}}\tan\left(\sqrt{\frac{2}{3}}\varepsilon_{h_w} T_w^* s^*\right)$$

Very surprising *tangent* profile!

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

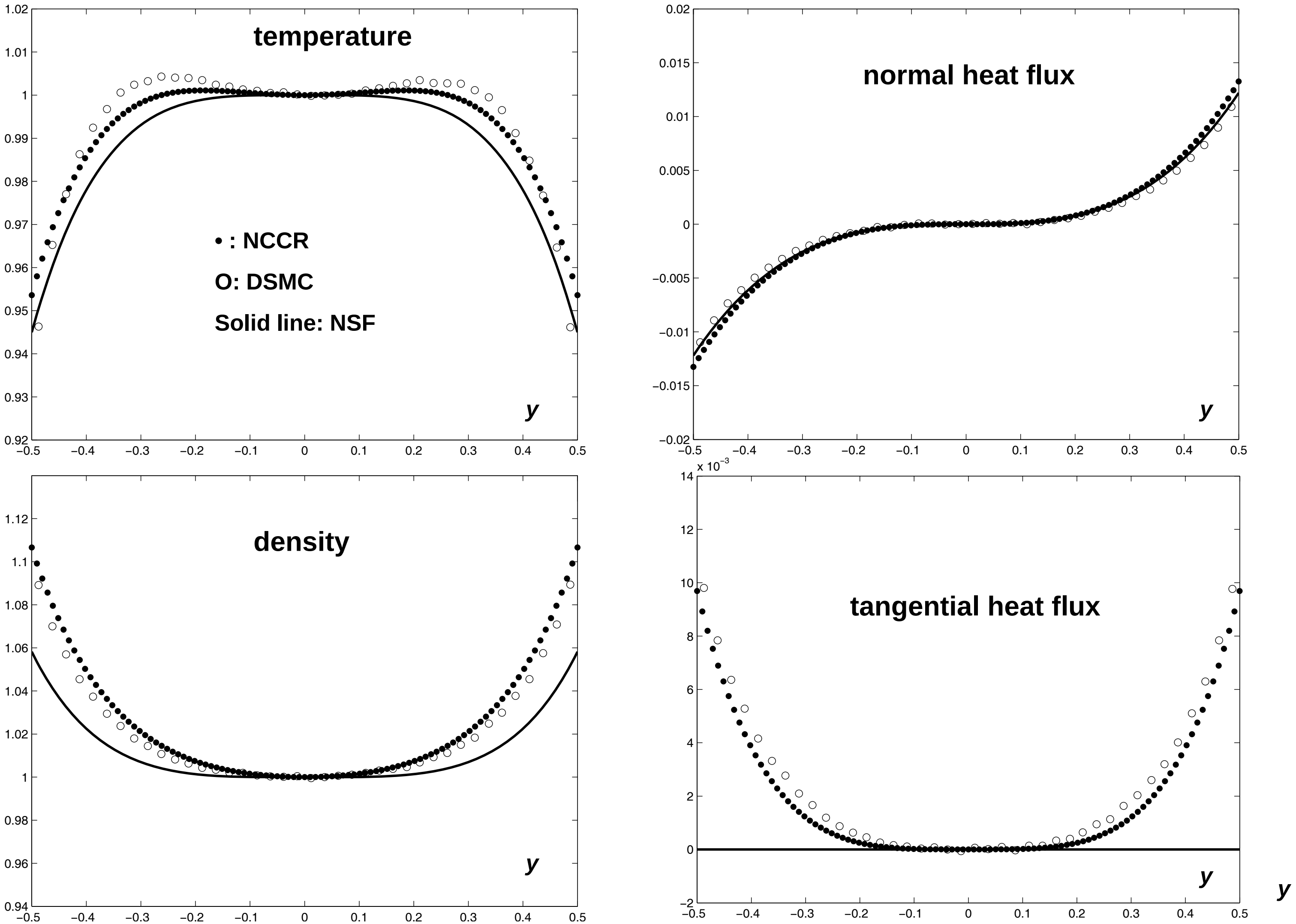
Exact analytic solutions: stresses

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



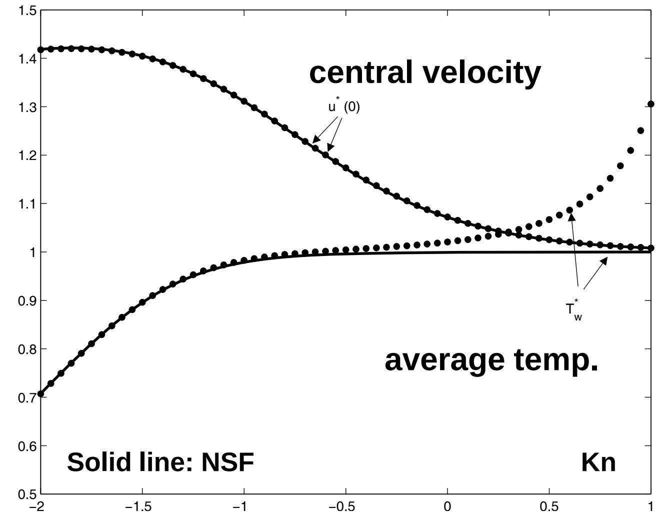
Exact analytic solutions: temp., density, heat fluxes

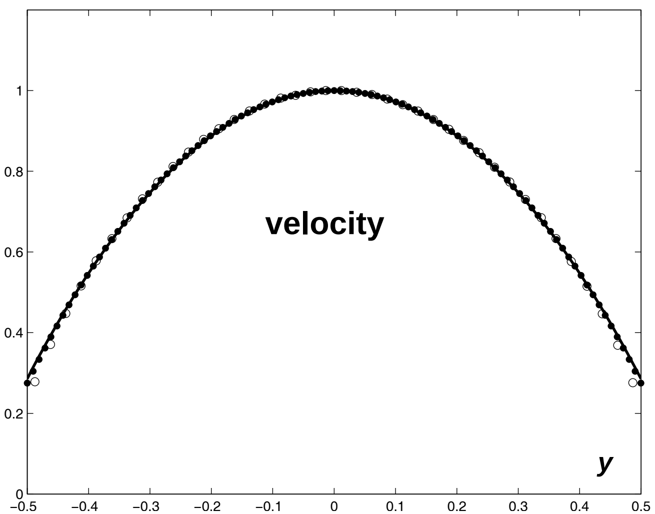
After applying the Langmuir slip/jump model

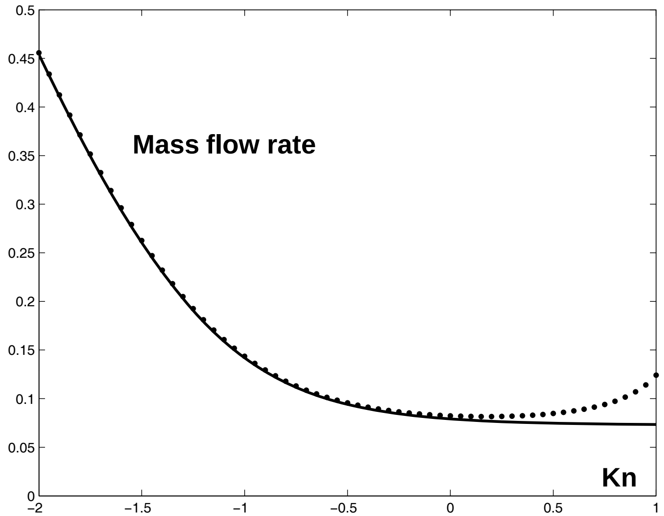


Exact analytic solutions: Knudsen minimum

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







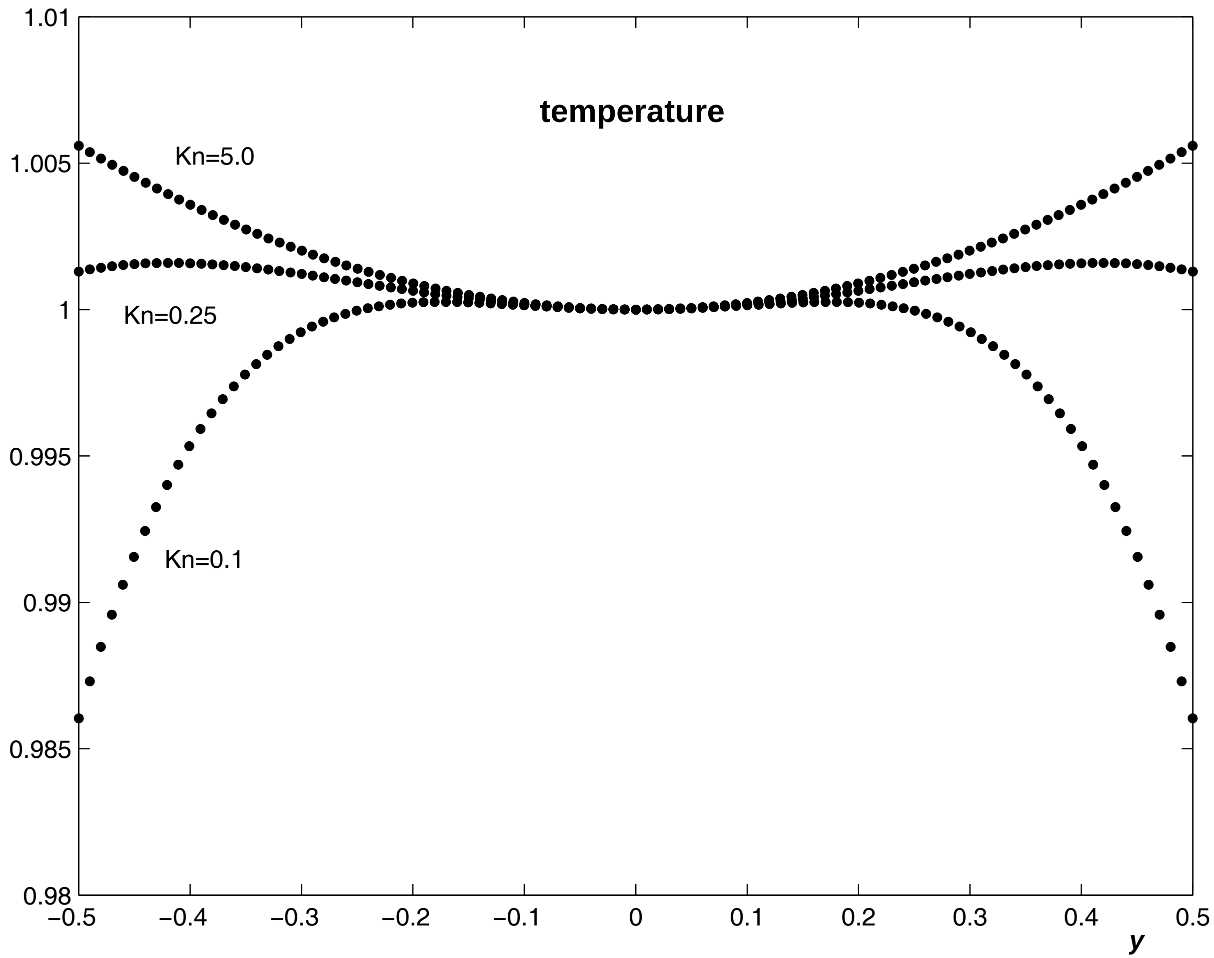
$$\frac{\dot{m}/2h}{\rho_r\sqrt{\gamma R T_w}} \equiv \frac{\int_0^{h/2} \rho u dy}{2\sqrt{\gamma R T_w}\int_0^{h/2} \rho dy}$$

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

slip | **central velocity** | **Stress constraint** | **average temperature**

Responsible for Knudsen minimum !

What happened here: Knudsen minimum

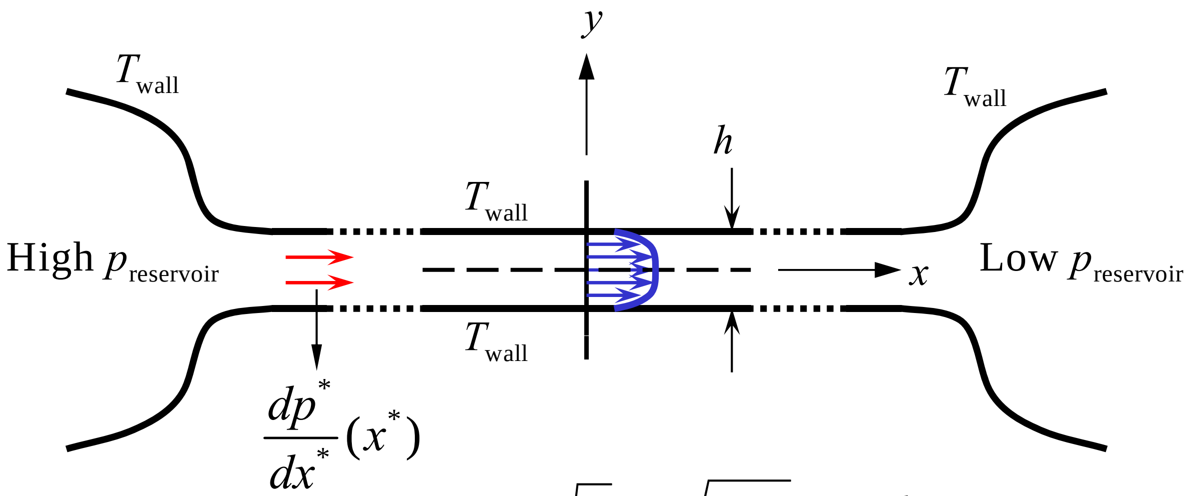


$$\frac{\dot{m}/2h}{\rho_r \sqrt{\gamma R T_w}} \sim \left(\frac{T_w}{T_{ave}} \right)^2$$

average temperature

Responsible for Knudsen minimum !

Pressure-driven compressible Poiseuille gas flow



Conservation laws

with

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

nonlinear & coupled

$$\frac{p_{in}}{p_{out}}: \text{ pressure ratio, } \text{Kn} \equiv \sqrt{\frac{\pi}{2}}\frac{\eta_{\text{wall}}\sqrt{RT_{\text{wall}}}}{p_{\text{reservoir}}h},\ \varepsilon = \frac{h}{L}: \text{ length-to-height ratio}$$

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

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

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

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

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

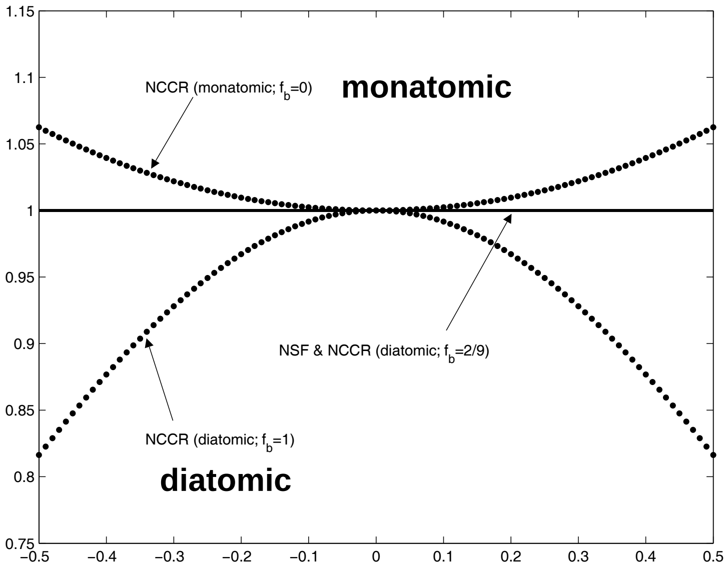
Surprisingly, there is even **no consensus** what the proper master kinetic equations would be for describing **diatomic gases** like nitrogen in thermal non-equilibrium.

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

$\Delta:$ excess normal stress

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

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



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?)

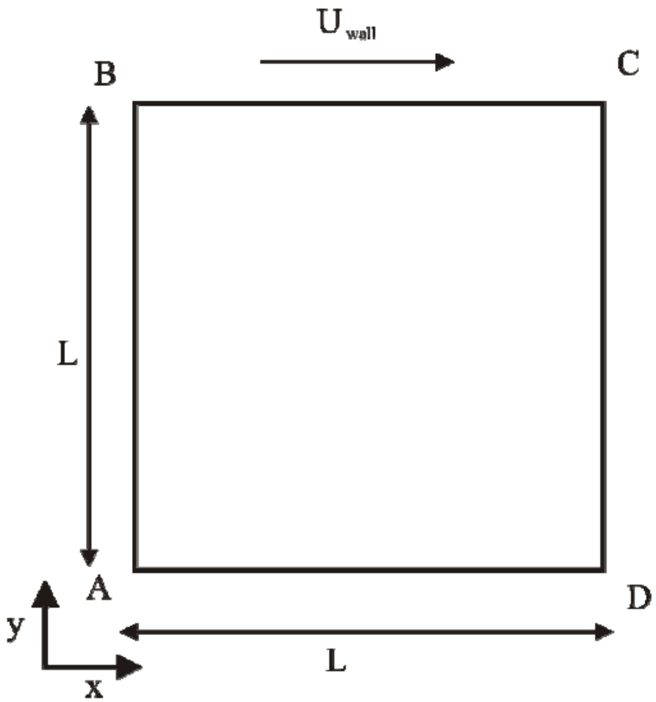
Lack of theories:

- 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.

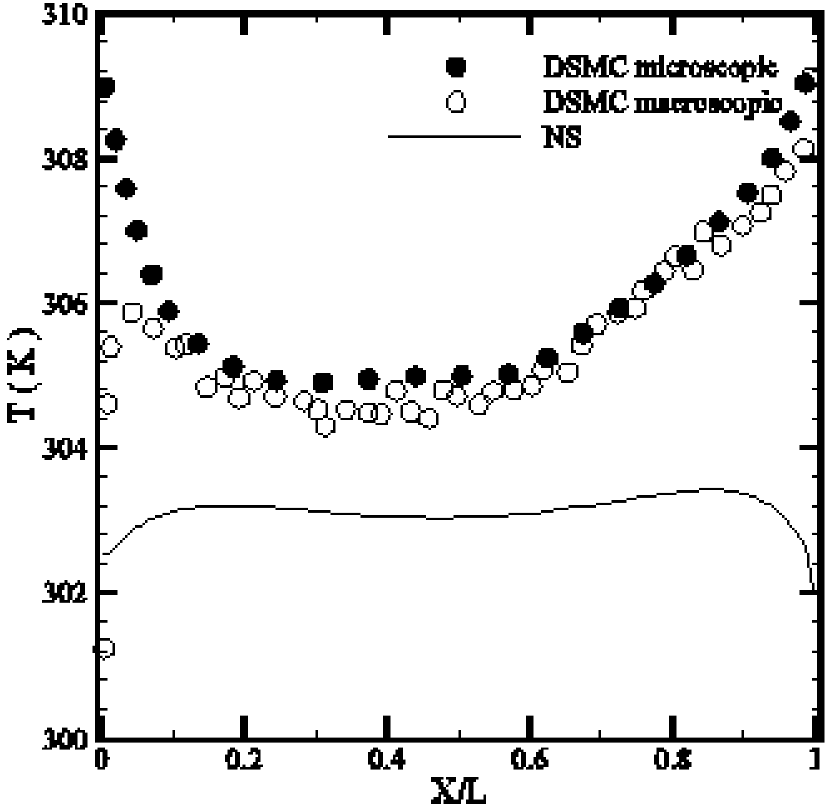


Microscopic sampling vs macroscopic (courtesy of Dr. Roohi)

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

vs

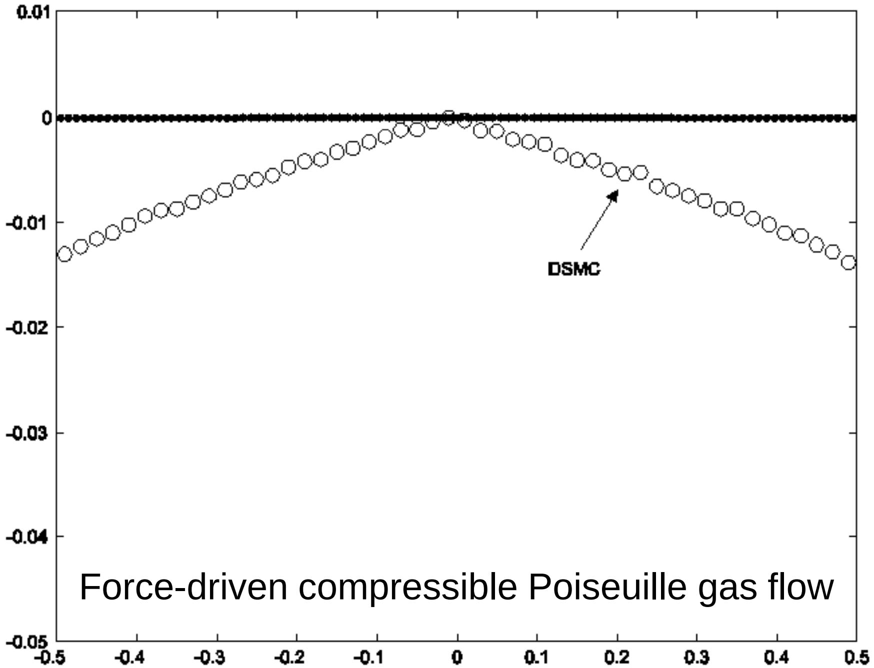
macroscopic approach that accounts for all molecules in the adjacent cell



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).



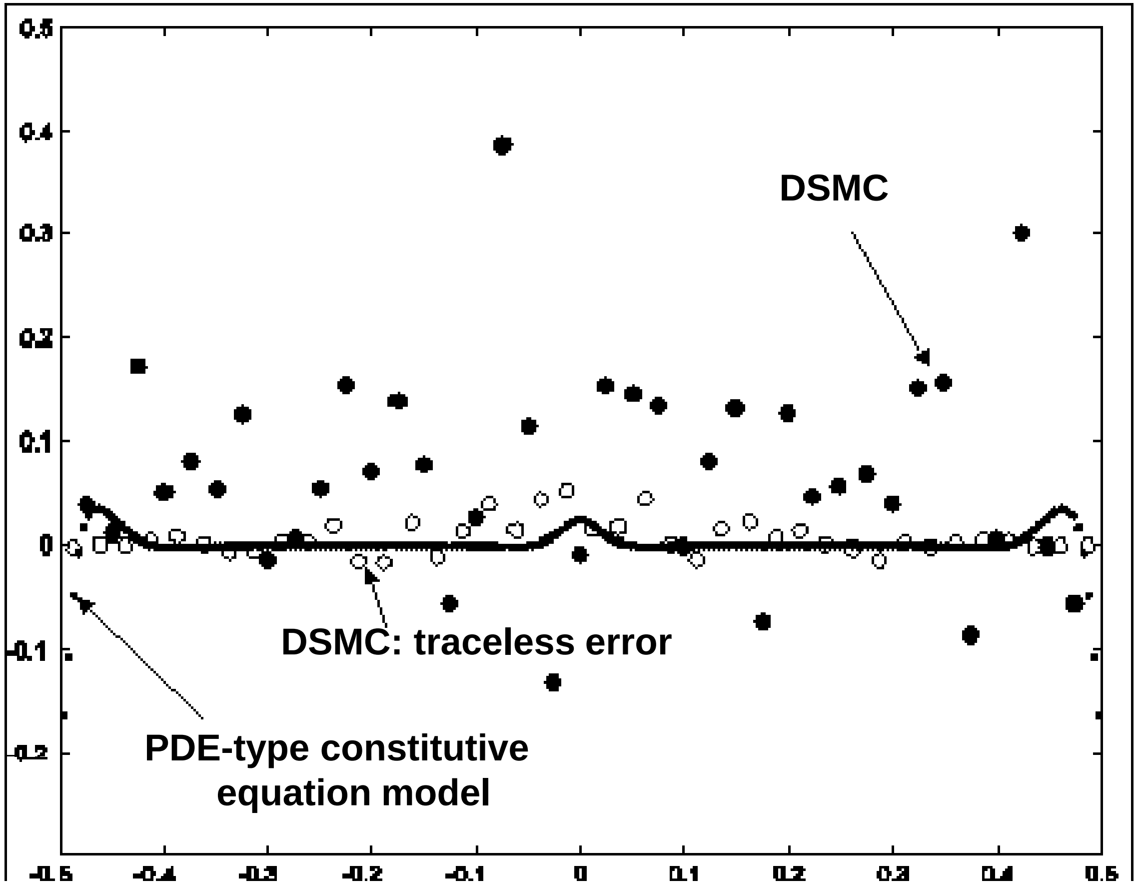
wall wall

$$\text{error}_{x\text{-momentum}} \equiv \frac{\Pi_{xy}(y) - \int_0^y \rho(y) a\, dy}{\rho(0) a h}$$

$$\text{error}_{\text{energy}} \equiv \frac{\Pi_{xy}(y) u(y) + Q_y(y) - \int_0^y \rho(y) u(y) a\, dy}{\rho(0) a h u(0)}$$

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

Assessment of internal errors: Another examples



wall wall

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.