Analytical and Numerical Normal Solutions of the Boltzmann Equation for Highly Nonequilibrium Fourier and Couette Flows

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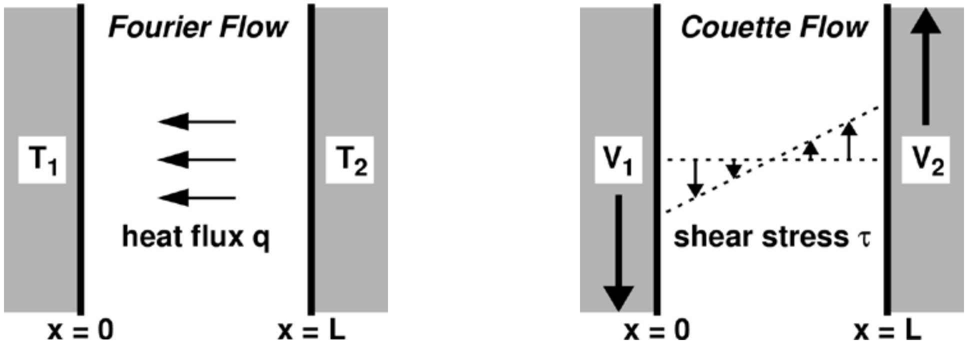
Canonical Gas Flows



Investigate Fourier flow and Couette flow

- One-dimensional steady heat flux, shear stress

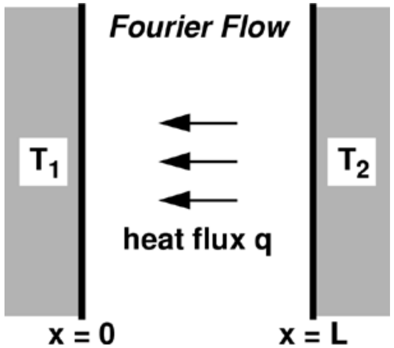
Determine normal solutions (outside Knudsen layers)

- Spatial/temporal dependence only via hydrodynamic fields
- Analytical method : Moment-Hierarchy (MH)
- Numerical method : Direct Simulation Monte Carlo (DSMC)

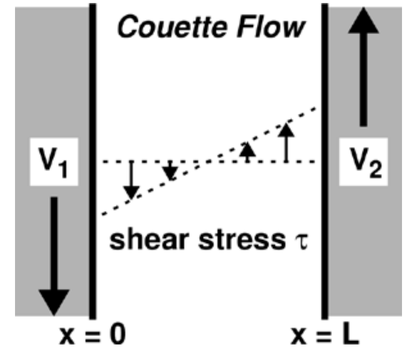
Consider high heat flux, shear stress

- Thermal conductivity, viscosity; velocity distribution
- Departure from Chapman-Enskog (CE) theory

Knudsen Number Definitions



System: $\mathrm{Kn}_L = \dfrac{\lambda}{L}$



Heat-flux: $\mathrm{Kn}_q = \dfrac{q}{mnc_m^3}$ Speed: $c_m = \sqrt{\dfrac{2k_B T}{m}}$ Shear-stress: $\mathrm{Kn}_\tau = \dfrac{\tau}{mnc_m^2}$

Three Knudsen numbers for Fourier-Couette flow

- System: thickness of Knudsen layers, wall effects
- Heat-flux, shear-stress: local, finite gradient over λ

Constraints on Kn_L, Kn_q, Kn_τ

- CE, MH normal solutions: $\mathrm{Kn}_L << 1$
- CE (additional): $\mathrm{Kn}_q << 1$, $\mathrm{Kn}_\tau << 1$
- DSMC: computational intensity grows as $\mathrm{Kn} \to 0$

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Chapman-Enskog Theory

$$f = f^{(0)}(1+\Phi^{(1)}+\Psi^{(1)}) \qquad \Phi^{(1)} = -(8/5)\tilde{A}[\tilde{c}](\tilde{\mathbf{c}}\cdot\tilde{\mathbf{q}}) \qquad \Psi^{(1)} = -2\tilde{B}[\tilde{c}](\tilde{\mathbf{c}}^{\circ}\tilde{\mathbf{c}}:\tilde{\tau})$$

$$S_j^{(k)}[x] = \sum_{i=0}^{k} \frac{(j+k)!\,(-x)^i}{(j+i)!\,i!\,(k-i)!} \qquad \tilde{A}[\tilde{c}] = \sum_{k=1}^{\infty}(a_k/a_1)S_{3/2}^{(k)}[\tilde{c}^2] \qquad \tilde{B}[\tilde{c}] = \sum_{k=1}^{\infty}(b_k/b_1)S_{5/2}^{(k-1)}[\tilde{c}^2]$$

$$K_{\mathrm{ref}} = \frac{K_\infty}{K_1}\frac{\mu_1}{\mu_\infty}\frac{15k_B}{4m}\mu_{\mathrm{ref}} \qquad \mathbf{q} = -K\nabla T \qquad \tau = \mu\left\{(\nabla\mathbf{V}+\nabla\mathbf{V}^{\mathrm{T}})-(2/3)(\nabla\cdot\mathbf{V})\mathbf{I}\right\}$$

- **Chapman-Enskog (CE) velocity distribution function**
  - **Normal solution (outside Knudsen layers)**
  - **Expansion for small heat flux q and shear stress τ (relative to molecular quantities)**
- **CE values for IPL molecules (inverse-power-law)**
  - **Thermal conductivity and viscosity: K and μ**
  - **Sonine-polynomial coefficients: a_k/a_1 and b_k/b_1**
  - **Applicable when $\mathrm{Kn}_L \ll 1$, $\mathrm{Kn}_q \ll 1$, $\mathrm{Kn}_\tau \ll 1$**

Moment-Hierarchy Method

$$M_{k_1k_2k_3} = \int \tilde{c}_x^{k_1}\tilde{c}_y^{k_2}\tilde{c}_z^{k_3}\,\tilde{f}[\tilde{\mathbf{c}}]d\tilde{\mathbf{c}} = \left\langle \tilde{c}_x^{k_1}\tilde{c}_y^{k_2}\tilde{c}_z^{k_3} \right\rangle \qquad J_{k_1k_2k_3} = \int \tilde{c}_x^{k_1}\tilde{c}_y^{k_2}\tilde{c}_z^{k_3} J[\tilde{\mathbf{c}} \mid \tilde{f}, \tilde{f}]d\tilde{\mathbf{c}}$$

$$J_{k_1k_2k_3} = \mathrm{Bilinear}\left[\left\{M_{k_1k_2k_3}\right\}\right] \qquad M_{k_1k_2k_3}[\mathrm{Kn}_q, \mathrm{Kn}_\tau] = \sum_{j=0}^{k_1+k_2+k_3-2} \mu_{k_1k_2k_3}^{(j)}[\mathrm{Kn}_\tau]\mathrm{Kn}_q^j$$

$$K_{\mathrm{eff}}/K = F_K[\mathrm{Kn}_\tau] = 1 - c_K\mathrm{Kn}_\tau^2 + \mathrm{O}[\mathrm{Kn}_\tau^4] \qquad \mu_{\mathrm{eff}}/\mu = F_\mu[\mathrm{Kn}_\tau] = 1 - c_\mu\mathrm{Kn}_\tau^2 + \mathrm{O}[\mathrm{Kn}_\tau^4]$$

$$a_k/a_1 = (-1)^{k-1}\sum_{j=1}^{k-1} A_{kj}\mathrm{Kn}_q^{2j} \qquad b_k/b_1 = (-1)^{k-1}\sum_{j=1}^{k-1} B_{kj}\mathrm{Kn}_q^{2j}$$

Moment-Hierarchy (MH) normal solution

- **MH solution extends CE solution to finite Kn_q and Kn_τ**
- **Solve Boltzmann eqn recursively for Maxwell molecules**
- **Collision-term moments bilinear in distribution moments**
- **Tij, Santos, and co-workers: theory, computer algebra**

Compare MH and DSMC for Maxwell molecules

- **Differences between IPL, VSS, VHS Maxwell molecules**
- **Dependence of K_{eff}, μ_{eff}, a_k/a_1, b_k/b_1 on Kn_q and Kn_τ**

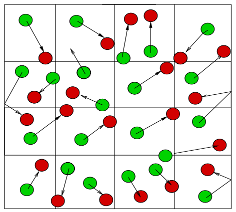
DSMC Method of Bird

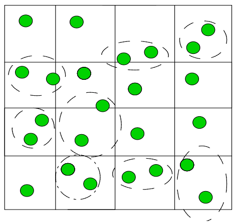
$$q = K_{\text{eff}} \left(\frac{\partial T}{\partial x} \right) \qquad \frac{a_k}{a_1} = \sum_{i=1}^{k} \left(\frac{(-1)^{i-1} k!(5/2)!}{(k-i)!i!(i+(3/2))!} \right) \left(\frac{\langle \tilde{c}^{2i} \tilde{c}_x \rangle}{\langle \tilde{c}^{2} \tilde{c}_x \rangle} \right) \qquad \tilde{\mathbf{c}} = \frac{\mathbf{v} - \mathbf{V}}{c_m}$$

$$\tau = \mu_{\text{eff}} \left(\frac{\partial V}{\partial x} \right) \qquad \frac{b_k}{b_1} = \sum_{i=1}^{k} \left(\frac{(-1)^{i-1} (k-1)!(5/2)!}{(k-i)!(i-1)!(i+(3/2))!} \right) \left(\frac{\langle \tilde{c}^{2(i-1)} \tilde{c}_x \tilde{c}_y \rangle}{\langle \tilde{c}_x \tilde{c}_y \rangle} \right) \qquad c_m = \sqrt{\frac{2k_B T}{m}}$$

DSMC moments of velocity distribution function

- **Temperature T, velocity V**
- **Heat flux q, shear stress τ**
- **Higher-order moments**

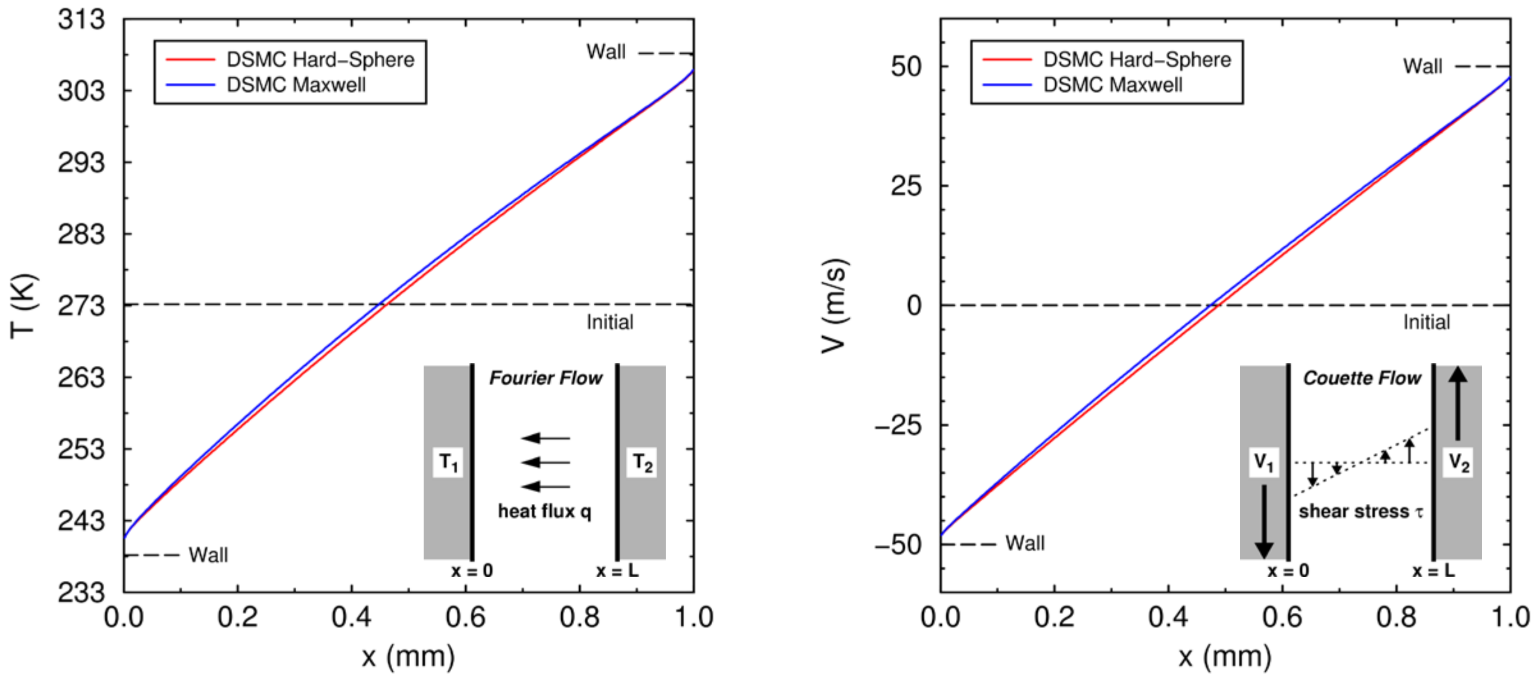




DSMC values for VSS molecules (variable-soft-sphere)

- **Thermal conductivity and viscosity: K_{eff} and μ_{eff}**
- **Sonine-polynomial coefficients: a_k/a_1 and b_k/b_1**
- **Applicable for arbitrary Kn_L, Kn_q, Kn_τ**

Temperature and Velocity Profiles

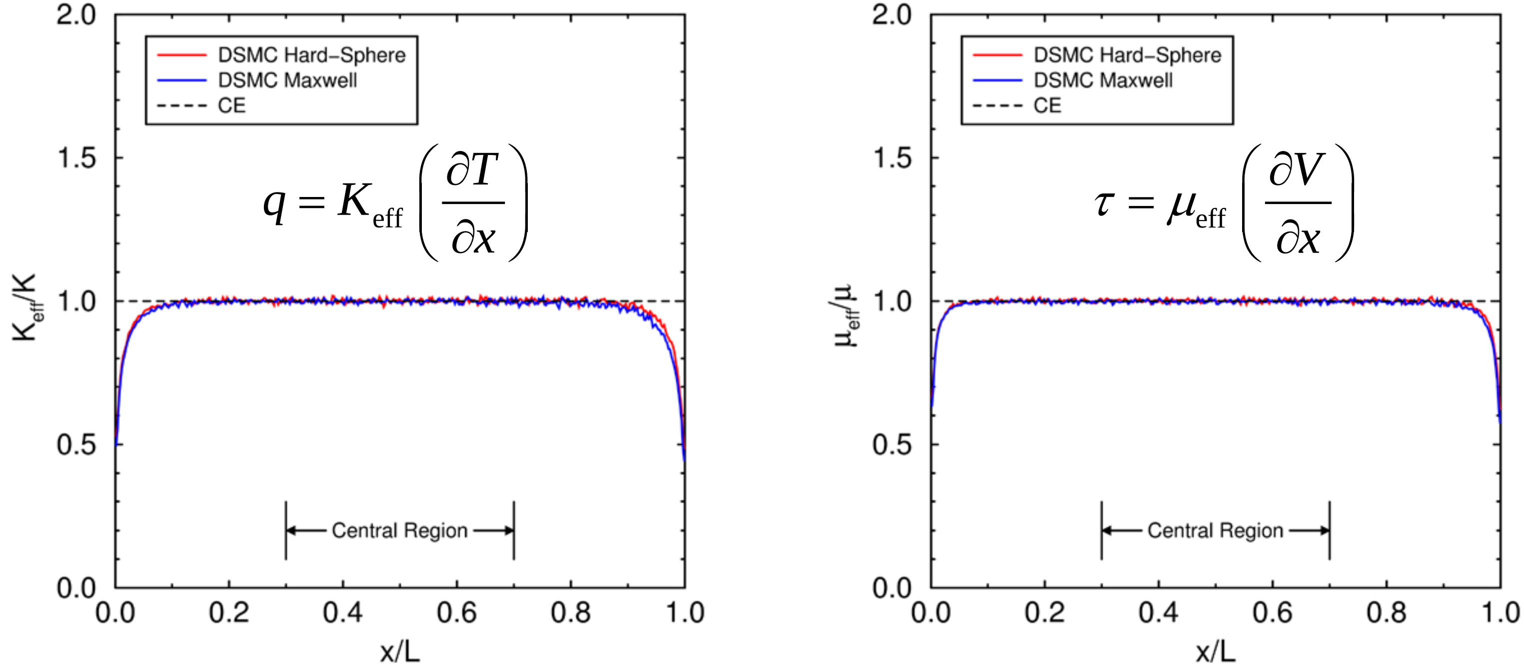


Low heat flux and shear stress: $Kn_q = 0.006$, $Kn_\tau = 0.003$

Small temperature jumps, velocity slips

- **Argon-like: initial $T = 273.15$ K, $p = 266.644$ Pa, $\lambda = 24$ μm**
- **Walls: $L = 1$ mm $= 42\lambda$, $\Delta T = 70$ K, $\Delta V = 100$ m/s**
- **$N_c = 120$, $\Delta t = 7$ ns, $\Delta x = 2.5$ μm, ~10^9 samples/cell, 32 runs**

Transport Coefficient Profiles

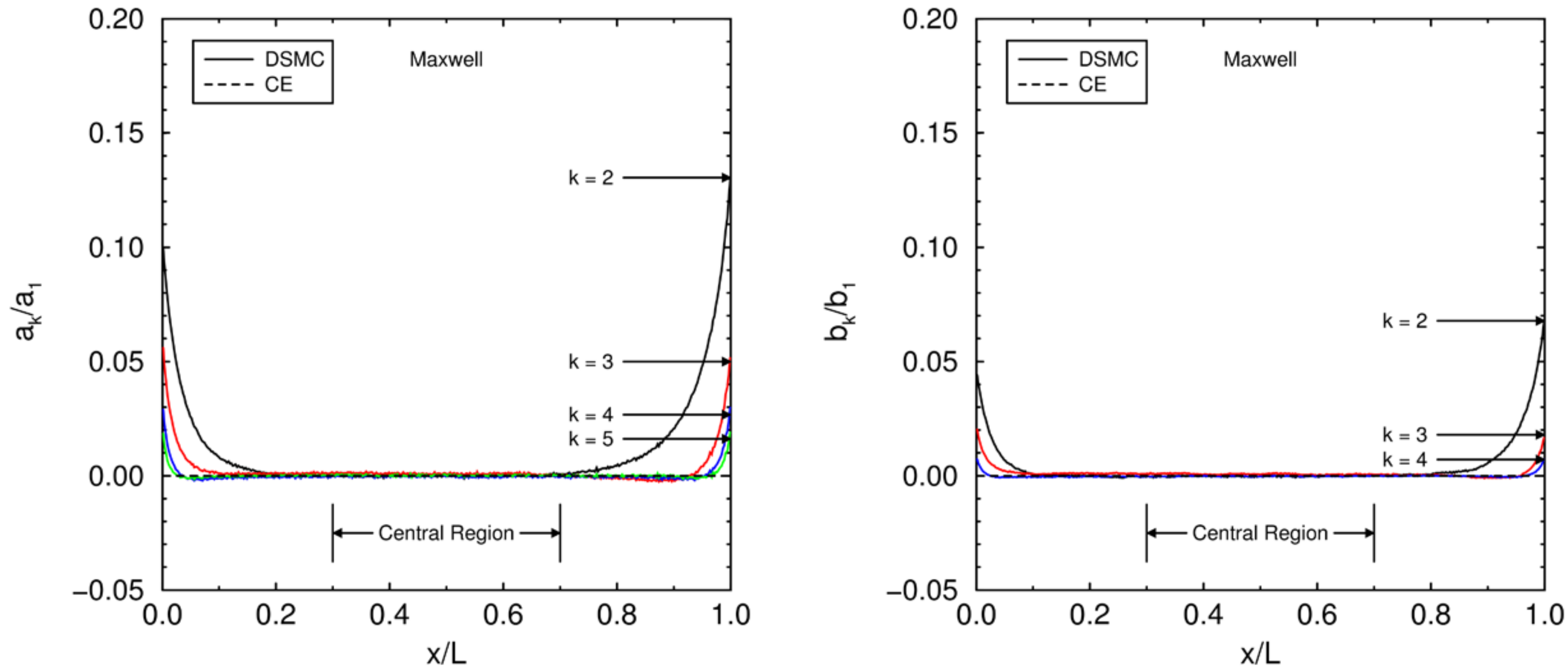


Low heat flux, low shear stress: $\mathbf{Kn_q = 0.006}$, $\mathbf{Kn_\tau = 0.003}$

Thermal conductivity K and viscosity μ

- **CE and DSMC agree in central region: normal solution**
- **Knudsen layers at walls: ~10% of domain each**

Maxwell Sonine-Coefficient Profiles

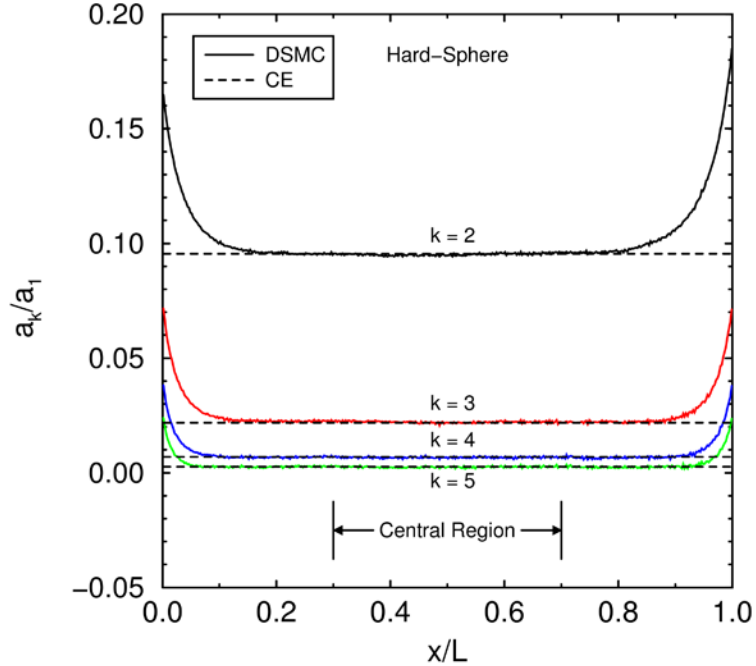


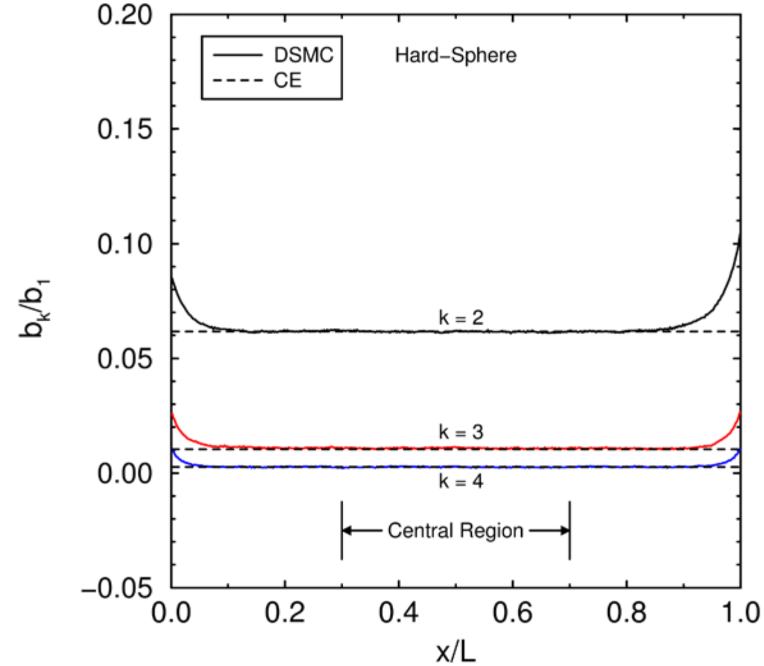
Low heat flux, low shear stress: $\mathrm{Kn}_q = 0.006$, $\mathrm{Kn}_\tau = 0.003$

Maxwell Sonine-polynomial coefficients a_k/a_1, b_k/b_1

- **CE and DSMC agree in central region: normal solution**
- **Knudsen layers at walls: ~10% of domain each**

Hard-Sphere Sonine-Coefficient Profiles



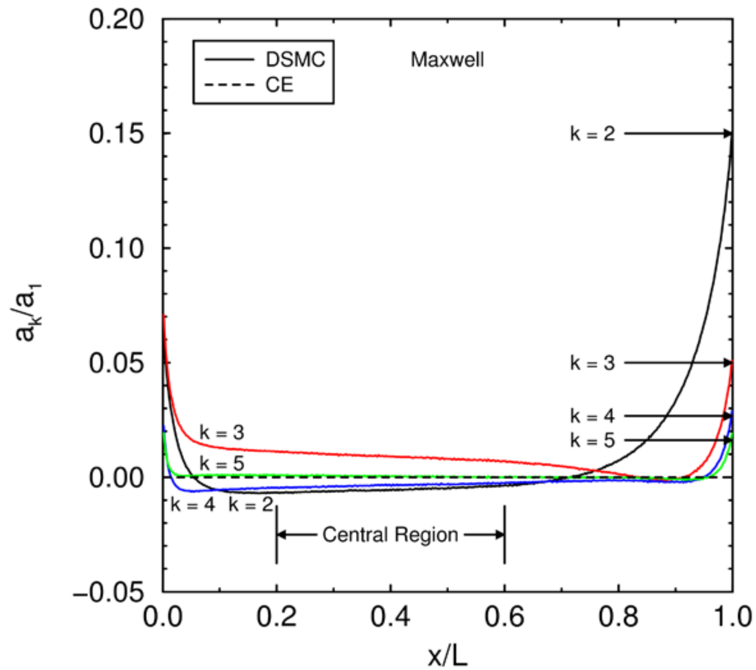


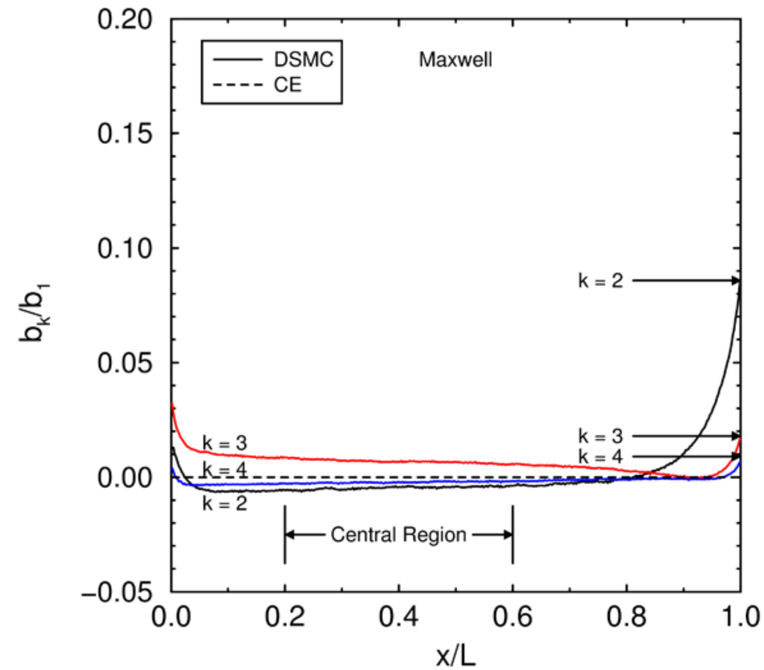
Low heat flux, low shear stress: $\mathrm{Kn}_q = 0.006$, $\mathrm{Kn}_\tau = 0.003$

Hard-sphere Sonine-polynomial coefficients a_k/a_1, b_k/b_1

- **CE and DSMC agree in central region: normal solution**
- **Knudsen layers at walls: ~10% of domain each**

Maxwell Sonine-Coefficient Profiles





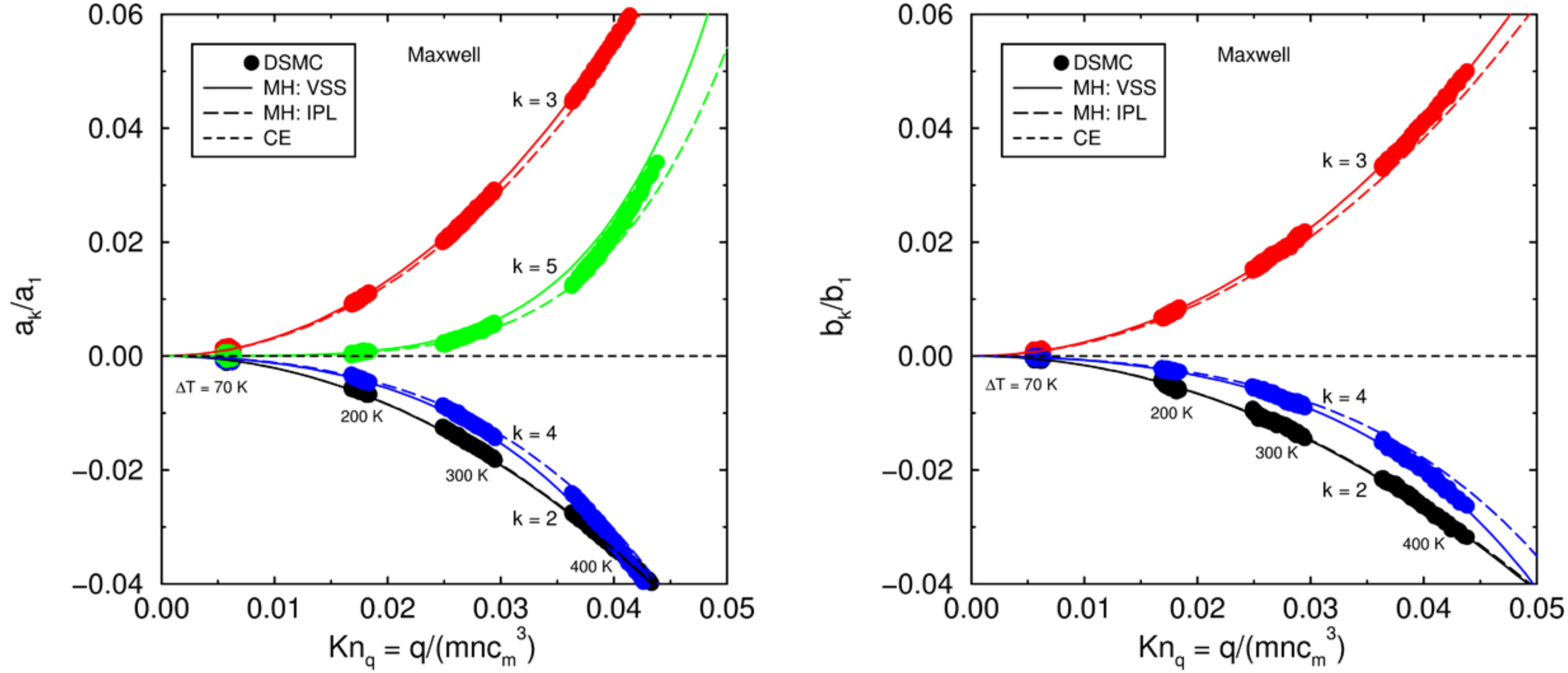
Finite heat flux, low shear stress: $\mathrm{Kn}_q \sim 0.017$, $\mathrm{Kn}_\tau = 0.003$

Maxwell Sonine-polynomial coefficients a_k/a_1, b_k/b_1

- **CE and DSMC differ in central region: Kn_q not small**
- **Normal solution is nonuniform: $\mathrm{Kn}_q \sim T^{-1/2}$ and $T = T[x]$**

Plot DSMC values vs. Kn_q from central region

Maxwell Sonine Coefficients

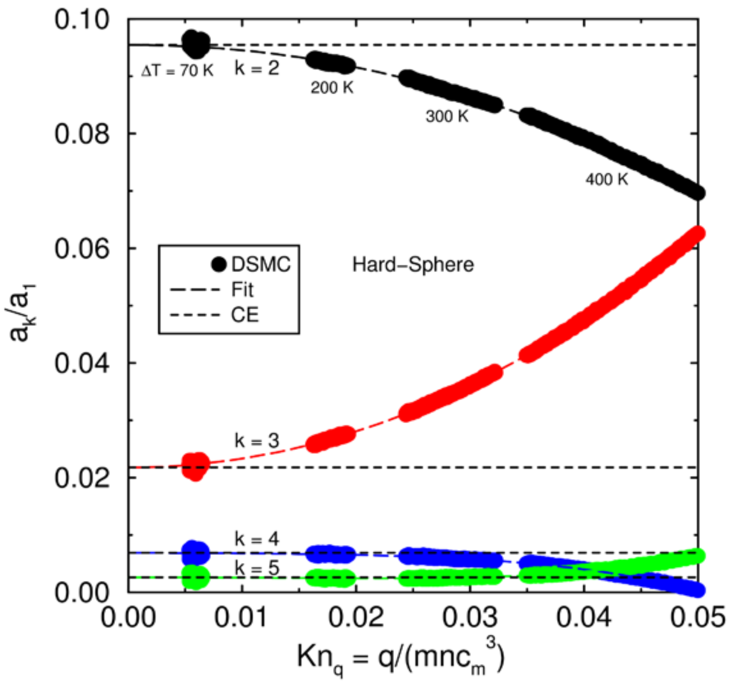


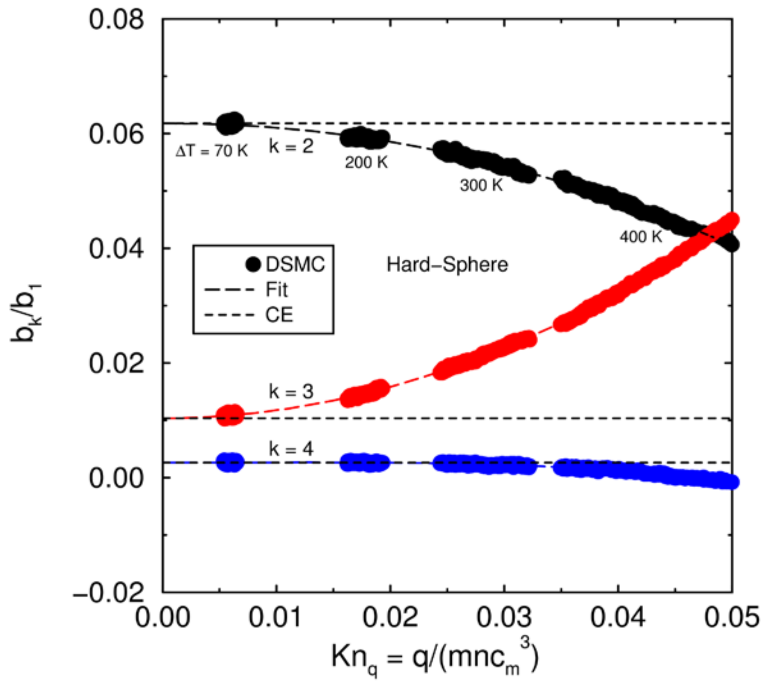
Maxwell normal solutions for a_k/a_1 and b_k/b_1

MH VSS-Maxwell and DSMC VSS-Maxwell agree

- **Four DSMC simulations: ΔT = 70, 200, 300, 400 K**
- **VHS-Maxwell and VSS-Maxwell are almost identical**
- **VSS-Maxwell and IPL-Maxwell differ noticeably**

Hard-Sphere Sonine Coefficients



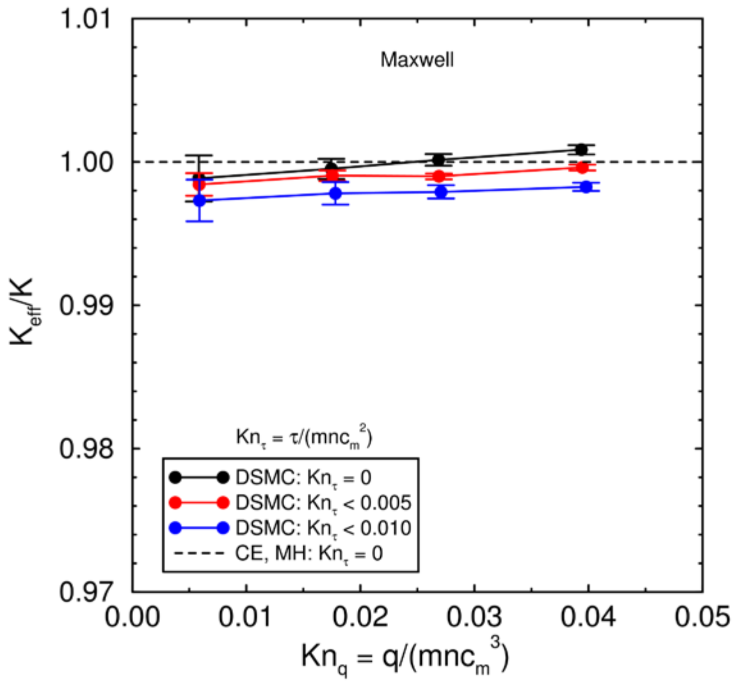


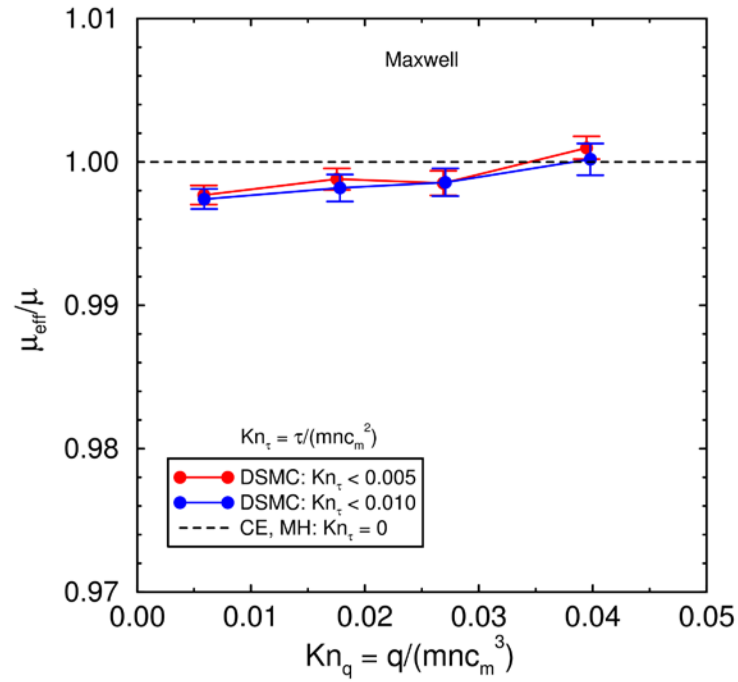
Hard-sphere normal solutions for a_k/a_1 and b_k/b_1

DSMC hard-sphere and VSS-Maxwell have same trends

- **Four DSMC simulations at same conditions as Maxwell**
- **No exact results available: MH does not apply**
- **Even-k terms decrease, odd-k terms increase**

Maxwell Transport Coefficients



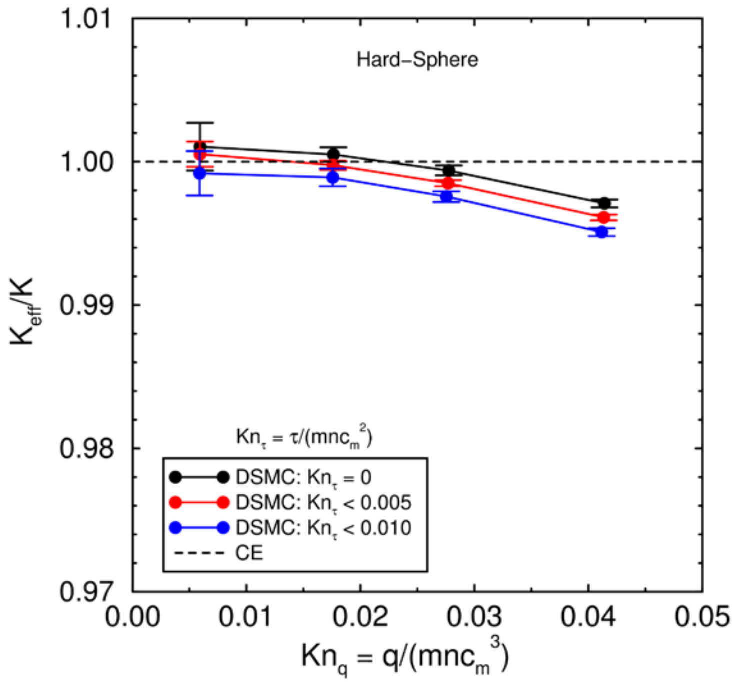


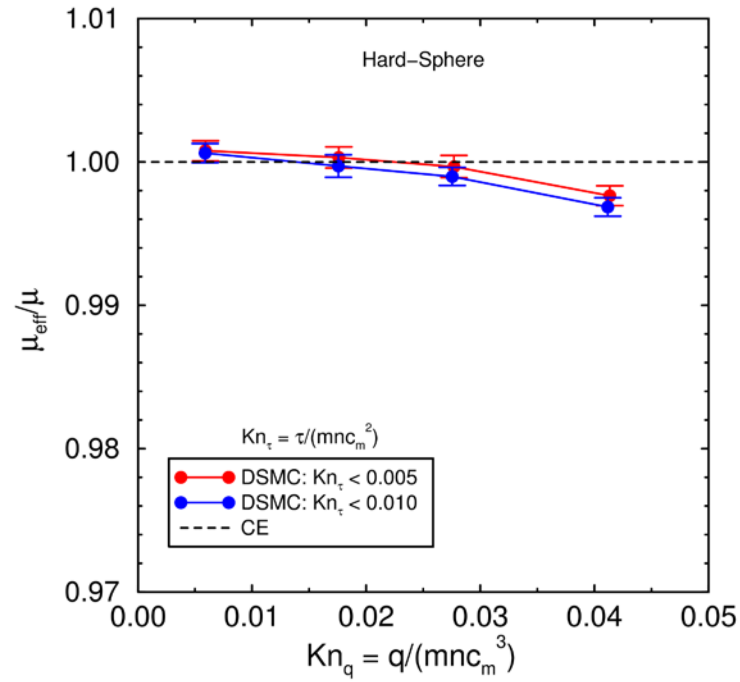
Maxwell normal solutions for K and μ

Maxwell transport coefficients are flux-independent

- **MH values for $\mathrm{Kn}_\tau = 0$ are independent of Kn_q**
- **DSMC values approach MH values as $\mathrm{Kn}_\tau \to 0$**
- **Difference is within discretization error**

Hard-Sphere Transport Coefficients





Hard-sphere normal solution for K and μ

Hard-sphere gas is "flux-insulating" and "flux-thinning"

- **No exact theoretical results available**
- **DSMC values decrease slightly with Kn_q**
- **Marginally greater than discretization error**

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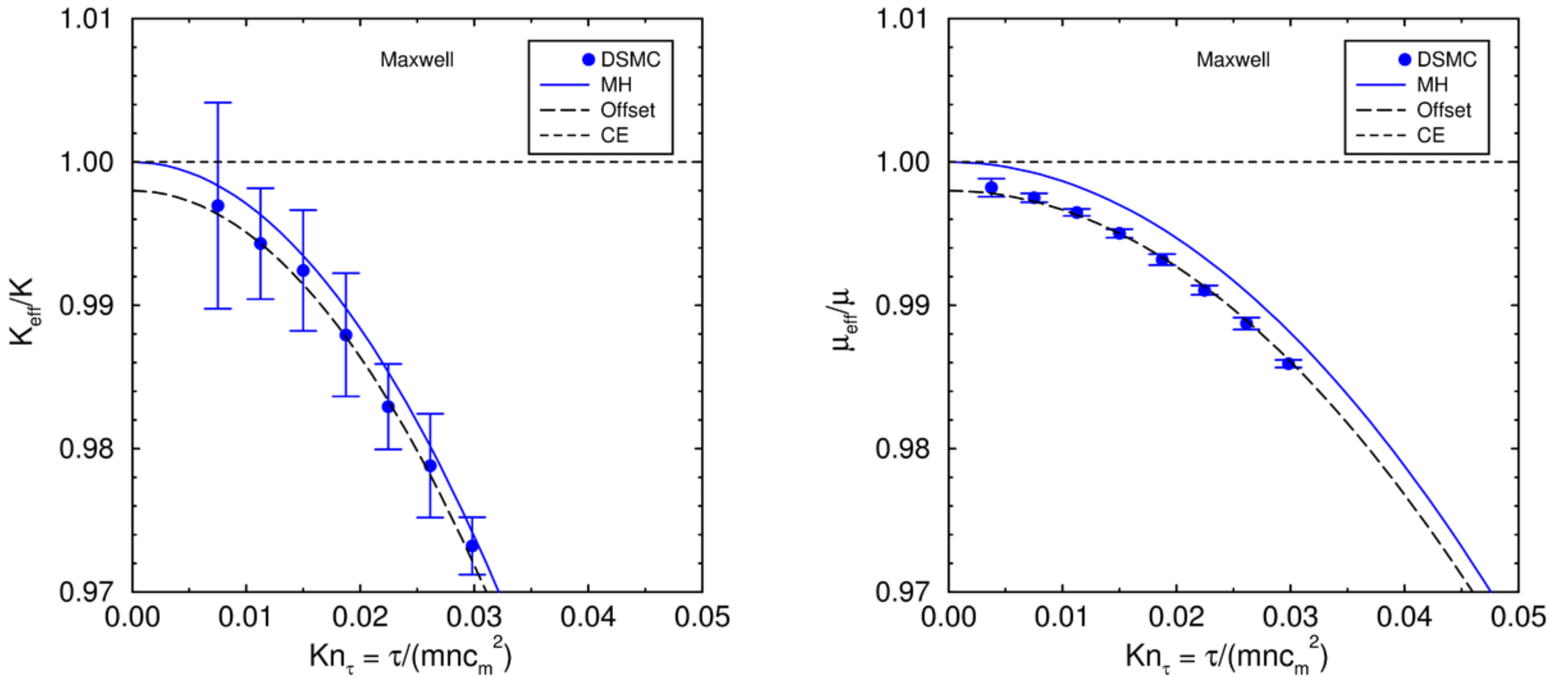
Maxwell Transport Coefficients



Maxwell normal solutions for K and μ

MH and DSMC agree to within discretization error

- **Eight DSMC simulations: $\Delta V = 100, \ldots, 800$ m/s**
- **Thermal conductivity from viscous heating, larger errors**
- **Offset MH to account for DSMC discretization error**

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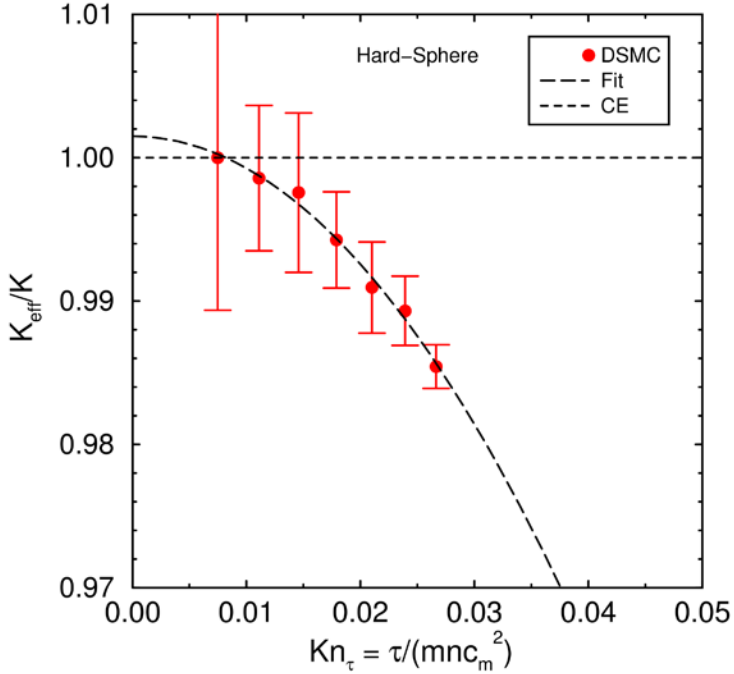
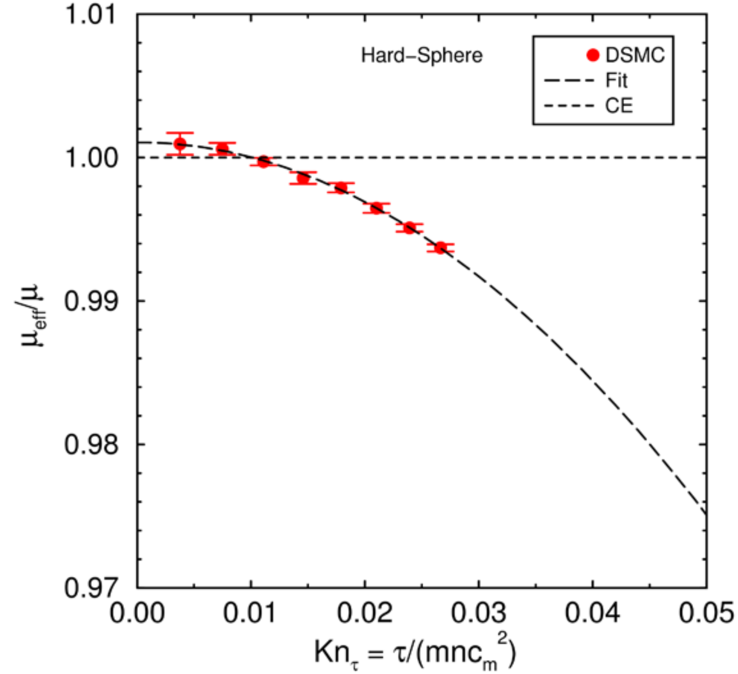
Hard-Sphere Transport Coefficients



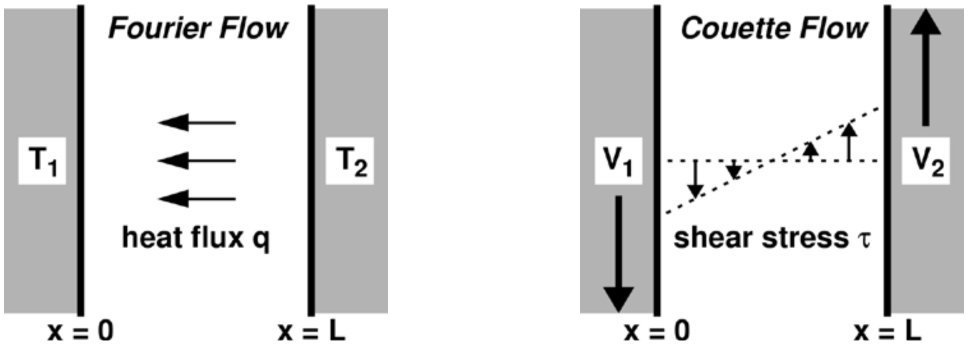


DSMC hard-sphere normal solution for K and μ

- **Finite Kn_τ (shear stress), low Kn_q (heat flux)**
- **No exact results available: MH does not apply**
- **DSMC values decrease with Kn_τ (like Maxwell)**

Hard-sphere gas: “shear-insulating” and “shear-thinning”

Conclusions



MH and DSMC have been applied to canonical gas flows
- Fourier flow: one-dimensional steady heat flux
- Couette flow: one-dimensional steady shear stress

MH and DSMC are in excellent agreement
- Chapman-Enskog at small heat flux, shear stress
- Maxwell molecules at finite heat flux, shear stress

Transport properties depend on heat flux, shear stress
- Maxwell: flux-independent, shear-insulating/thinning
- Hard-sphere: flux/shear-insulating/thinning

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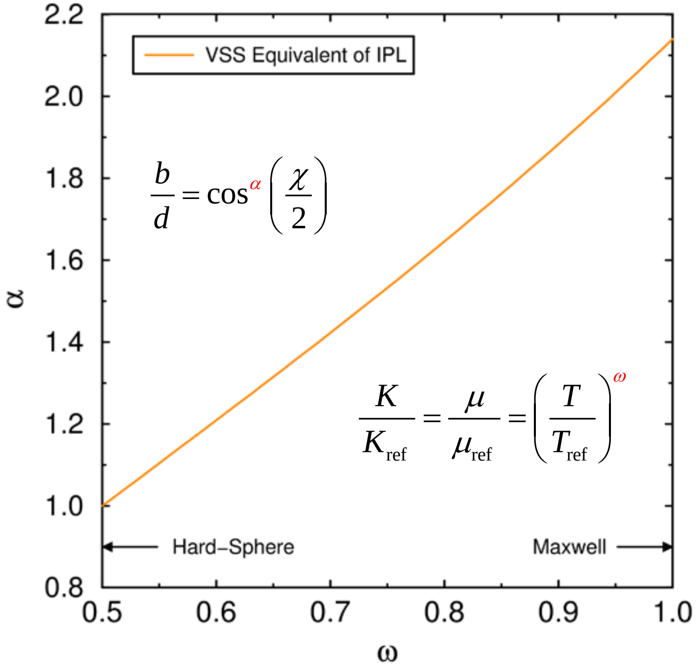
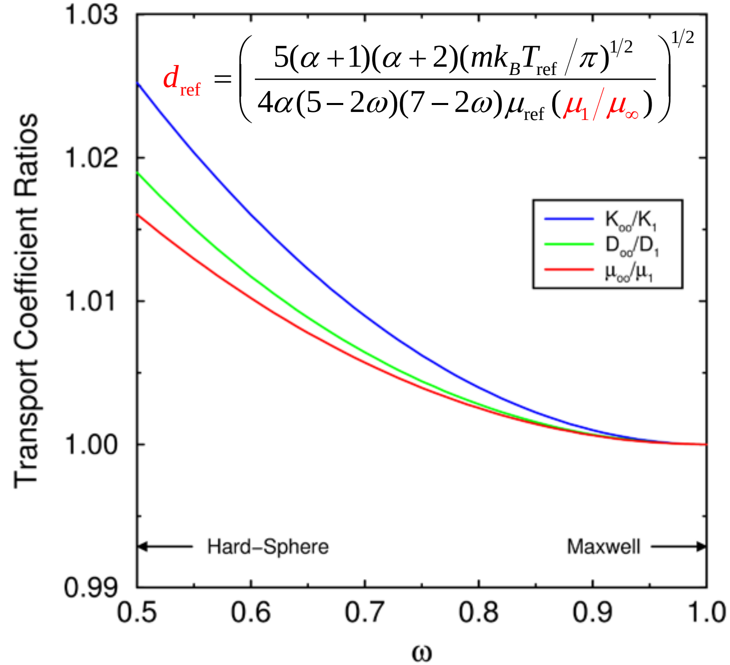
Backup Slides

IPL and VSS Molecules





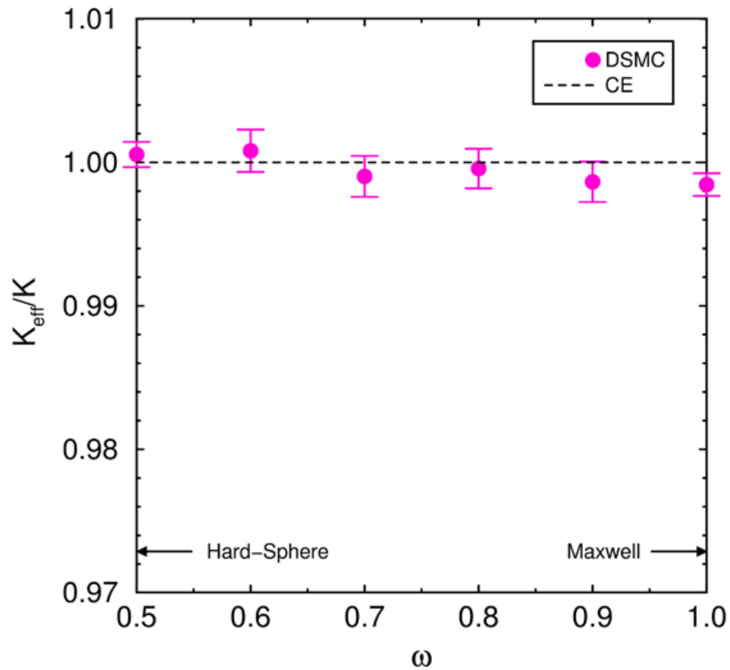
Best VSS ω, α to match IPL ω by equating diffusivities

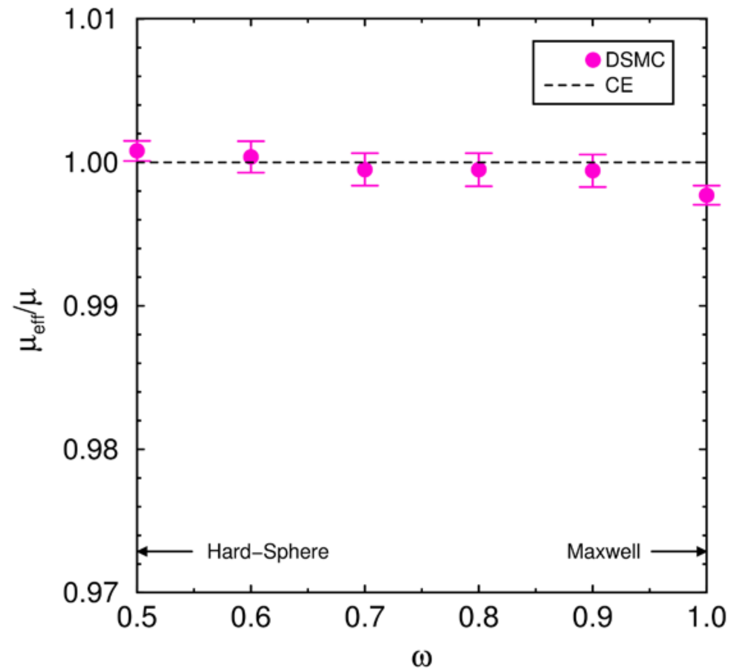
- **Identical match only for hard-sphere**
- **VSS-Maxwell ≠ IPL-Maxwell (they are very similar)**

Infinite-approximation CE changes K and μ by O(0.03)

- **Affects reference diameter d_{ref} very slightly**

Transport Coefficients



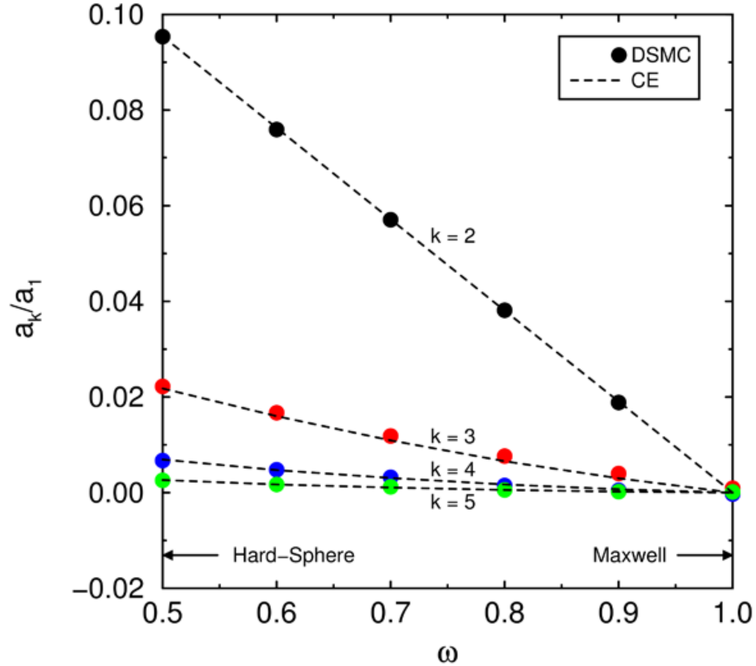


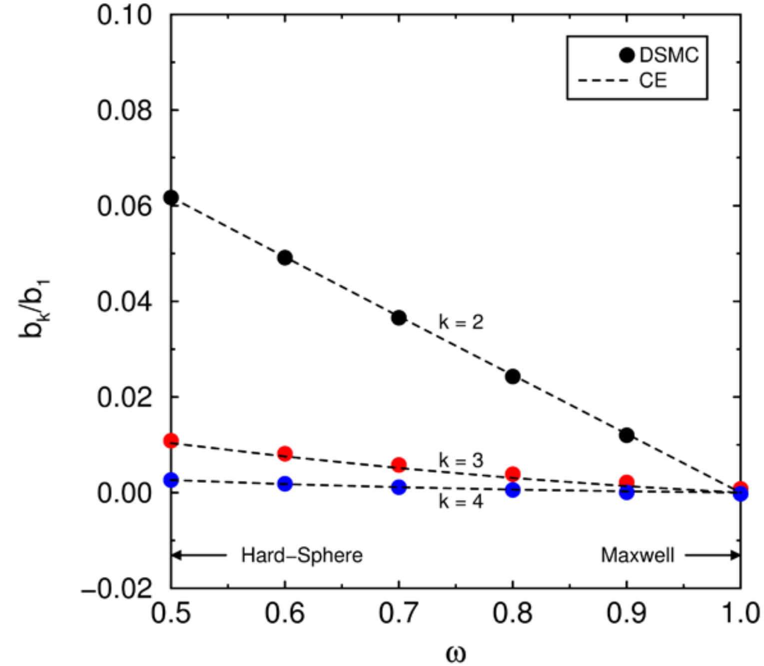
Thermal conductivity and viscosity for IPL molecules

- **Intermolecular force: hard-sphere through Maxwell**
- **Stochastic and discretization errors: ±0.002 each**
- **CE infinite-to-first-approximation difference: O(0.03)**

Excellent agreement between DSMC and CE

Sonine Coefficients





Sonine coefficients a_k/a_1 and b_k/b_1 for IPL molecules

- **Intermolecular force: hard-sphere through Maxwell**
- **Stochastic, discretization errors: smaller than symbols**

Good agreement between DSMC and CE

- **Higher-k coefficients have similar agreement**
- **Slight difference for $k = 3$, Kn_q not small enough**

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