The Limits of Navier-Stokes Theory and Kinetic Extensions for Describing Small Scale Gaseous Hydrodynamics

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Introduction

- Our interest in small scale hydrodynamics:
  - Motivated by the recent significant interest in micro/nano science and technology
  - Lies in the scientific challenges associated with breakdown of Navier-Stokes description

- In simple fluids, Navier-Stokes description expected to break down when the characteristic flow lengthscale approaches the fluid "internal scale" λ

- In a dilute gas, λ is typically identified with the molecular mean free path $\gg d$ (molecular diameter–measure of molecular interaction range)

- $\lambda_{air} \approx 0.05\mu$m (atmospheric pressure). Kinetic phenomena appear in air at micrometer scale.

Breakdown of Navier-Stokes description (gases)

Breakdown of Navier-Stokes $\neq$ breakdown of continuum assumption.

In the regime on interest, hydrodynamic fields (e.g. flow velocity, stress) can still be defined (e.g. taking moments of the underlying molecular description [Vincenti & Kruger, 1965])

Navier-Stokes description fails because collision-dominated tranport models, i.e. constitutive relations such as

$$\tau_{ij} = \mu \left(\frac{\partial u_i}{\partial x_j} + \frac{\partial u_j}{\partial x_i} \right), \quad i \neq j$$

fail

Without "closures", conservation laws such as the momentum conservation law

$$\rho \frac{D\mathbf{u}}{Dt} = -\frac{\partial P}{\partial \mathbf{x}} + \frac{\partial \tau}{\partial \mathbf{x}} + \rho \mathbf{f}$$

cannot be solved

Practical applications*

Examples include:

- Design and operation of small scale devices (sensors/actuators [Gad-el-Hak, 1999], pumps with no moving parts [Muntz et al., 1997-2004; Sone et al., 2002], MIT's NANOGATE,...)
- Processes involving nanoscale transport (Chemical vapor deposition [e.g. Cale, 1991-2004], micromachined filters [Aktas & Aluru, 2001&2002], flight characteristics of hard-drive read/write head [Alexander et al., 1994], damping/thin films [Park et al., 2004; Breuer, 1999],...)
- Vacuum science/technology: Recent applications to small-scale fabrication (removal/control of particle contaminants [Gallis et al., 2001&2002],...)
- Similar challenges associated with nanoscale heat transfer in the solid state (phonon transport)

*These are mostly low-speed, internal, incompressible flows, in contrast to the external, high-speed, compressible flows studied in the past in connection with high-altitude aerodynamics

Outline

- Introduction to dilute gases
  - Background
  - Kinetic description for dilute gases: Boltzmann Equation
  - Direct simulation Monte Carlo (DSMC)
- Review of slip-flow theory
- Physics of flow beyond Navier-Stokes
  - Knudsen's pressure-driven-flow experiment
  - Recent theoretical results: Wave propagation in 2-D channels, convective heat transfer, lubrication-type flows
- Kinetic extensions of Navier-Stokes: Second-order slip
- Recent developments in simulation

Introduction to Dilute Gases* I

In dilute gases (number density (n) normalized by atomic volume is small, i.e. $nd^3 \ll 1$):

- The mean intermolecular spacing $\delta \approx 1/n^{1/3}$ is large compared to the atomic size, i.e. $\delta/d \approx (1/nd^3)^{1/3} \gg 1$
- Interaction negligible most of the time $\Rightarrow$ particles travel in straight lines except when "encounters" occur
- The hydrodynamically relevant inner scale is the average distance between encounters (mean free path) $\lambda \approx 1/(\sqrt{2}\pi n d^2)$
- Because $\lambda/d = 1/(\sqrt{2}\pi n d^3) \gg 1$ or $\lambda \gg \delta \gg d$, time between encounters $\gg$ encounter duration $\Rightarrow$treat particle interactions as collisions
- Motivates simple model such as hard sphere as reasonable approximation (for discussion and more complex alternatives see [Bird, 1994])

*Air at atmospheric pressure meets the dilute gas criteria

Introduction to Dilute Gases II

Deviation from Navier-Stokes is quantified by $Kn = \lambda/H$
H is flow characteristic lengthscale

Flow regimes (conventional wisdom):

- $Kn \lll 0.1$, Navier-Stokes (Transport collision dominated)
- $Kn \lesssim 0.1$, Slip flow (Navier-Stokes valid in body of flow, slip at the boundaries)
- $0.1 \lesssim Kn \lesssim 10$, Transition regime
- $Kn \gtrsim 10$, Free molecular flow (Ballistic motion)

Kinetic description for dilute gases*

Boltzmann Equation†: Evolution equation for $f(\mathbf{x}, \mathbf{v}, t)$:

$$\frac{\partial f}{\partial t} + \mathbf{v} \cdot \frac{\partial f}{\partial \mathbf{x}} + \mathbf{F} \cdot \frac{\partial f}{\partial \mathbf{v}} = \int \int (f^* f_1^* - f\, f_1) |\mathbf{v}_r|\, \sigma\, d^2\Omega\, d^3\mathbf{v}_1$$

$f(\mathbf{x}, \mathbf{v}, t) d^3\mathbf{v} d^3\mathbf{x} =$ number of particles (at time t) in phase-space volume element $d^3\mathbf{v} d^3\mathbf{x}$ located at $(\mathbf{x}, \mathbf{v})$

Connection to hydrodynamics:

$$\rho(\mathbf{x}, t) = \int_{\text{all}\,\mathbf{v}} m\, f d\mathbf{v}, \qquad \mathbf{u}(\mathbf{x}, t) = \frac{1}{\rho(\mathbf{x}, t)} \int_{\text{all}\,\mathbf{v}} m\mathbf{v}\, f d\mathbf{v}, \ldots$$

The BGK approximation:

$$\int \int (f^* f_1^* - f f_1) |\mathbf{v}_r| \sigma d^2\Omega d^3\mathbf{v}_1 \approx -(f - f^{eq})/\tau$$

*References: Y. Sone, Kinetic theory and fluid dynamics, 2002; C. Cercignani, The Boltzmann equation and its applications, 1988.

†Subsequently shown to correspond to a truncation of the BBGKY Hierarchy for dense fluids to the single-particle distribution by using the (Molecular Chaos) approximation $P(\mathbf{v}, \mathbf{v}_1) = f(\mathbf{v})\, f(\mathbf{v}_1) = f\, f_1$.

Direct Simulation Monte Carlo (DSMC) [Bird]

- **Smart molecular dynamics**: no need to numerically integrate essentially straight line trajectories.
- System state defined by $\{\mathbf{x}_i, \mathbf{v}_i\}$, $i = 1, ...N$
- Split motion:
  - Collisionless advection for Δt $(\mathbf{x}_i \to \mathbf{x}_i + \mathbf{v}_i \Delta t)$:

$$\frac{\partial f}{\partial t} + \mathbf{v} \cdot \frac{\partial f}{\partial \mathbf{x}} + \mathbf{F} \cdot \frac{\partial f}{\partial \mathbf{v}} = 0$$

  - Perform collisions for the same period of time Δt:

$$\frac{\partial f}{\partial t} = \int \int (f^* f_1^* - f\, f_1) |\mathbf{v}_r|\, \sigma\, d^2\Omega\, d^3\mathbf{v}_1$$

    Collisions performed in cells of linear size Δx. Collision partners picked randomly within cell

- **Significantly faster than MD** (for dilute gases)
- In the limit $\Delta t, \Delta x \to 0$, $N \to \infty$, DSMC solves the Boltzmann equation [Wagner, 1992]
- DSMC (solves Boltzmann)$\neq$ Lattice Boltzmann (solves NS)

Variance reduction

[Baker & Hadjiconstantinou, 2005]

- Statistical convergence ($E \propto N^{-1/2}$) associated with field averaging process

- For example

$$E_u = \frac{\sigma_u}{u_o} = \frac{1}{\sqrt{\gamma} Ma} \frac{1}{\sqrt{NM}}, \quad Ma = u_o / \sqrt{\gamma R T}$$

  [Hadjiconstantinou, Garcia, Bazant & He, 2003]
  Typical MEMS flows at $Ma < 0.01$ require enormous number of samples.
  e.g. to achieve a 1% statistical uncertainty, in a 1m/s flow, $\approx 5 \times 10^8$ samples are required.

Slip flow

- Maxwell's slip boundary condition:

$$u_{gas}|_{wall} - u_w = \frac{2-\sigma_v}{\sigma_v}\lambda\frac{du}{d\eta}|_{wall} + \frac{3}{4}\frac{\mu}{\rho T}\frac{\partial T}{\partial s}$$

  Temperature jump boundary condition:

$$T_{gas}|_{wall} - T_w = \frac{2-\sigma_T}{\sigma_T}\frac{2\gamma}{\gamma+1}\frac{\lambda}{Pr}\frac{dT}{d\eta}|_{wall}$$

  $\eta =$ wall normal
  $s =$ wall tangent
  $\sigma_v =$ tangential momentum accommodation coefficient
  $\sigma_T =$ energy accommodation coefficient

- For the purposes of this talk $\sigma_v = \sigma_T =$ fraction of diffusely (as opposed to specularly) reflected molecules (see Cercignani (1998) for more details)
- These relations **are an oversimplification** and responsible for a number of misconceptions
- Slip-flow theory can be **rigorously derived** from asymptotic analysis of the Boltzmann equation [Grad, 1969; Sone, 2002]

Main elements of first-order asymptotic analysis

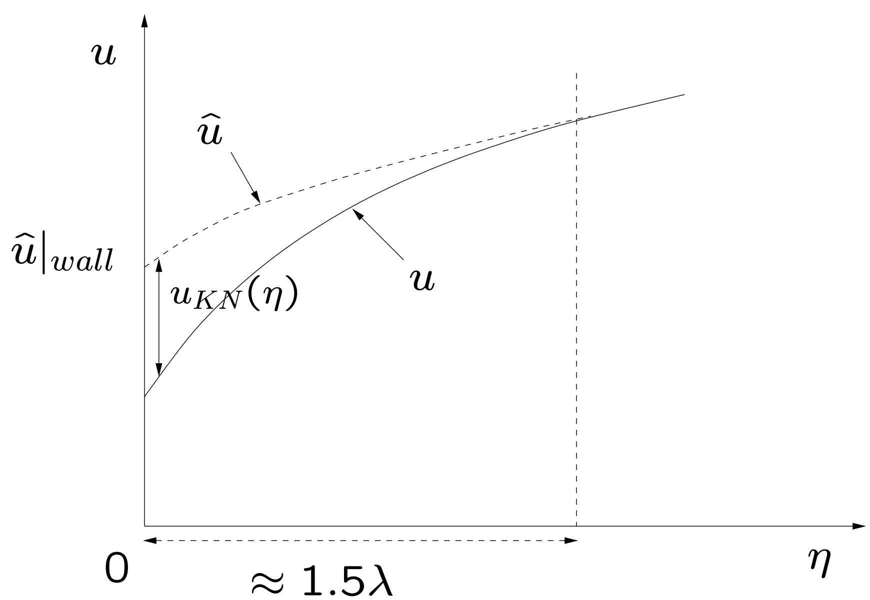
(Discuss isothermal flow; see [Sone, 2002] for details and non-isothermal case)

- The (Boltzmann solution for) tangential flow speed, u, is given by

$$u = \widehat{u} + u_{KN}$$

  - $\widehat{u}$ = Navier-Stokes component of flow
  - u_{KN} = Knudsen layer correction, $\to 0$ as $\eta/\lambda \to \infty (\gg \lambda)$

- Slip-flow conditions provide effective boundary conditions for $\widehat{u}$, the Navier-Stokes component of the flow



- Constitutive relation remains the same (by definition!).
- Slip-flow relation:

$$\hat{u}_{gas}|_{wall} - u_w = \alpha(\sigma_v, gas)\lambda \frac{d\hat{u}}{d\eta}|_{wall}$$

  Some results:

  – For $\sigma_v \to 0$

$$\alpha(\sigma_v \to 0, gas) \to \frac{2}{\sigma_v}$$

  – For $\sigma_v = 1$

$$\alpha(\sigma_v = 1, BGK) = 1.1467 \;\; \text{[Cercignani, 1962]}$$

$$\alpha(\sigma_v = 1, HS) = 1.11 \;\; \text{[Ohwada et al., 1989]}$$

  Fairly insensitive to molecular model but still different from Maxwell model

$$\alpha(\sigma_v = 1) = \frac{2 - \sigma_v}{\sigma_v}|_{\sigma_v = 1} = 1$$

- Experiments: For engineering (dirty) surfaces in air suggest that σ_v is close to one [Bird, 1994]
  Recent results: $\sigma_v \approx 0.85 - 0.95$ (see e.g. [Karniadakis & Beskok, 2002])
  HOWEVER recent experiments typically use Maxwell form

$$\alpha = \frac{2 - \sigma_v}{\sigma_v}$$

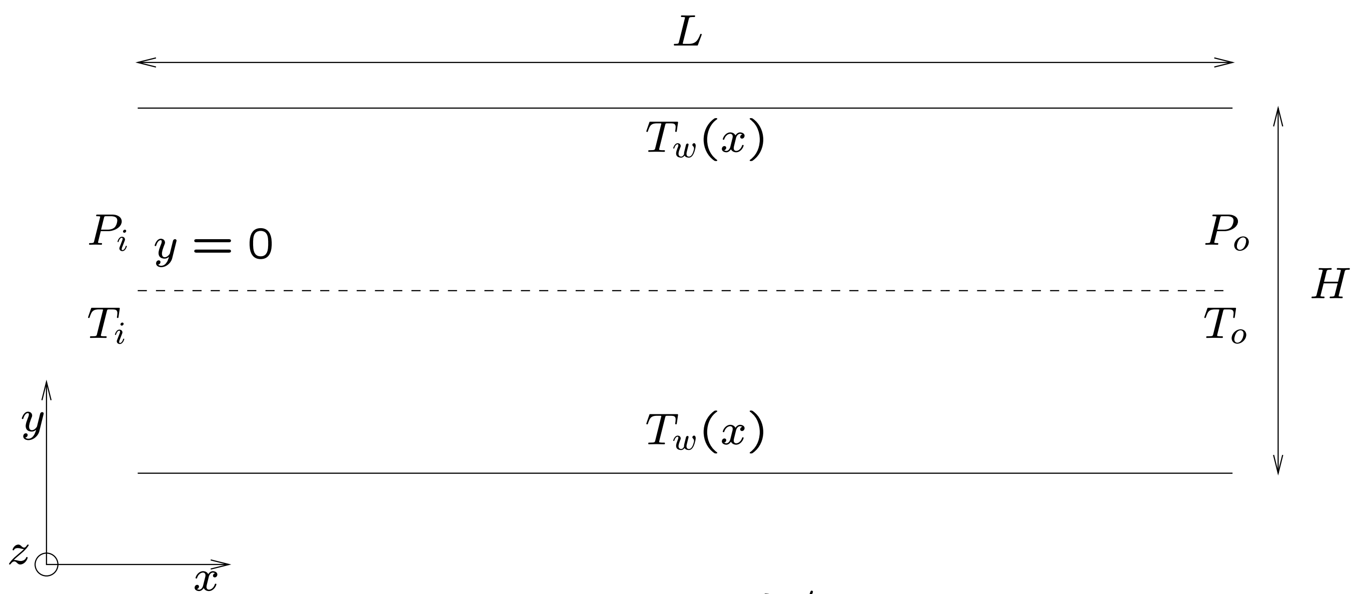
  which is **inconsistent with Boltzmann theory** in the $\sigma_v \to 1$ limit

  – Note: the upper limit 0f 0.95 is probably not an accident but perhaps a manifestation of the fact that $\alpha(\sigma_v = 1) \approx$ 1.1...*

*(2-0.95)/0.95=1.11!

Flow Physics beyond Navier-Stokes

Microchannels are the predominant building blocks in small scale devices. For simple problems studied here assume $\sigma_v = \sigma_T = 1$.

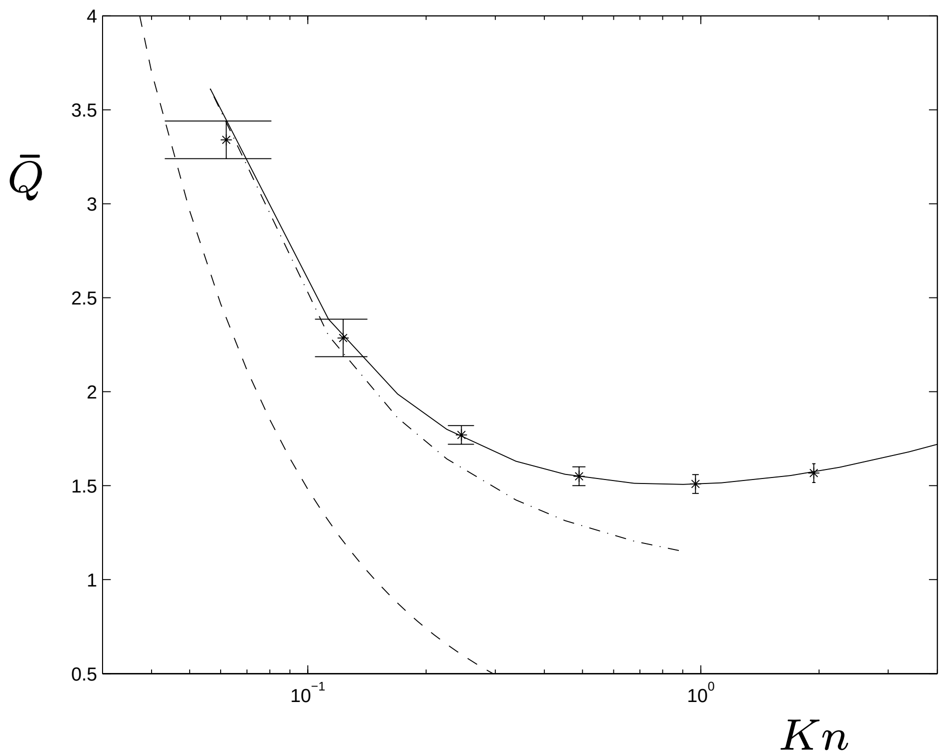


$$Kn = \lambda / H$$

Example: Pressure-driven flow in a channel

(Linear regime)

"Poiseuille" flowrate for arbitrary Knudsen number can be scaled using the following expression [Knudsen (1909)] (experiments)



$$\bar{Q} = \frac{\dot{Q}}{-\frac{1}{P}\frac{dP}{dx}H^2\sqrt{\frac{RT}{2}}}$$

Navier-Stokes/slip-flow result (dashed line/dash-dotted line)

$$\dot{Q} = -\frac{H^3}{12\mu}\frac{dP}{dx}(1 + 6\alpha Kn)$$

$$\Rightarrow \bar{Q} = \frac{\sqrt{\pi}}{12Kn}(1 + 6\alpha Kn)$$

Solid line: Numerical solution of the Boltzmann equation [Ohwada, Sone & Aoki, 1989]

Stars: DSMC simulation

“Wave” propagation in channels

Plane axial waves: Steady state response to oscillatory forcing

- Solution based on realization that in transition regime channels, for reasonable frequencies, inertia will be negligible.
- In Navier-Stokes regime, inertia is negligible when $S = \sqrt{\omega H^2/\nu} \ll 1$. When $S \ll 1$, solution is effectively quasi-steady [Lamb (1898)]; because $Pr \approx 1$ for a gas, flow is also isothermal.
- At $H \approx 1\mu$m inertia negligible for $\omega \lesssim O(10^6) rad/s$.
- When inertia is negligible, equation of motion

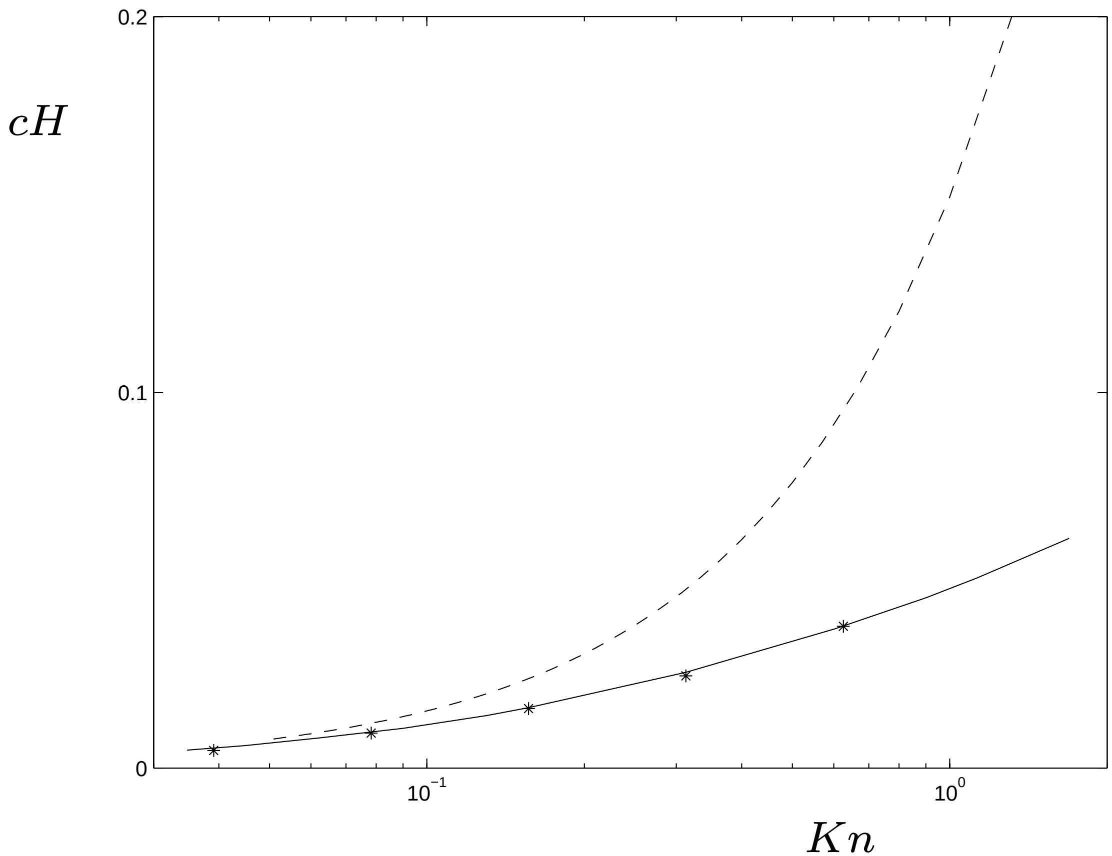
$$\rho \frac{\partial u}{\partial t} = \frac{\partial \tau_{xy}}{\partial y} - \frac{\partial P}{\partial x} \quad \text{becomes} \quad \frac{\partial \tau_{xy}}{\partial y} = \frac{\partial P}{\partial x}$$

  i.e. oscillatory response *locally* governed by steady pressure-driven flow characteristics.
- Integrate across channel to formulate in terms of “Knudsen’s $\bar{Q}$” (no need to know the velocity field) [Hadjiconstantinou, 2002&2003]

Theoretical result (after using kinematics):

$$\beta^2 H^2 = (c + i\mathcal{K})^2 H^2 = \frac{8i\sqrt{\pi}}{Kn\bar{Q}}\frac{\tau_c}{\mathcal{T}}$$

$\mathcal{T} = 2\pi/\omega$, $\tau_c =$ molecular collision time



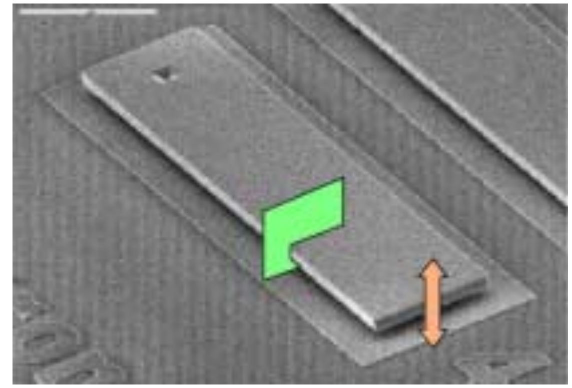
Solid line: Theory ($\bar{Q}$ tabulated)

Stars: DSMC

Dashes: Navier-Stokes (no slip)

Lubrication-type flows

Typical geometries of interest lend themselves naturally to lubrication-type analyses:



- e.g. Micro/nanocantilever motion close to a solid surface

  [Gallis & Torczynski, 2004]

- Extend Reynolds equation

$$\frac{d}{dx}\left[-\frac{\rho H^3}{12\mu}\frac{dP}{dx}+\frac{\rho HU}{2}\right]=-\frac{\partial(\rho H)}{\partial t}$$

  (here for 1-D, including "Couette" flow component) to arbitrary Kn [Fukui & Kaneko, 1988]:

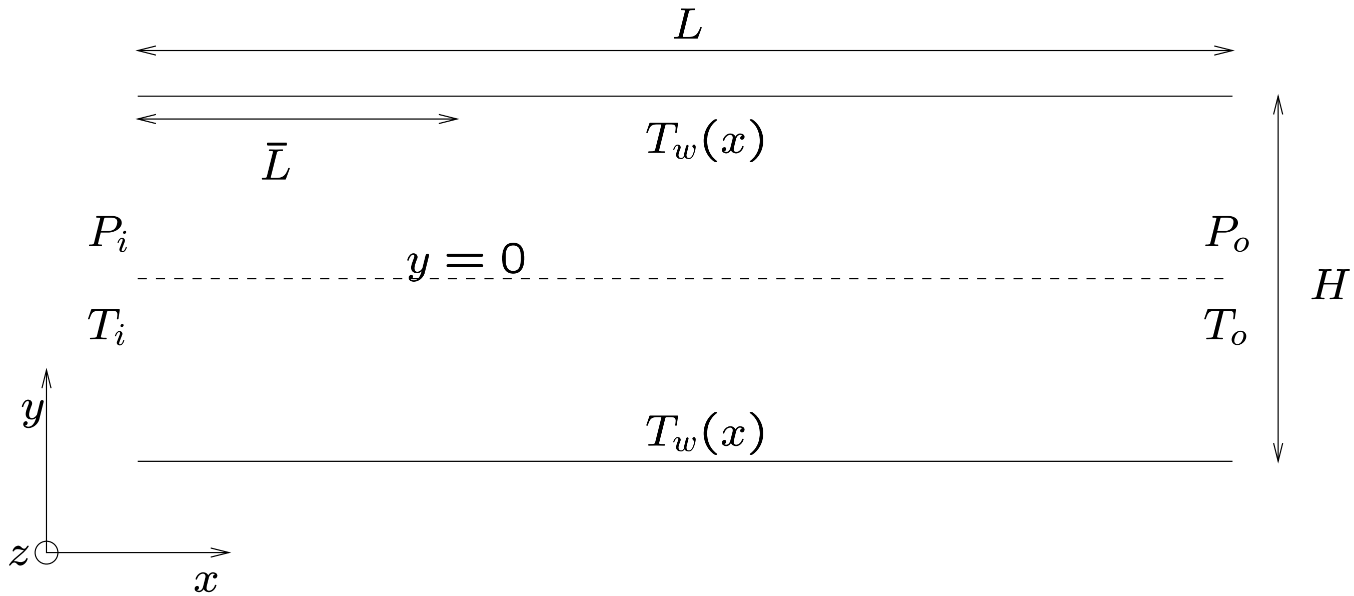
  – Couette flow rate unchanged by Knudsen number

  – $-\frac{\rho H^3}{12\mu}\frac{dP}{dx}$ replaced by $-\frac{\rho H^2}{P}\sqrt{\frac{RT}{2}}\bar{Q}(\sigma_v, Kn)\frac{dP}{dx}$

  – Thermal creep term may also be included (flowrate $\propto \bar{Q}_T(\sigma_T, Kn)\frac{dT}{dx}$)

Convective heat transfer in microchannels

"Graetz Problem"



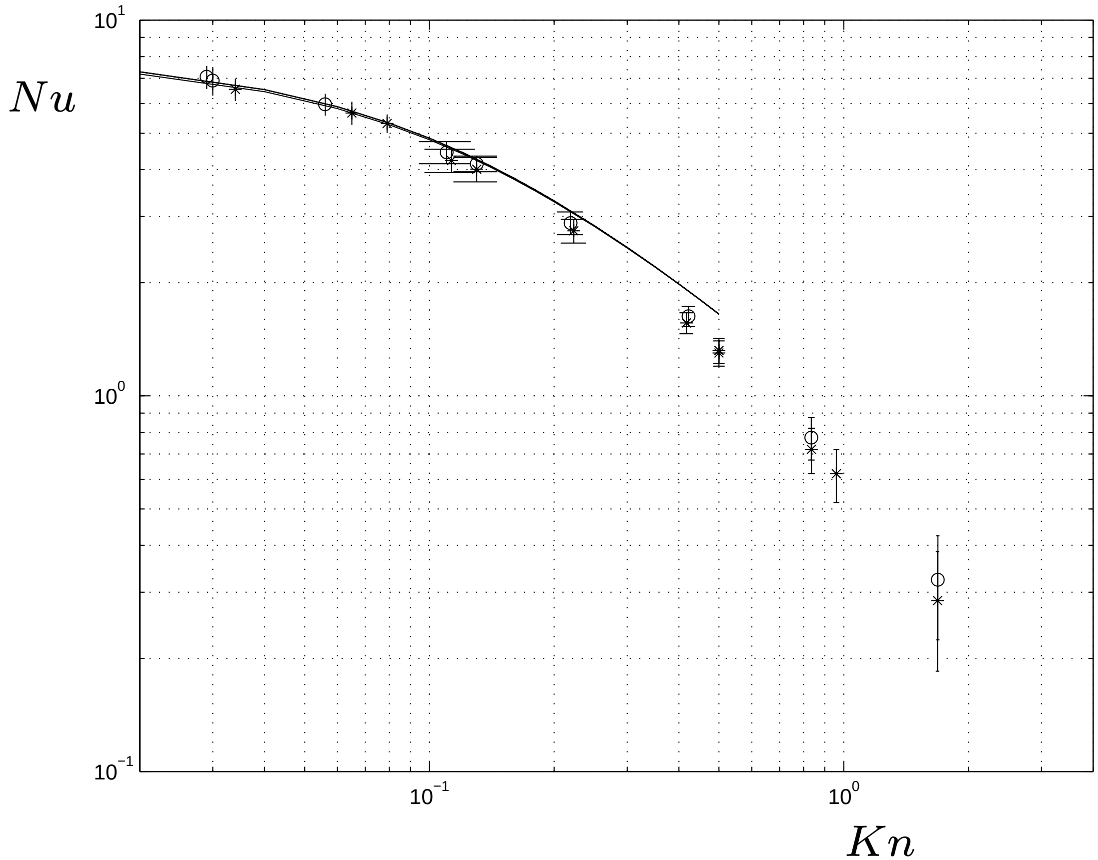
$$T_w(x) = T_i, \quad x < \bar{L}$$
$$T_w(x) = T_o, \quad x \geq \bar{L}$$

We are interested in the non-dimensional heat transfer coefficient between the gas and the wall (Nu)

$$h = \frac{q}{T_b - T_w}, \quad T_b = \frac{\int_A \rho u_x T dA}{\int_A \rho u_x dA}, \quad Nu = \frac{h2H}{\kappa} = \frac{q2H}{\kappa(T_b - T_w)}$$

Nusselt number as a function of Knudsen number

[Hadjiconstantinou & Simek, 2003]



*: DSMC $\frac{dT}{dx} > 0$

o: DSMC $\frac{dT}{dx} < 0$

- Slip flow accurate for $Kn \lesssim 0.1$
- Slip flow qualitatively robust beyond $Kn \approx 0.1$

Second-order slip models

Models which extend the Navier-Stokes description to $Kn \gtrsim 0.1$ (second-order slip models) are very desirable because:

- Numerical solutions of the Navier-Stokes description are orders of magnitude less costly than solutions of the Boltzmann equation
- The effort invested in Navier-Stokes simulation tools and solution theory for the last two centuries
- Improve accuracy of first-order slip-flow description around $Kn \approx 0.1$

A large number of empirical approaches have appeared (1969-2004) based on fitting parameters. **Do not work except for the flow they have been fitted for**

A second-order slip model for the hard-sphere gas
[Hadjiconstantinou, 2003&2005]

- RIGOROUS asymptotic theory worked out for BGK gas [Cercignani, 1964; Sone 1965-1971] but overlooked because...
- BGK model not good approximation to reality–Did not match experiments/typical simulations (hard-sphere, VHS,...)
- Model discussed here "conjectures" second-order BGK asymptotic theory can be used for hard spheres, appropriately modifies
  - Should get us close to experiments–currently lacking!
  - If successful, approach can be extended to other models
- Assumptions:
  - Steady flow–Not restrictive (see below)
  - 1-D–Can be relaxed
  - $M \ll 1 \quad (Re \sim \frac{M}{Kn} \ll 1)$
  - Flat walls–Can be relaxed to include wall curvature

The model
[Hadjiconstantinou, 2003 & 2005]

$$\hat{u}_{gas}|_{wall} - u_w = \alpha\lambda \frac{d\hat{u}}{d\eta}|_{wall} - \beta\lambda^2 \frac{d^2\hat{u}}{d\eta^2}|_{wall}$$ (Captures $\hat{u}$ component only!)

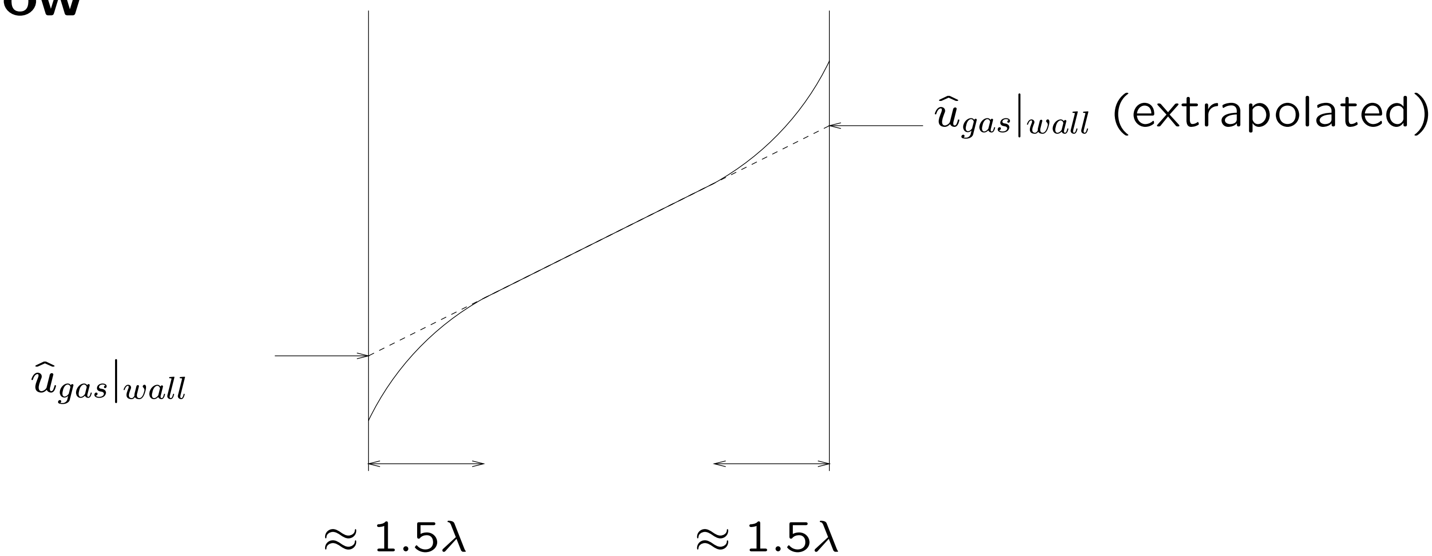
$$\bar{u} = \frac{1}{H}\int_{-H/2}^{H/2}\left[\hat{u} + \xi\lambda^2 \frac{\partial^2 \hat{u}}{\partial y^2}\right] dy$$ (includes Knudsen layer correction)

- $\alpha = 1.11$
- $\beta = 0.61$
- $\xi = 0.3$ (same as BGK value ...)
- **Coefficients NON-ADJUSTABLE**
- **Gas viscosity NON-ADJUSTABLE**

NOTE: Knudsen layer contribution to $\bar{u}$ is $O(Kn^2)$

Recall...

- **Slip-flow boundary conditions provide effective boundary conditions for $\hat{u}$, the Navier-Stokes component of the flow**



- For $Kn \gtrsim 0.1$ Knudsen layer covers a substantial part of the physical domain!

- Existence of Knudsen layer means that the correct second-order slip model is the one that **does not agree** with DSMC within 1.5λ from the walls! Explains why fitting DSMC data has not produced a reliable model.

Comments

- Results below: Steady flow=quasisteady *at the molecular collision time*
- In Poiseuille flow, where curvature of $\hat{u}$ is constant, a correction of the form

$$\bar{u} = \frac{1}{H}\int_{-H/2}^{H/2}\left[\hat{u} + \xi\lambda^2\frac{\partial^2\hat{u}}{\partial y^2}\right]dy$$

  results in an "effective" second-order slip coefficient of $\beta - \xi$. In other words, while

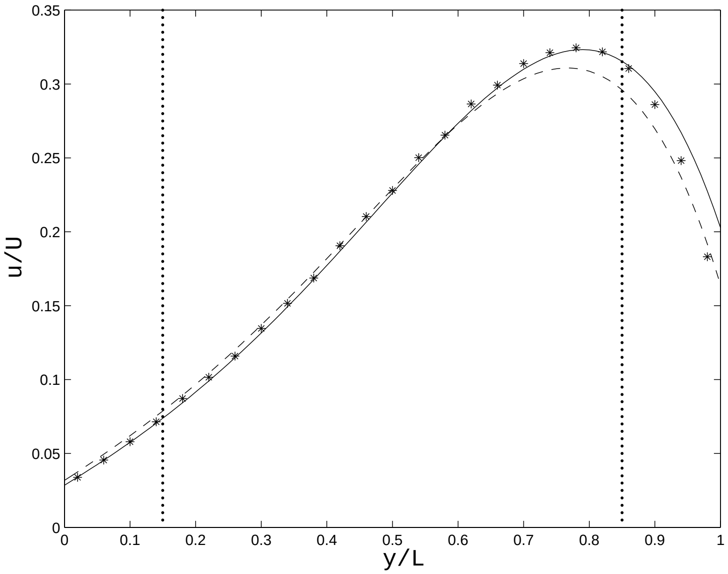
$$\frac{1}{H}\int_{-H/2}^{H/2}\hat{u}dy = -\frac{H^2}{2\mu}\frac{dP}{dx}\left(\frac{1}{6} + \alpha Kn + 2\beta Kn^2\right)$$

$$\bar{u} = \frac{1}{H}\int_{-H/2}^{H/2}\left[\hat{u} + \xi\lambda^2\frac{\partial^2\hat{u}}{\partial y^2}\right]dy = -\frac{H^2}{2\mu}\frac{dP}{dx}\left(\frac{1}{6} + \alpha Kn + 2(\beta - \xi)Kn^2\right)$$

- An experiment **measuring flowrate** in pressure-driven flows in order to measure β, **in fact** measures the **effective** second-order slip coefficient $\beta - \xi = 0.31$
- Recent experiments [Maurer et al., 2003] measure $''\beta''$(in reality $\beta - \xi$) $= 0.25 \pm 0.1$.

Comparison with DSMC simulations of oscillatory Couette flow

$Kn = 0.1,\ S \approx 4$



Flow profile at $t = \mathcal{T}/2$

Solid line: Second-order slip model

Dashed line: First-order slip model

Stars: DSMC

Vertical lines: Knudsen layer extent (approx)

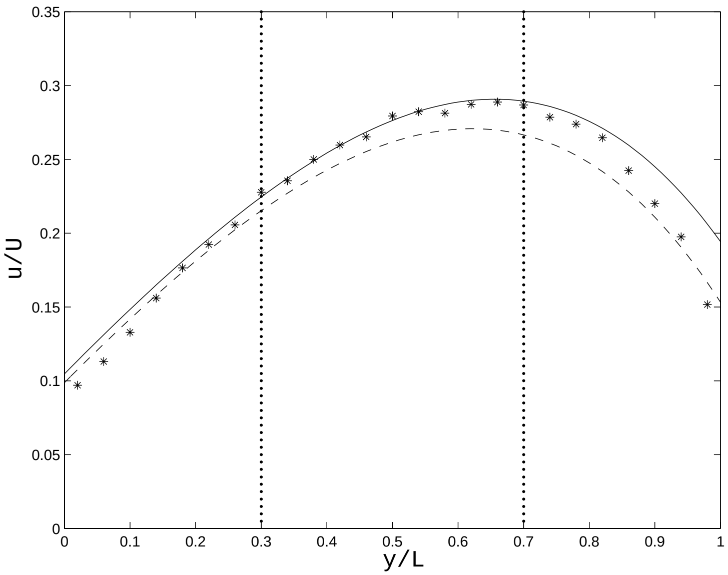
$\bar{u} = 0.196\ (DSMC: 0.200)$

$\tau_w^l = 0.27\ (DSMC: 0.28 \pm 0.04)$

$\tau_w^r = 1.33 (DSMC: 1.39 \pm 0.04)$

Comparison with DSMC simulations of oscillatory Couette flow

$Kn = 0.2,\ S \approx 2$

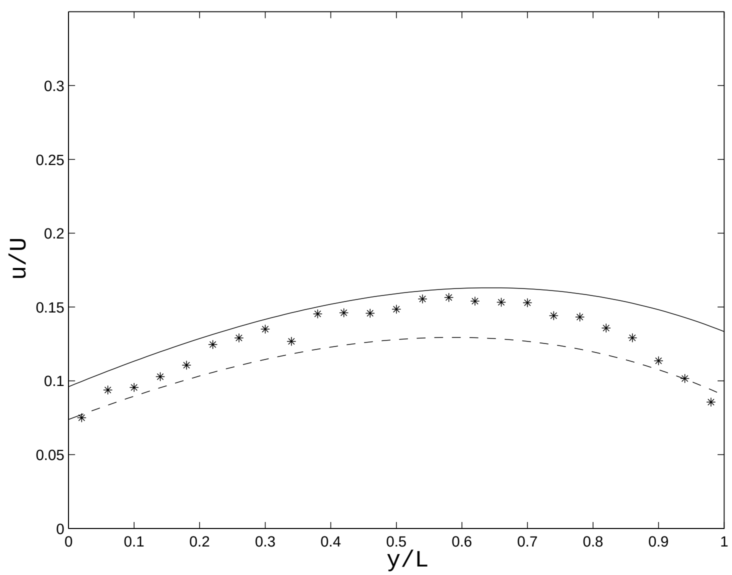


$\bar{u} = 0.221\ (DSMC : 0.226)$

$\tau_w^l = 0.45\ (DSMC : 0.43 \pm 0.02)$

$\tau_w^r = 0.62(DSMC : 0.62 \pm 0.02)$

$Kn = 0.4,\ S \approx 1$

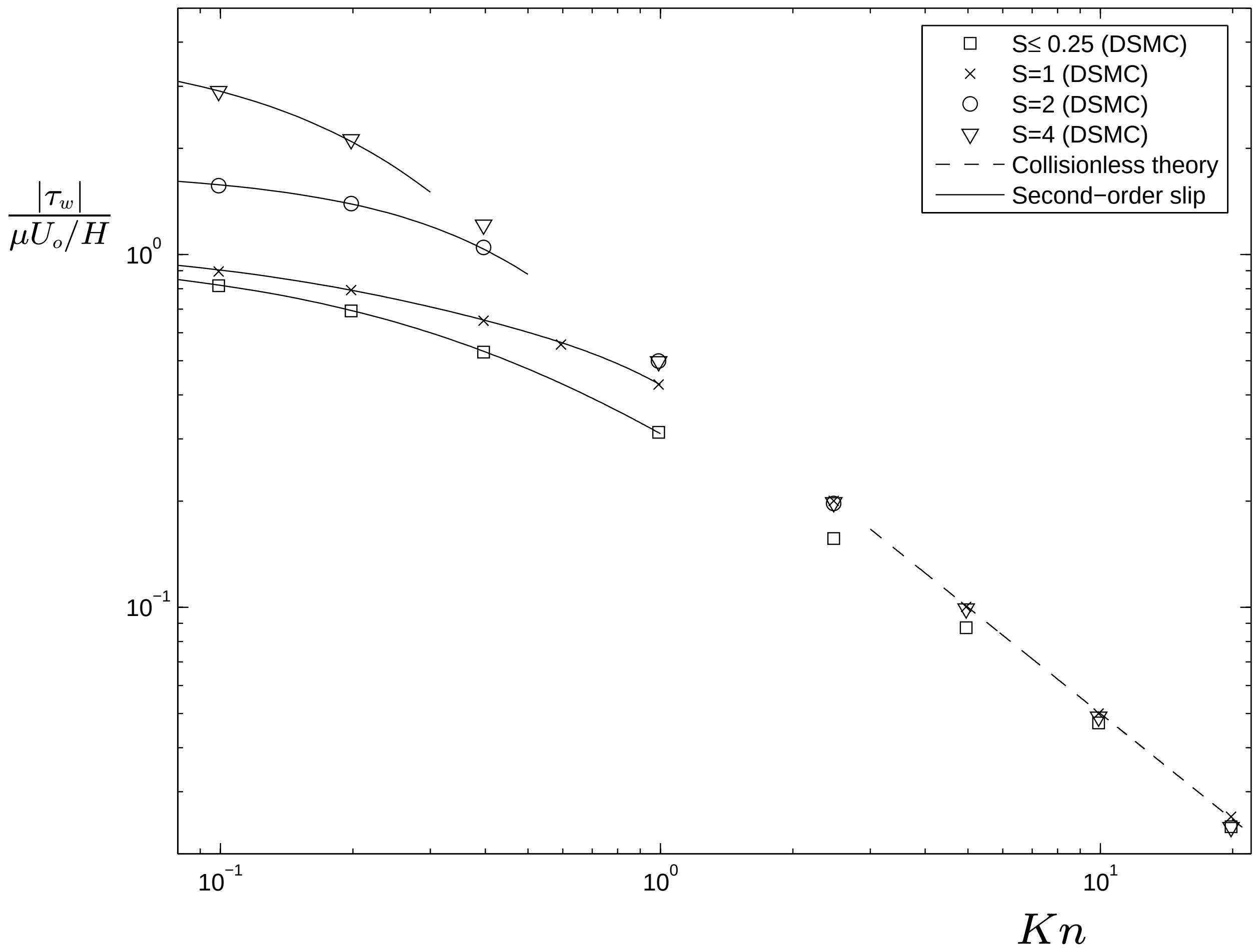


$\bar{u} = 0.127(DSMC : 0.128)$

$\tau_w^l = 0.18\ (DSMC : 0.18 \pm 0.01)$

$\tau_w^r = 0.175(DSMC : 0.18 \pm 0.01)$

Comparison for stress amplitude at the driven wall

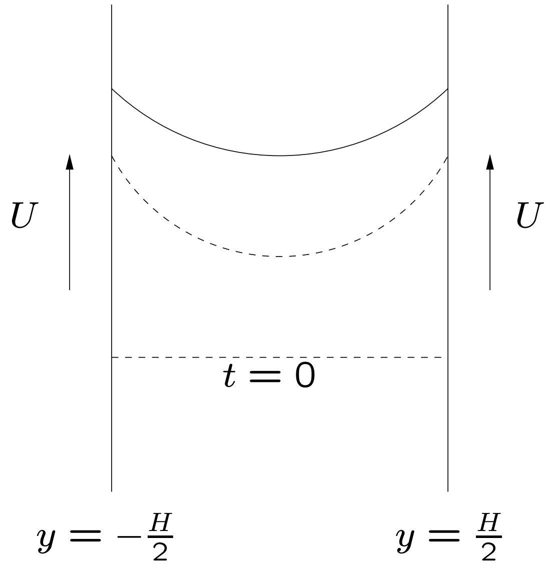


Collisionless Theory:

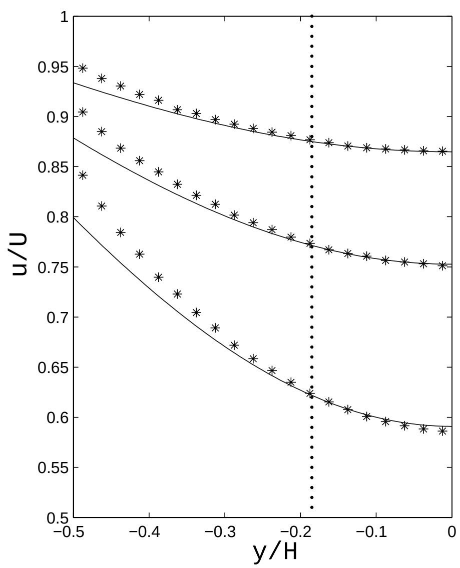
$$\frac{|\tau_w|}{\mu U_o/H} = \frac{1}{2Kn}$$

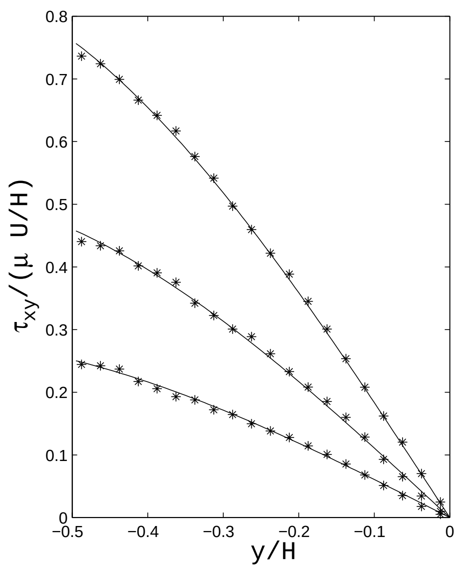
In some cases, second-order slip combined with a collisionless theory **comes close** to bridging the gap

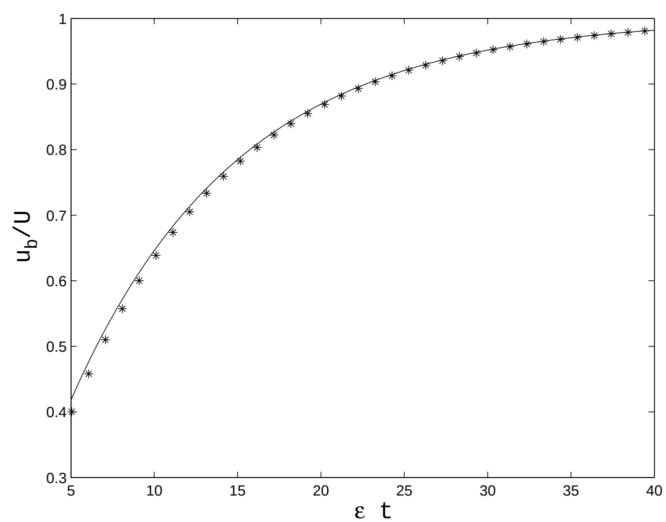
Comparison for an "Impulsive Start Problem" at $Kn = 0.21$



Half-domain $-0.5 \leq y/H \leq 0$ shown



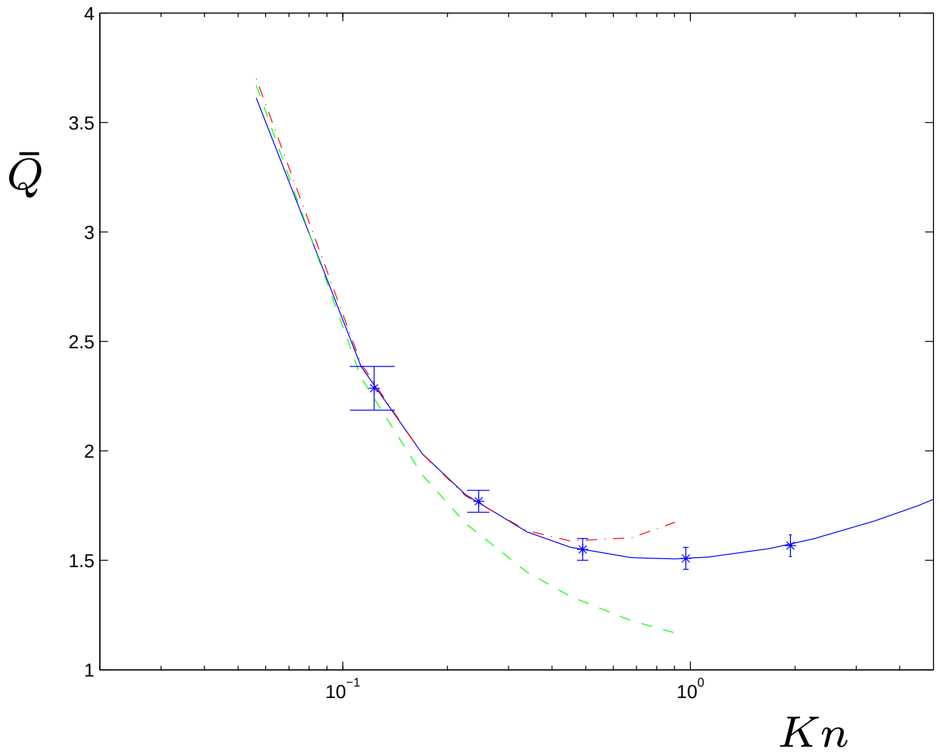




Normalized velocity   Normalized Stress   Average velocity ($\bar{u}$) vs time

Three snapshots at $t = 4.1\tau_c,\ 7.5\tau_c,\ 14.2\tau_c$

Comparison for pressure-driven flow in a channel



Solid line: Boltzmann equation solution by Ohwada et al.

Stars: DSMC

Dashed line: First order slip model, $\alpha = 1.11,\ \beta = 0$

Dash-dotted line: Second order slip model, $\alpha = 1.11,\ \beta = 0.61\ \xi = 0.3$

Recent Developments in Simulation

- DSMC: Solves the Boltzmann equation in the limit of vanishing discretization [Wagner, 1992]
- DSMC second-order accurate transport coefficients in Δx [Alexander, Garcia & Alder, 1998]
- Symmetrized splitting scheme in DSMC is second-order accurate in time [Ohwada, 1998]
- DSMC second-order accurate transport coefficients in Δt (symmetrized) [Hadjiconstantinou, 2000; Garcia&Wagner, 2000]
- Transport of small spherical particles in DSMC [Gallis, Torczynski & Rader, 2001]
- Higher moments of the Chapman-Enskog distribution captured accurately by DSMC [Gallis, Rader &Torczynski, 2004]
- Variance reduction [Baker & Hadjiconstantinou, 2005]
- Quasi-Newton methods for steady states using variance reduction [Al-Mohssen, Hadjiconstantinou & Kevrekidis, 2005]

Final Remarks

- Viscous constitutive relation robust up to $Kn \approx 0.5$ (provided kinetic effects are taken into account). No place for adjustable viscosity
- Second-order slip requires even more care than first-order slip: e.g.
  - Second-order slip coefficient different for flow in tubes (wall curvature)
  - To second-order in Kn there exists slip (flow) normal to the wall
  - Knudsen layer contribution $\sim O(Kn^2)$ (to flow average)
- Gas-surface interaction: More complex models?
  $\alpha(\sigma_v \neq 1, HS/...) =?$
- Review by Sharipov & Seleznev (1998): useful compilation of basic facts/results (known at that time)

- Thanks for your attention
- Happy Thanksgiving!