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Convergence Behavior of Bird's Sophisticated DSMC Algorithm

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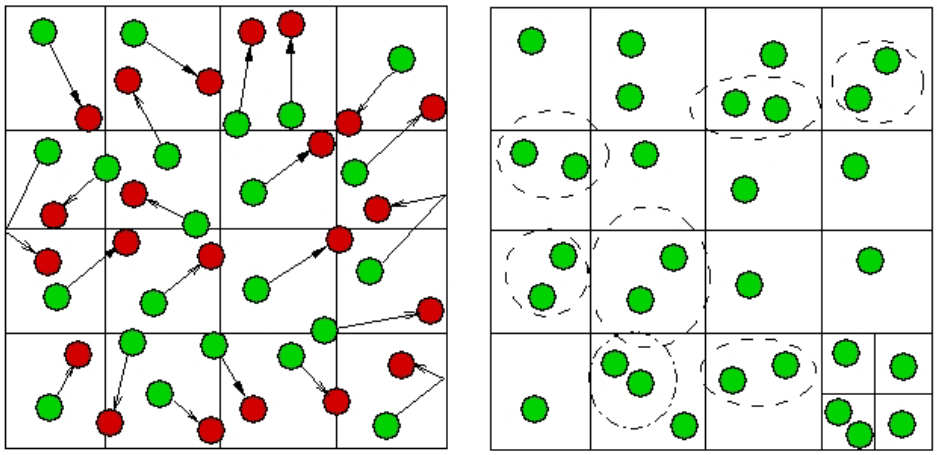
DSMC Procedures

- Since the original inception of the DSMC algorithm (1963), there have been no major changes to it
- DSMC has been shown to provide solutions to the Boltzmann equation more accurately than any other numerical method
- The original 1994 DSMC algorithm (DSMC94) has been criticized as being computationally inefficient
- Recently, a new DSMC algorithm (DSMC07) was proposed by Bird that addresses these concerns while maintaining the accuracy of the method
- The aim of this work is to demonstrate the benefits of using the new procedures

Sophisticated DSMC (DSMC07)

- Basic features of DSMC algorithm retained
  - Move-collide separation, molecular models, collision frequency calculation
- Changes in collide
  - Virtual collision cells: nearest-neighbor (*NN*) collisions, N^2 search operation
  - Adaptive transient collision cells based on a background grid ($N > 30$)
  - Exclusion of latest collision partner: physically realistic requirement for *NN* schemes
- Changes in temporal advection
  - Global time step
  - Cell-based time step
- Changes in time-tracking
  - Global time
  - Cell time
  - Molecule time



- Separate sampling and collision cells

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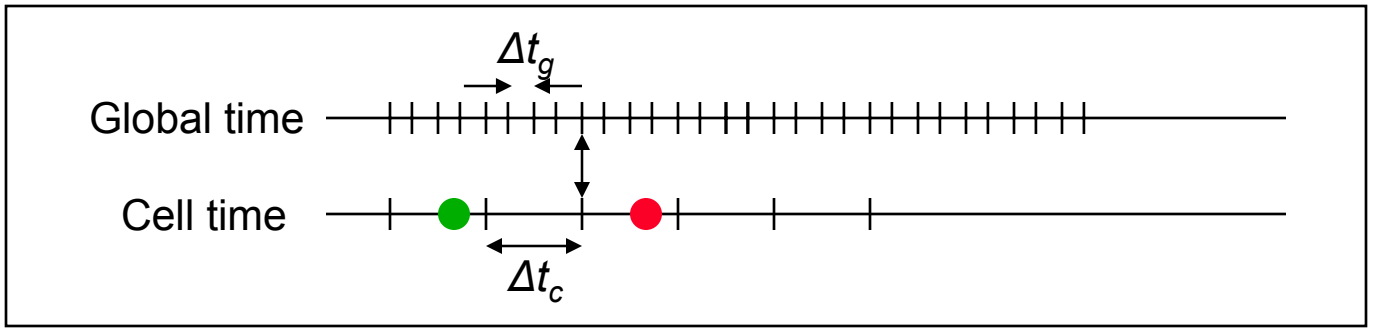
DSMC07 Temporal Advection

- Global time advances with small global time steps (Δt_g)
  Uniform throughout the domain, similar to DSMC94 time step

- Cell time step (Δt_c) is local (cell-based) and is a fraction of the local mean collision time (*MCT*) and the mean cell transit time (*MTT*)

- *With this (cell-based) time step:*
  - Cells perform collisions only when their "time" (cell time) falls more than $\Delta t_c/2$ behind global time
  - Molecules move only when their "time" (molecule time) falls more than $\Delta t_c/2$ behind global time



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DSMC07 Time-Step Properties

- Local: Cell-based time step (Δt_c): function of the local collision frequency and average molecular speed
- Adaptive: Global time step (Δt_g): function of the smallest Δt_c (adjusted during run)
- Dynamic: Move and collision phases are not synchronized for the whole domain (large low-collisionality regions)

- Collisions are considered for a cell
  Move is considered for a particular molecule

- Molecules cannot travel across a cell in one move without considering collisions

- Same pair cannot have sequential collisions

Motivation and Aim of this Work

- Wagner provided analytical support to the DSMC94 procedures
- No such proof (yet) for the new DSMC07 procedures

- Is this new implementation correct?

- We investigate the accuracy of the DSMC07 procedures by comparing to analytical solutions of the Boltzmann equation
  - Fourier-Couette benchmark problem
  - Near-equilibrium and far-from-equilibrium regimes
  - Chapman-Enskog (CE) and Moment-Hierarchy (MH) theories

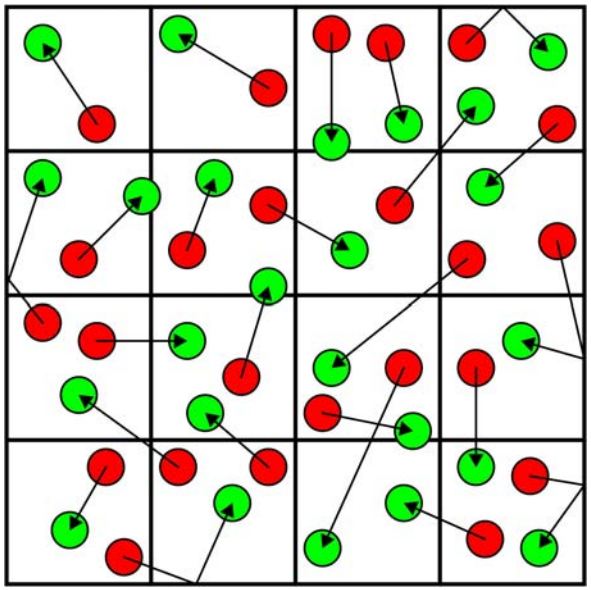
Equilibrium Collision Frequency

The collision frequency (number of collisions per molecule per unit time in a volume V) can be calculated from kinetic theory

The collision frequency can be calculated in a DSMC simulation

Test Case

- Flow in a closed box with fully accommodating walls
- Molecules VSS-Maxwell “argon”
- Walls fully accommodating
- Width 0.001 m (1 mm)
- Temperature 273.15 K
- Pressure 264.9 Pa (~2 torr)
  - $L/\lambda \sim 42$
  - $t_o \sim 71$ ns



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Equilibrium Collision Frequency

Average Sims/cell	Collision Freq DSMC/Theory
2	1.002
5	1.001
10	1.000
30	0.999
60	0.999

The new DSMC algorithm reproduces the correct collision frequency even for small number of simulators (as it should)

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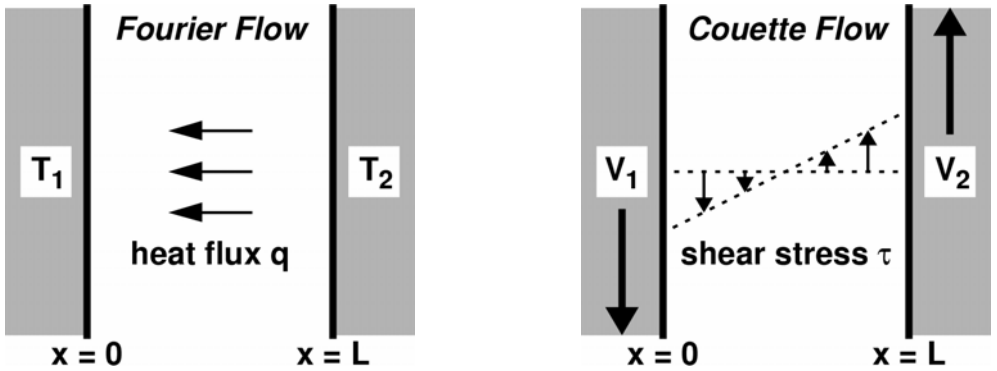
Fourier-Couette Benchmark Flow



- Molecules VSS-Maxwell “argon”
- Walls fully accommodating
- Width 0.001 m (1 mm)
- Pressure 264.9 Pa (~2 torr)
  - L/λ 42
  - t_o 71 ns (273.15 K)
  - ΔT 70-400 K
  - ΔV 100 m/s

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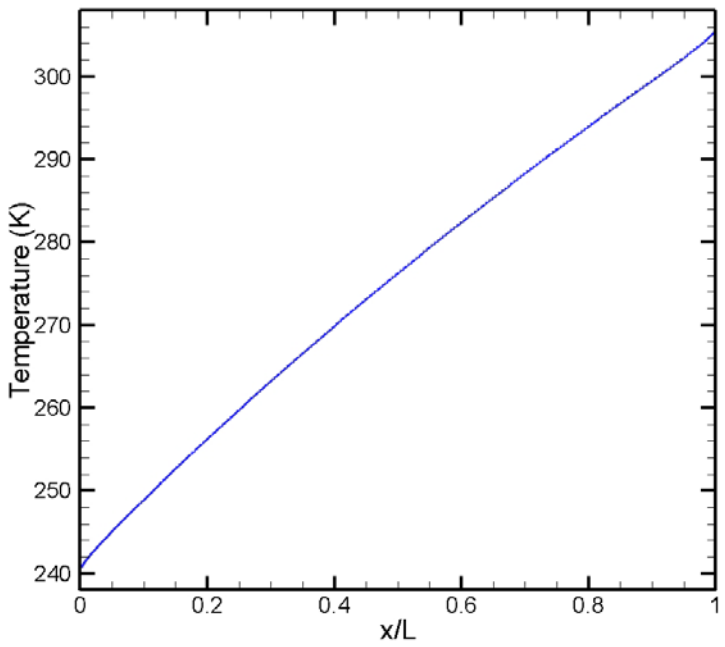
Comparing DSMC07 to Theory



Temperature profile (velocity profile is similar)

- Nearly linear
- Near-continuum, small jumps near walls
- Low level of statistical scatter

Compare CE-MH theory & DSMC07 results

- Thermal conductivity, viscosity: K, μ

$$q = K_{DSMC}\left(\frac{\partial T}{\partial x}\right) \qquad \tau = \mu_{DSMC}\left(\frac{\partial V}{\partial x}\right)$$

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

$$\left(\frac{a_k}{a_1}\right)_{DSMC} = \sum_{i=1}^{k}\left(\frac{(-1)^{i-1}k!(5/2)!}{(k-i)!i!(i+(3/2))!}\right)\left(\frac{\left\langle \tilde{c}^{2i}\tilde{c}_x\right\rangle}{\left\langle \tilde{c}^{2}\tilde{c}_x\right\rangle}\right)$$

$$\left(\frac{b_k}{b_1}\right)_{DSMC} = \sum_{i=1}^{k}\left(\frac{(-1)^{i-1}(k-1)!(5/2)!}{(k-i)!(i-1)!(i+(3/2))!}\right)\left(\frac{\left\langle \tilde{c}^{2(i-1)}\tilde{c}_x\tilde{c}_y\right\rangle}{\left\langle \tilde{c}_x\tilde{c}_y\right\rangle}\right)$$

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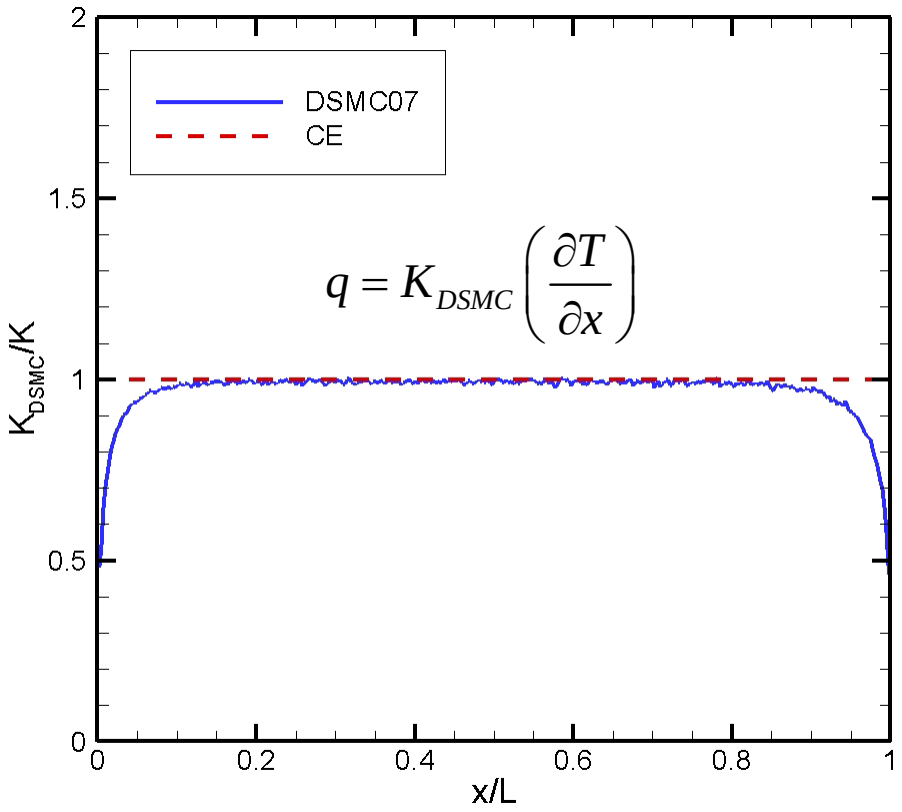
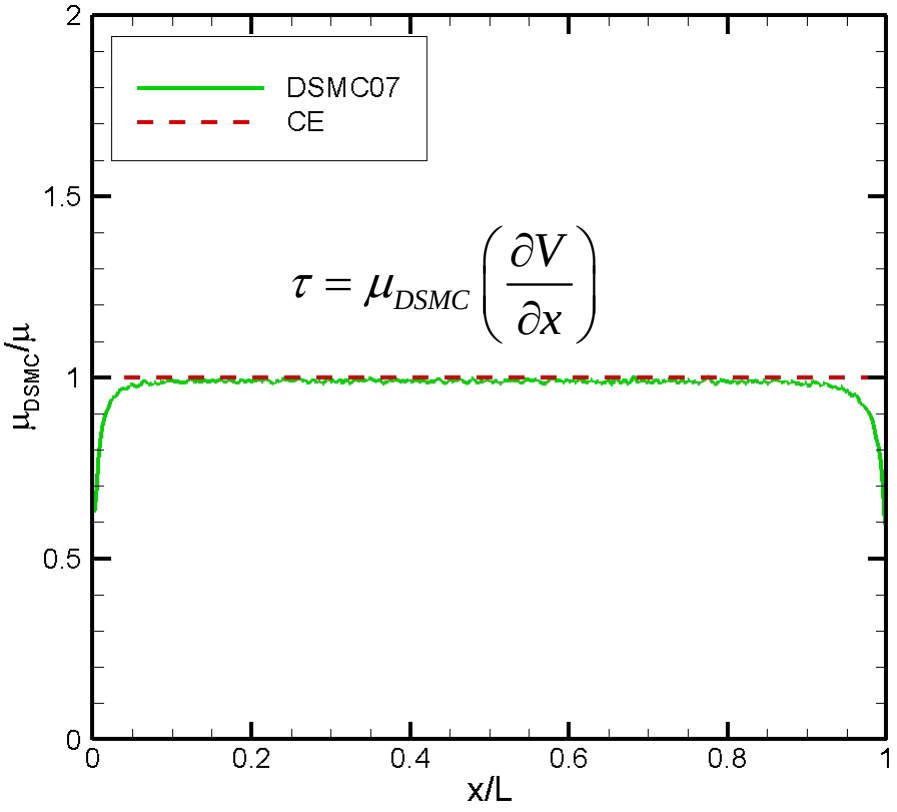
Maxwell
Transport Coefficient Profiles





- DSMC07 and CE thermal conductivity and viscosity
  - Low heat flux, low shear stress: $Kn_q = 0.006$, $Kn_\tau = 0.003$
  - Agreement in central region: normal solution

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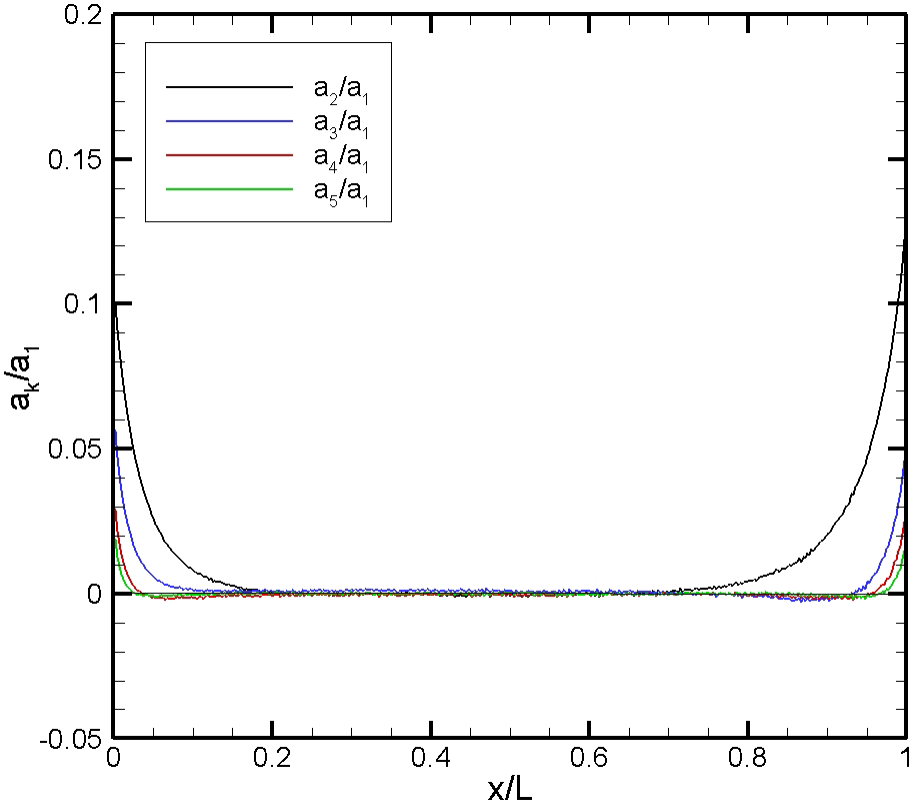
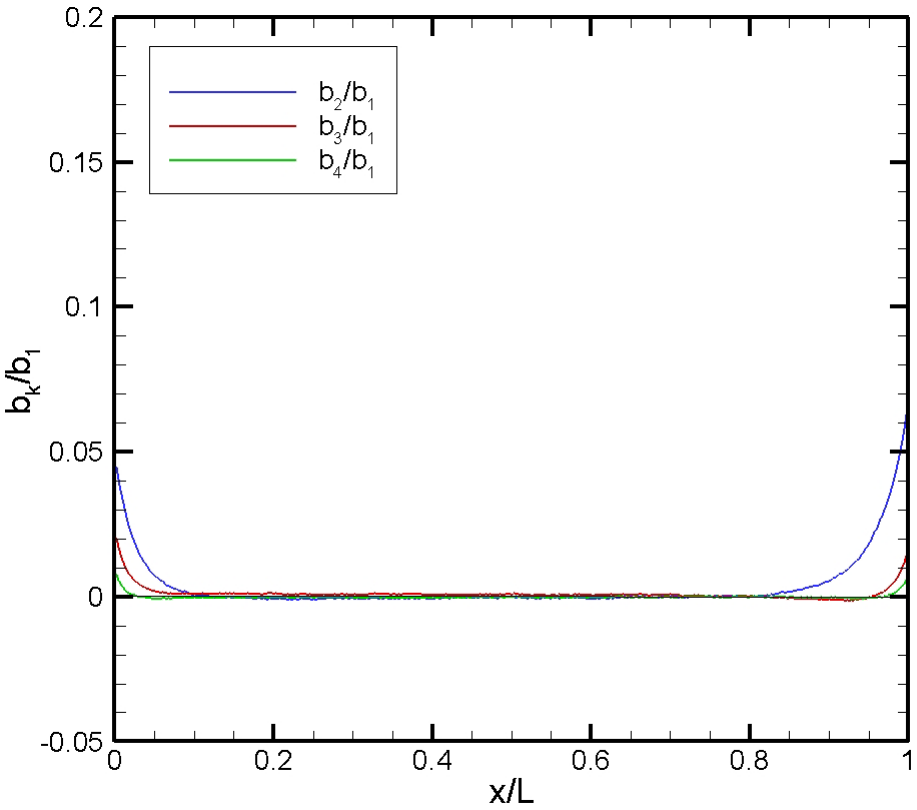
Maxwell
Sonine-Coefficient Profiles





- DSMC07 and CE Maxwell Sonine polynomial coefficients a_k/a_1 and b_k/b_1
  - Low heat flux, low shear stress: $Kn_q = 0.006$, $Kn_\tau = 0.003$
  - Good agreement in central region: normal solution
  - Demonstrates accuracy of molecular velocity distribution

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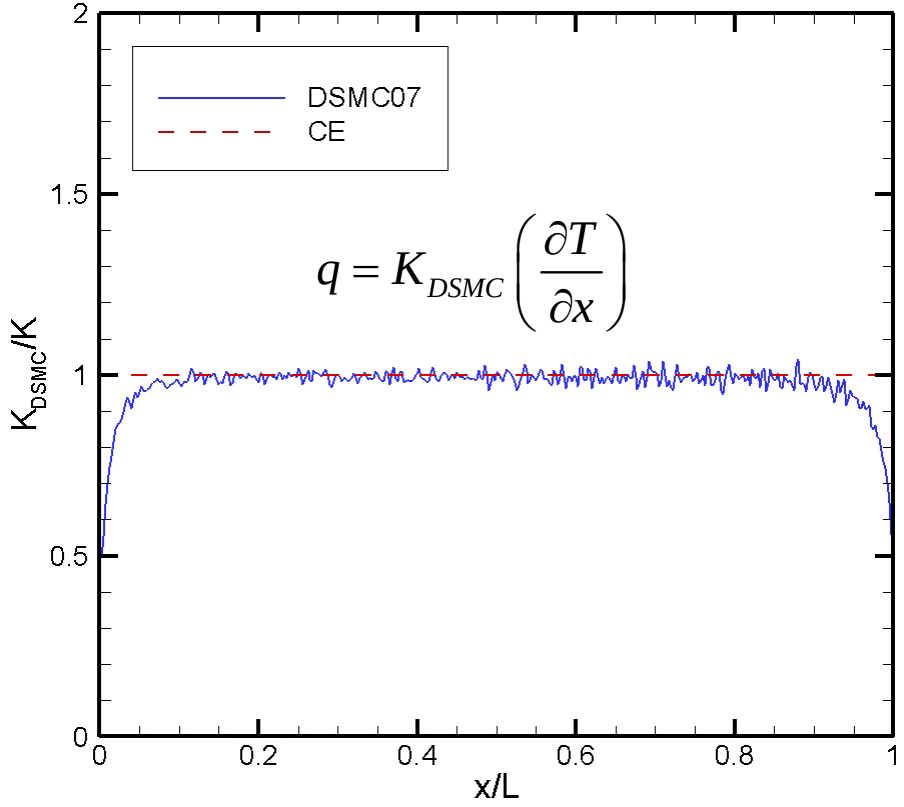
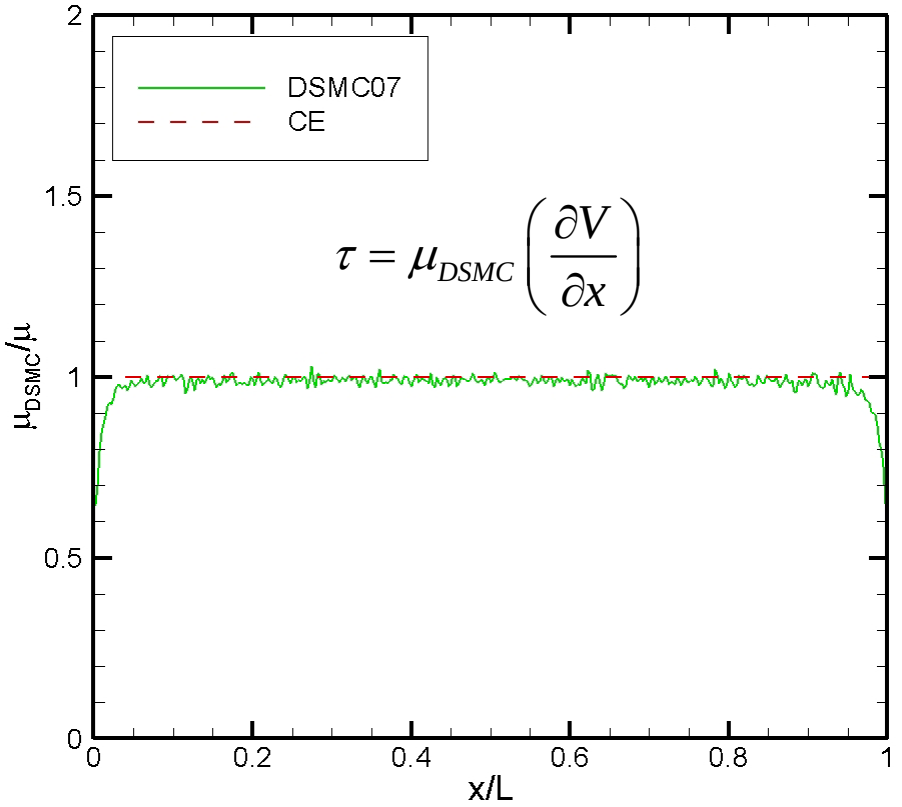
Hard-Sphere
Transport Coefficient Profiles





- DSMC07 and CE thermal conductivity and viscosity
  - Low heat flux, low shear stress: Kn_q = 0.006, Kn_τ = 0.003
  - Agreement in central region: normal solution

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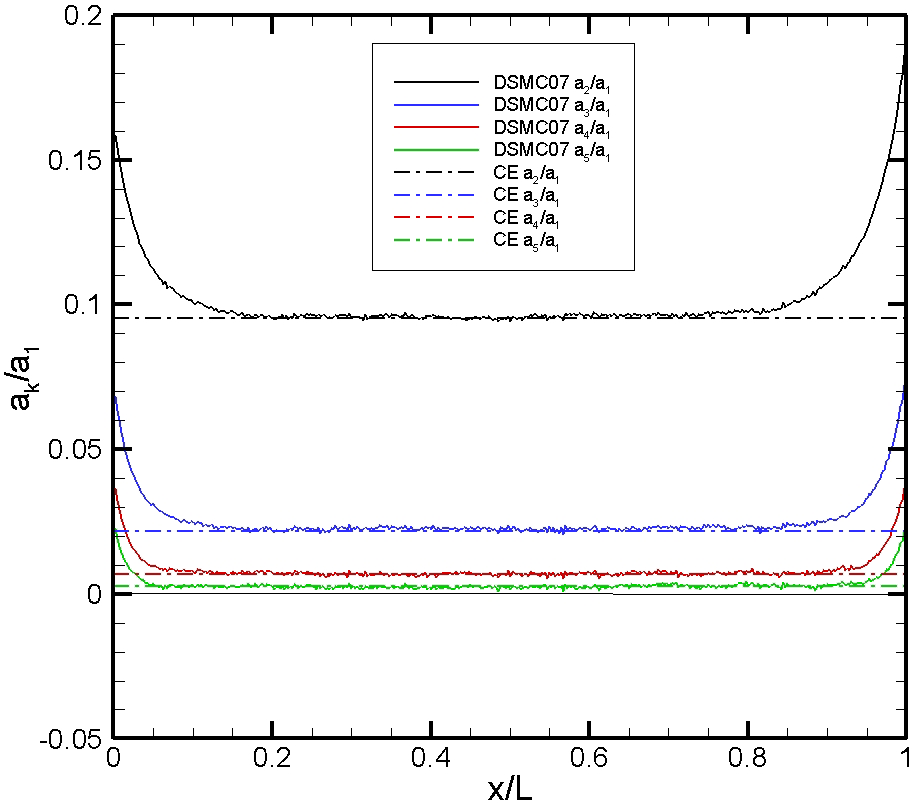
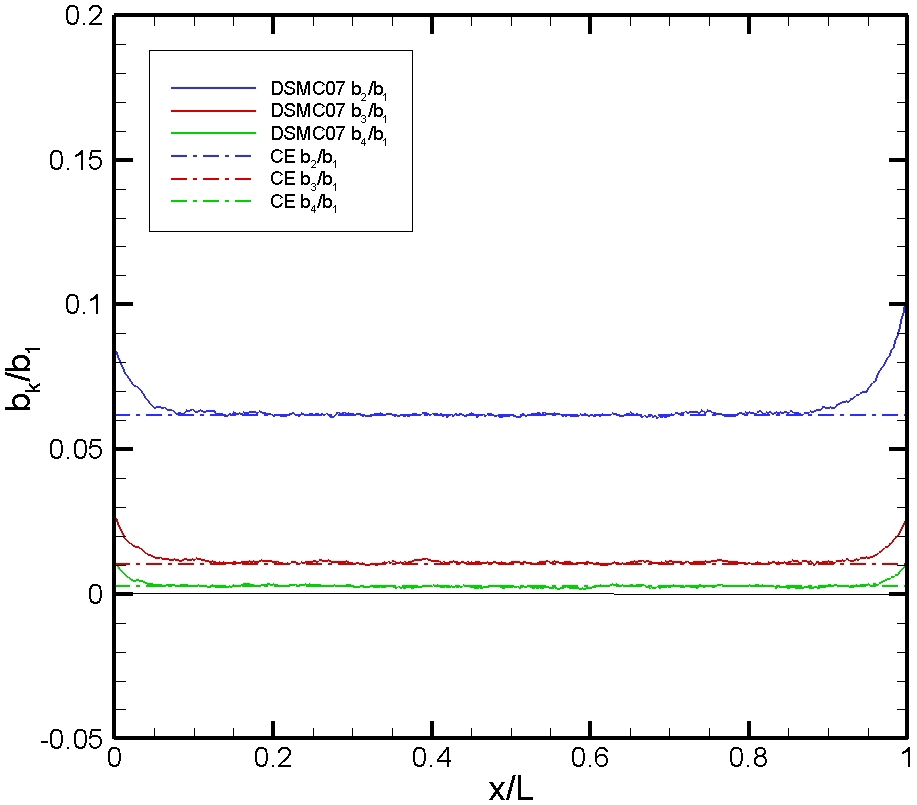
Hard-Sphere
Sonine-Coefficient Profiles





- DSMC07 and CE Hard-Sphere Sonine polynomial coefficients a_k/a_1 and b_k/b_1
  - Low heat flux, low shear stress: $Kn_q = 0.006$, $Kn_\tau = 0.003$
  - Good agreement in central region: normal solution
  - Demonstrates accuracy of molecular velocity distribution

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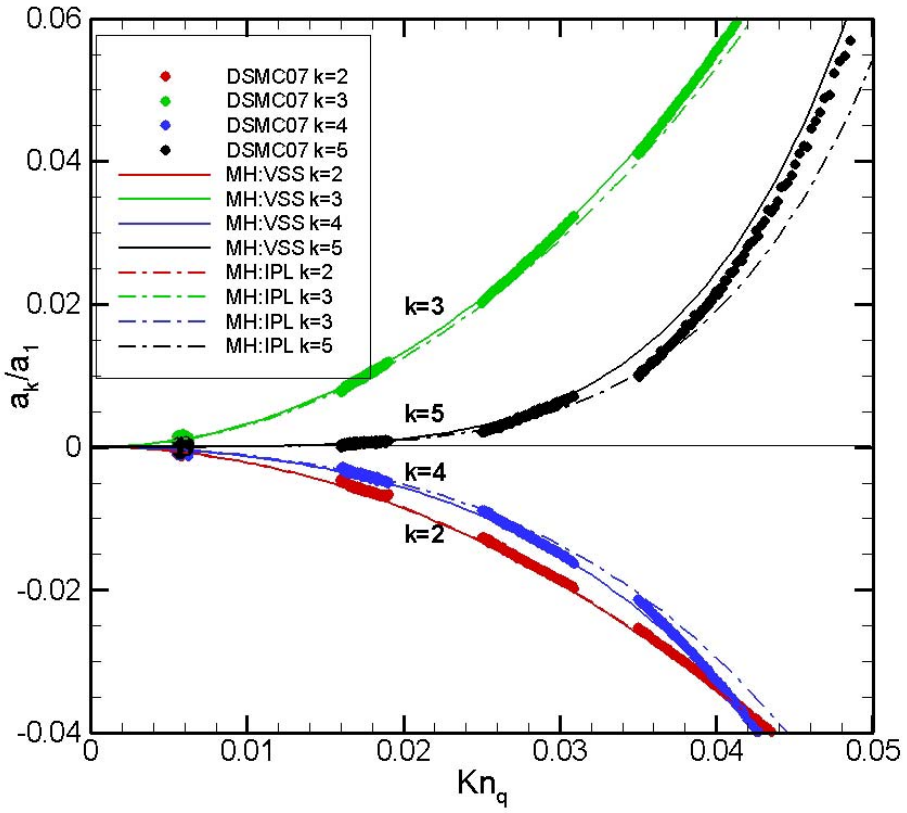
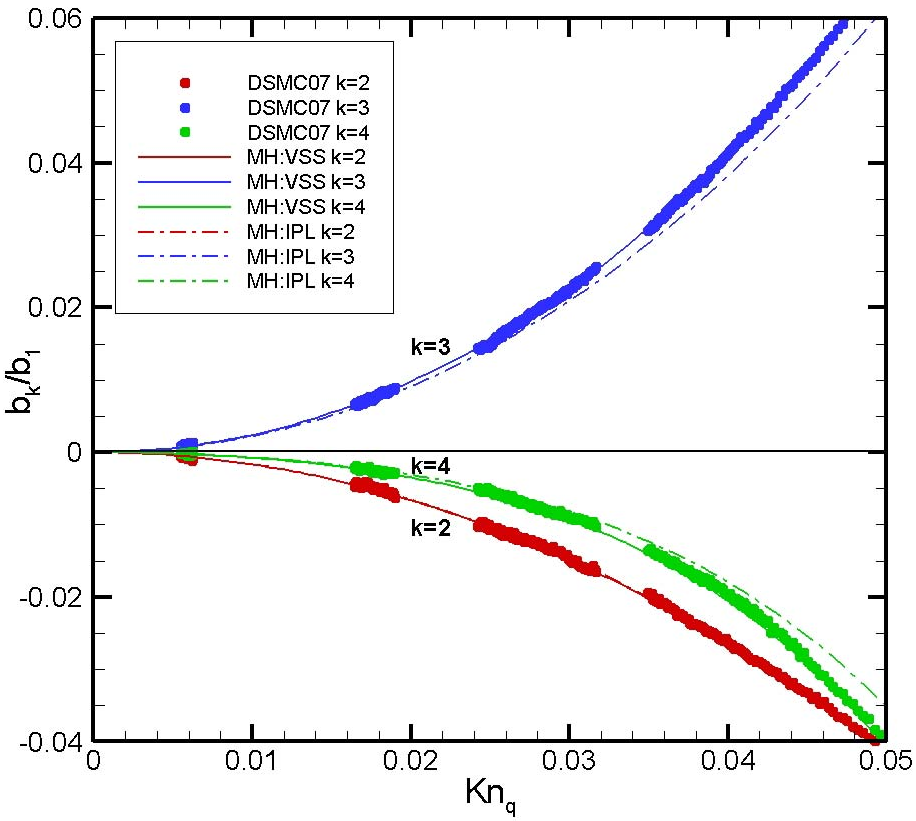
Maxwell
Normal Sonine Coefficients





- DSMC07 and MH Maxwell normal solutions for a_k/a_1 and b_k/b_1
  - Four DSMC07 simulations: ΔT = 70, 200, 300, 400 K
  - MH: VSS-Maxwell (solid) and IPL-Maxwell (dashed) differ
  - DSMC07 and MH VSS-Maxwell normal solutions agree

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Conclusions

Accuracy of a new DSMC algorithm investigated

The sophisticated DSMC algorithm reproduces the:

- Correct collision frequency at equilibrium conditions
- Correct distribution function and transport properties at near-equilibrium for Hard Sphere and Maxwell molecular models
- Correct distribution function and transport properties at non-equilibrium conditions for Maxwell molecular models