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Convergence Behavior of a New DSMC Algorithm

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Direct Simulation Monte Carlo: Theory, Methods, and Applications
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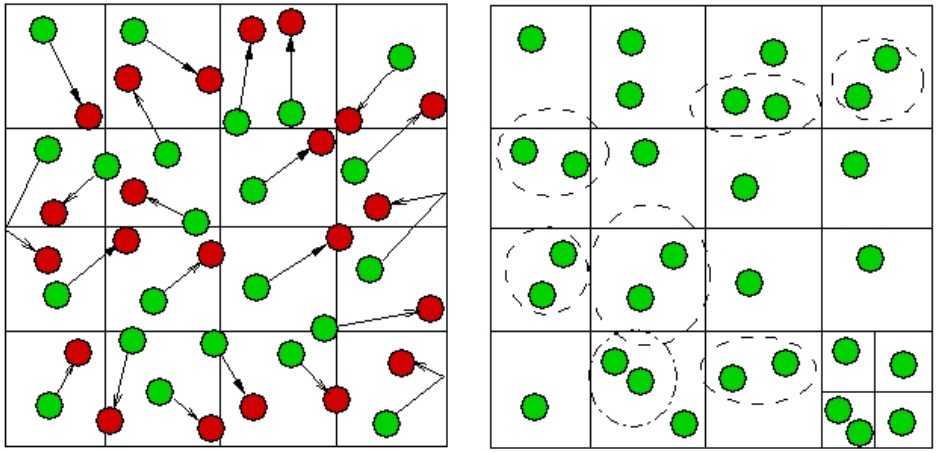
DSMC Procedures

- 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 move and collision cells



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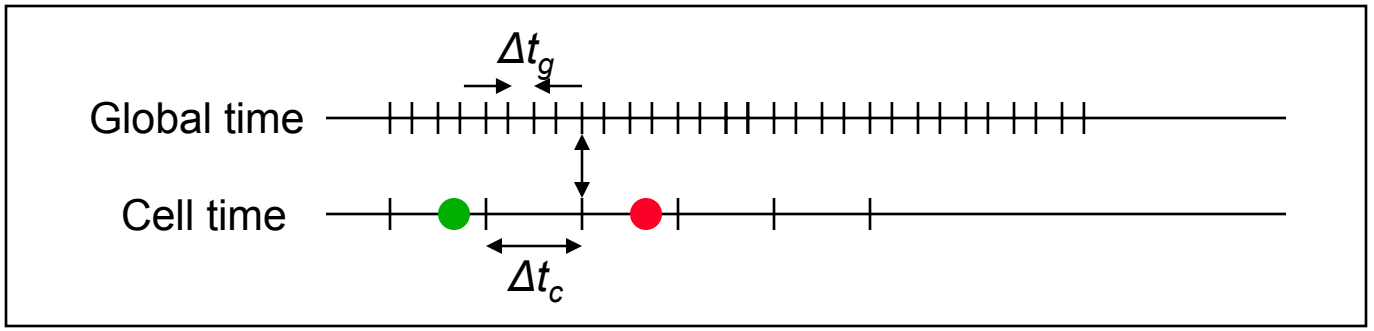
DSMC07 Temporal Advection

- 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 transient 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

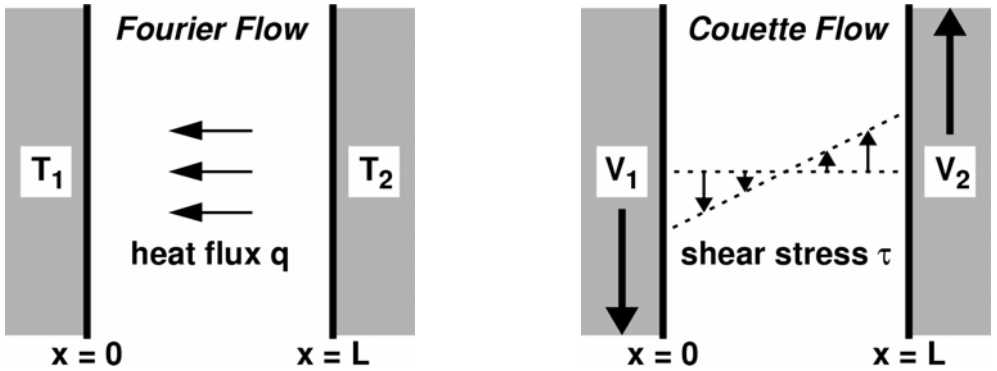
- Wagner provided analytical support to the DSMC94 procedures
- No such proof (yet) for the new DSMC07 procedures

- Is this new implementation correct?
- How do the new procedures affect the convergence behavior?

- 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

- We examine the convergence of DSMC07 compared to DSMC94 using a Fourier-flow benchmark problem

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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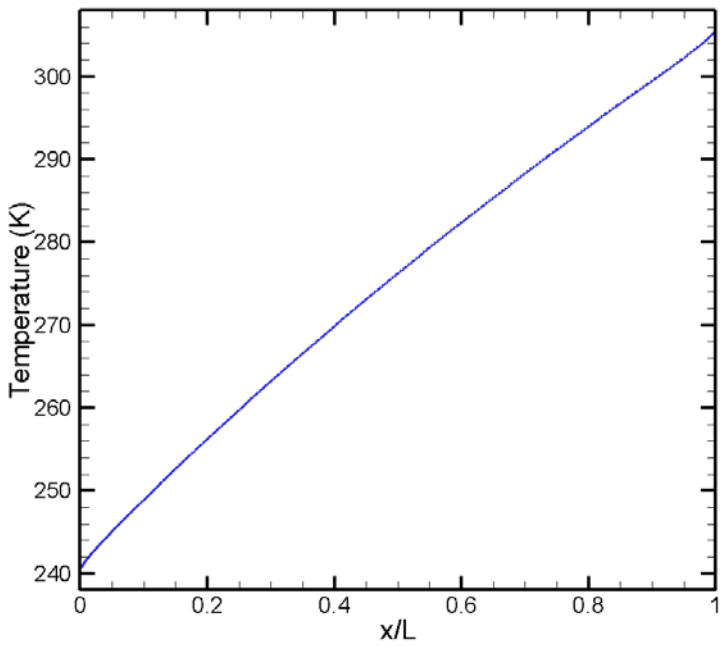
Comparing DSMC07 to Theory



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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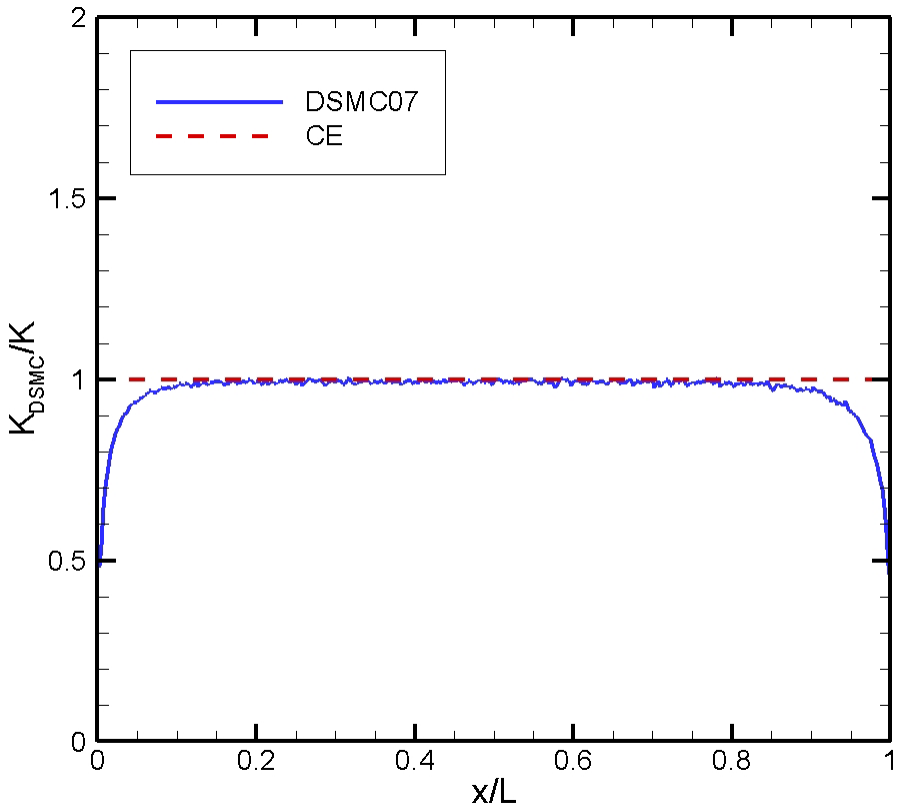
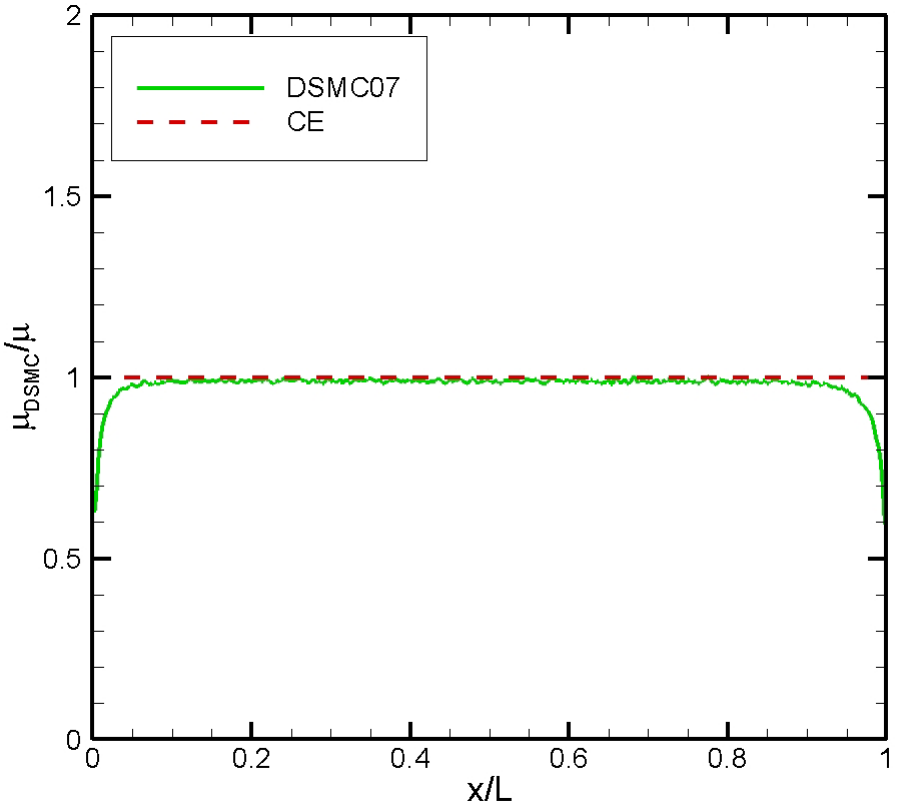
Transport Coefficient Profiles





- 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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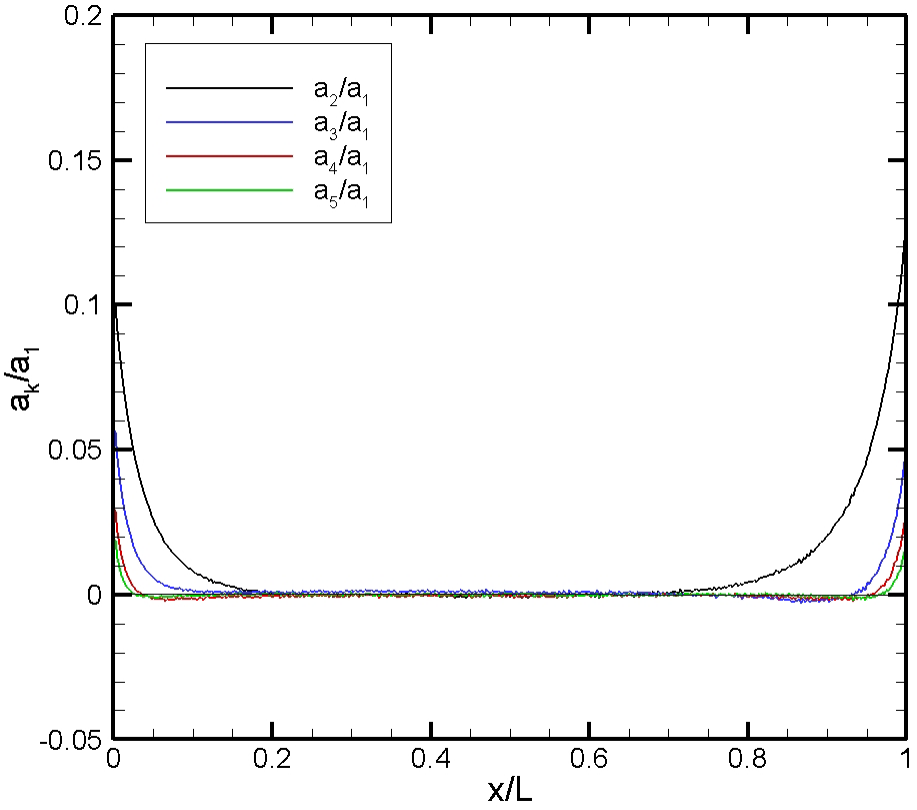
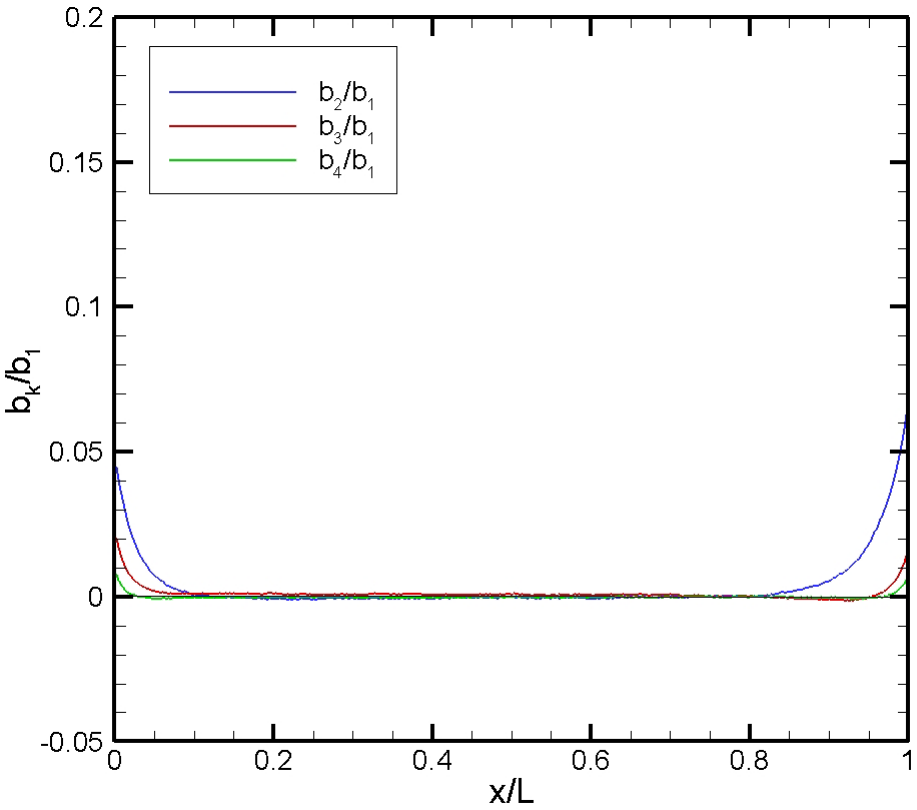
Maxwell Sonine-Coefficient Profiles





- 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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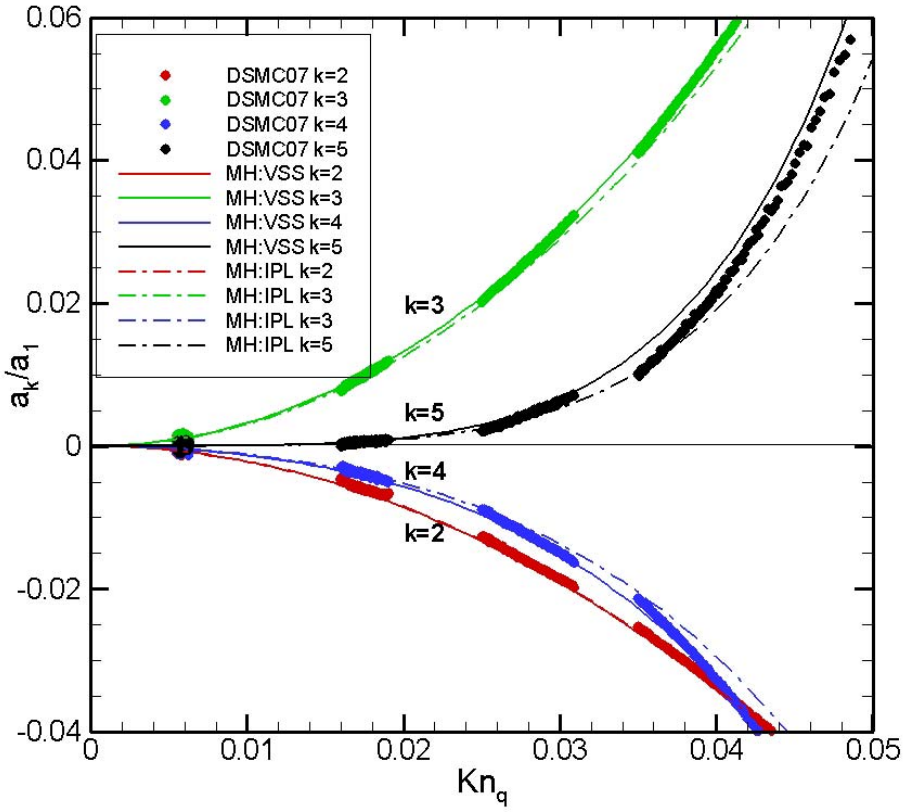
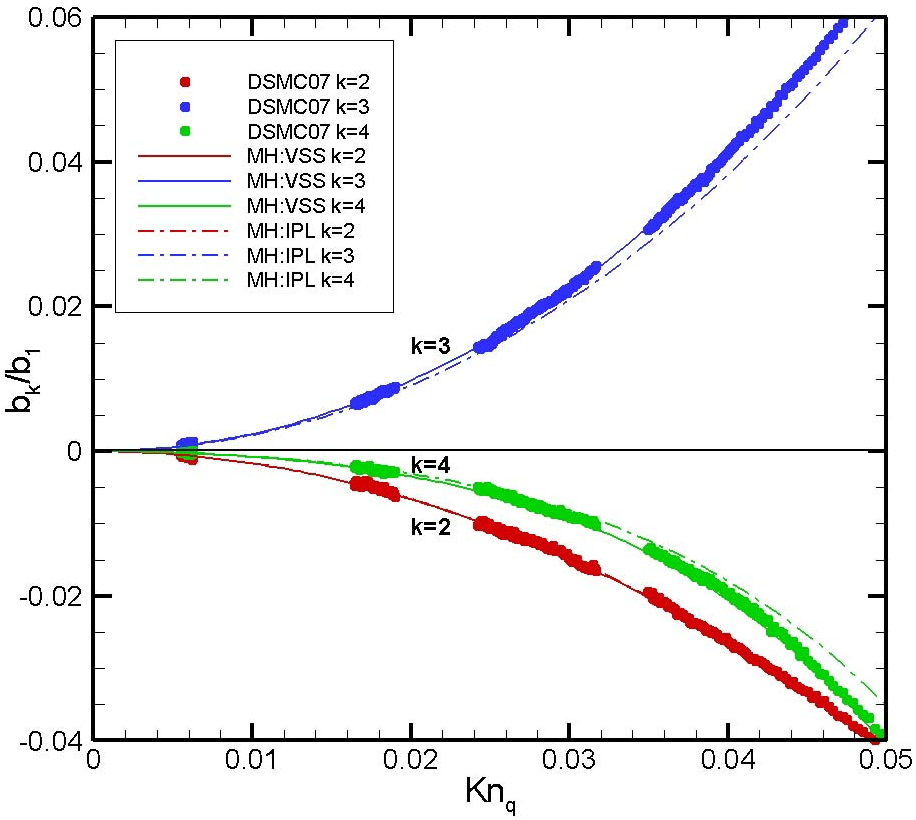
Maxwell Normal Sonine Coefficients





- 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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Numerical Error in DSMC Procedures

Four parameters control DSMC numerical error

- Sample size per cell (M_c) → statistical error
- Simulators per cell (N_c)
- Cell size (Δx) → discretization error
- Time step (Δt)

Error related to cell width, Δx

- Collision partners selected from anywhere in same cell
- Some potential partners move into adjacent cells
- Some invalid partners move into the same cell

Error related to time step, Δt

- Collisions occur at the end of time step
- Collisions should be uniformly distributed over time step

Previous DSMC94 Error Analyses

Fallavollita, Chen, Boyd: Journal of Computational Physics, 1993-1996

- Statistical error analysis

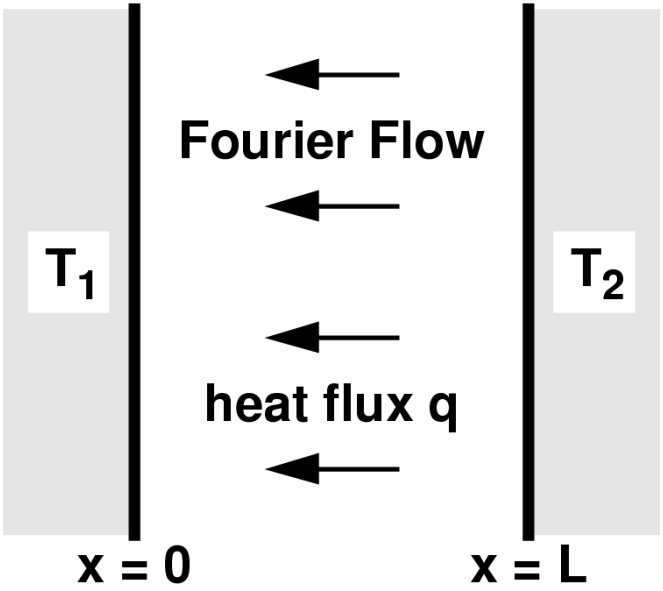
Alexander, Garcia, Alder, Wagner, Hadjiconstantinou: Physics of Fluids, 1998-2000

- Green-Kubo (GK) theory for steady transport in DSMC
- Gave expressions for viscosity & thermal conductivity

Rader, Gallis, Torczynski, Wagner: Physics of Fluids, 2006

- Quantified discretization error of thermal conductivity
  - Cell size Δx
  - Time step Δt
  - Molecules/cell N_c

DSMC94 Convergence Analysis for Fourier Flow



One-dimensional gas-phase conduction

Temperature, heat flux calculated from DSMC molecular velocity distribution

- Continuum gas, HS "Argon"
- Small gradient-Kn: *Chapman-Enskog* in interior
- Large gradient-Kn: *Non-equilibrium* in interior

$$q = -K(T)\frac{dT}{dx}$$

K = thermal conductivity
T = gas temperature

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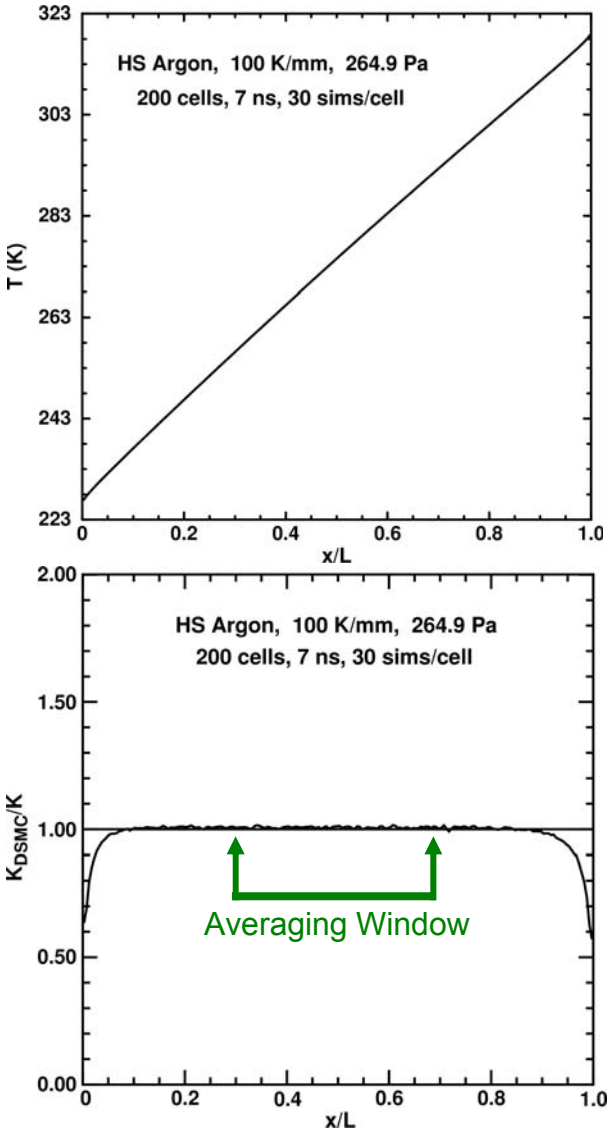
Assessing DSMC94 Convergence



Temperature Profile

- Nearly linear
- Near-continuum
- Small jumps near walls

Thermal conductivity from CE theory and DSMC94 results

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

Average over central 40% of domain to obtain a single convergence metric

K_{DSMC}/K

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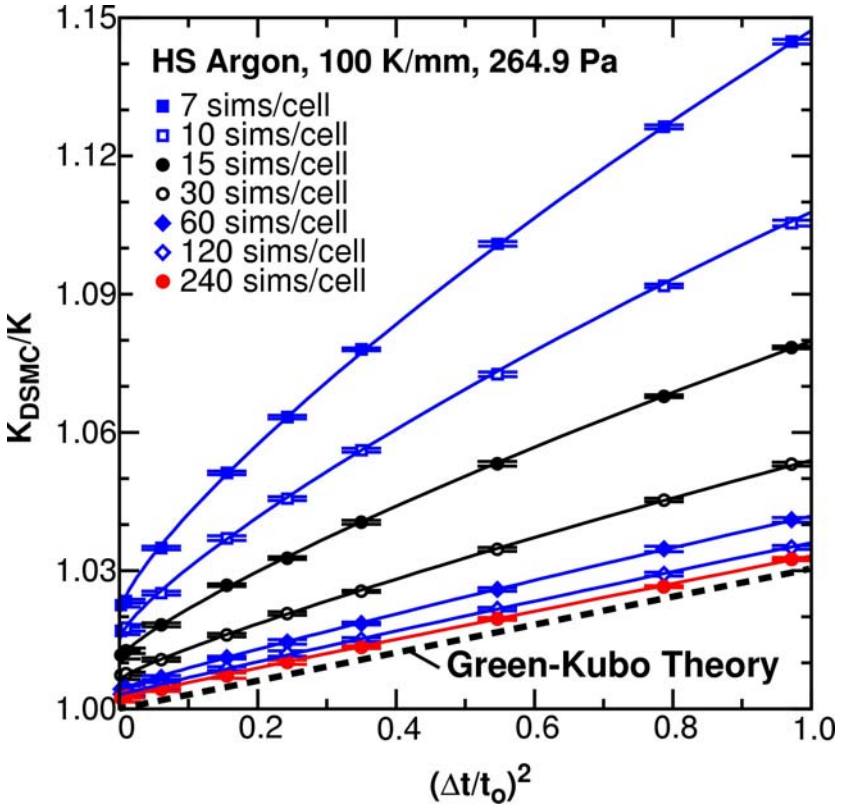
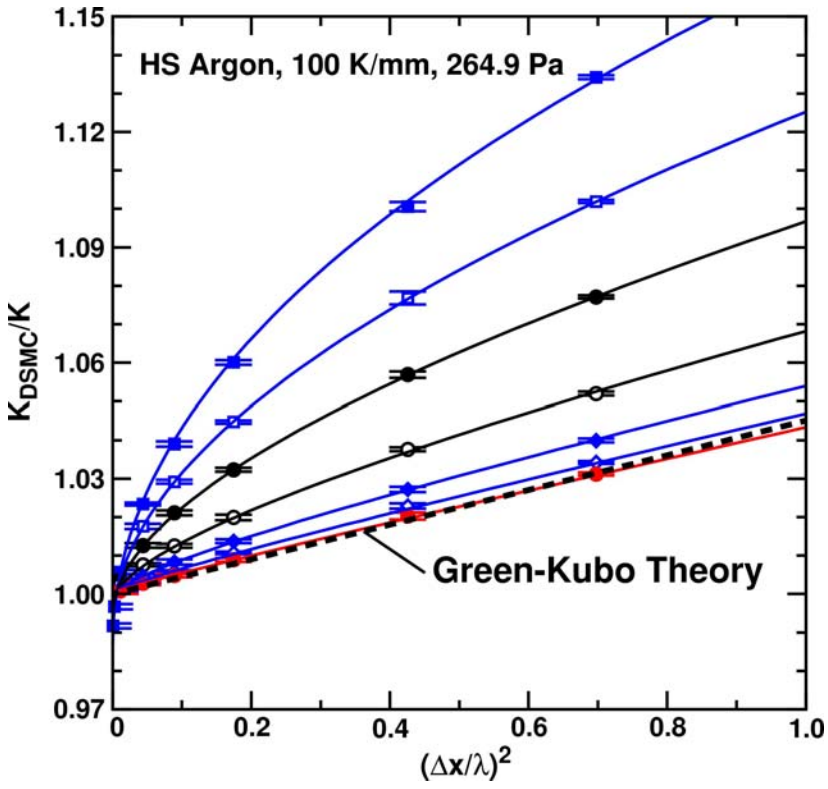
DSMC94
Cell-Size & Time-Step Convergence





Quadratic dependence on cell size and time step observed only for large N_c

Quadratic coefficients agree with GK theory in the limit $N_c \rightarrow \infty$

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DSMC94
Functional Form of Error

Best-fit correlation function for DSMC94

$$\frac{K_{DSMC}}{K} = 1.0001 + 0.0286\left(\frac{\Delta t}{t_o}\right)^2 + 0.0411\left(\frac{\Delta x}{\lambda}\right)^2$$

$$-0.01\left(\frac{\Delta t}{t_o}\right)^2\left(\frac{\Delta x}{\lambda}\right)^2 - 0.147\frac{1}{N_c} + \frac{1}{N_c}F\left[\frac{\Delta t}{t_o}, \frac{\Delta x}{\lambda}, \left(\frac{\Delta t}{t_o}\right)^2\right]$$

DSMC94 limiting convergence behavior is in agreement with GK theory

- Quadratic convergence in time step ($\Delta x/\lambda \to 0$, $N_c \to \infty$)
- Quadratic convergence in cell size ($\Delta t/t_o \to 0$, $N_c \to \infty$)
- Linear convergence in $1/N_c$ for $N_c \geq 30$ simulators/cell
- *Coefficients* in good agreement with GK theory
- Cross terms needed for finite discretization

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Sophisticated DSMC (DSMC07) Convergence Behavior

- The algorithm was implemented in a 1-D DSMC code
- To allow for a “fair” comparison:
  - Time step was based on mean collision time only
  - Identical collision and sampling cells
  - Virtual-subcells were used for any N_c
- To eliminate statistical noise, 100 simulations were performed for each data point
- 175 total simulations were performed to create the database for the analysis

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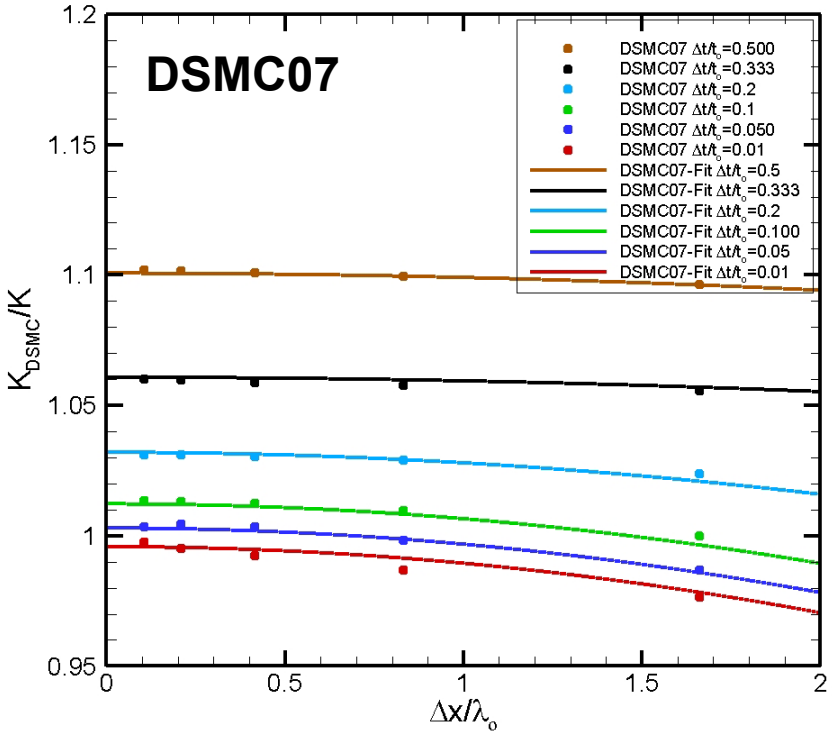
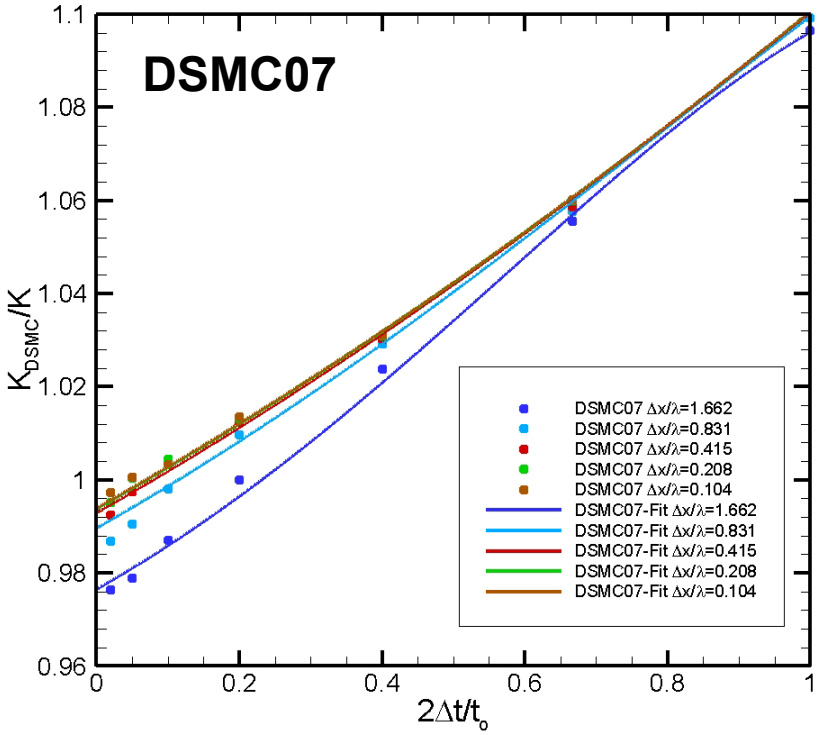
Convergence Behavior for $N_c \rightarrow \infty$





- The algorithm is
  - Insensitive to spatial resolution
  - Spatial resolution constraint: $\Delta x \leq \lambda$
  - Almost linearly dependent on time step

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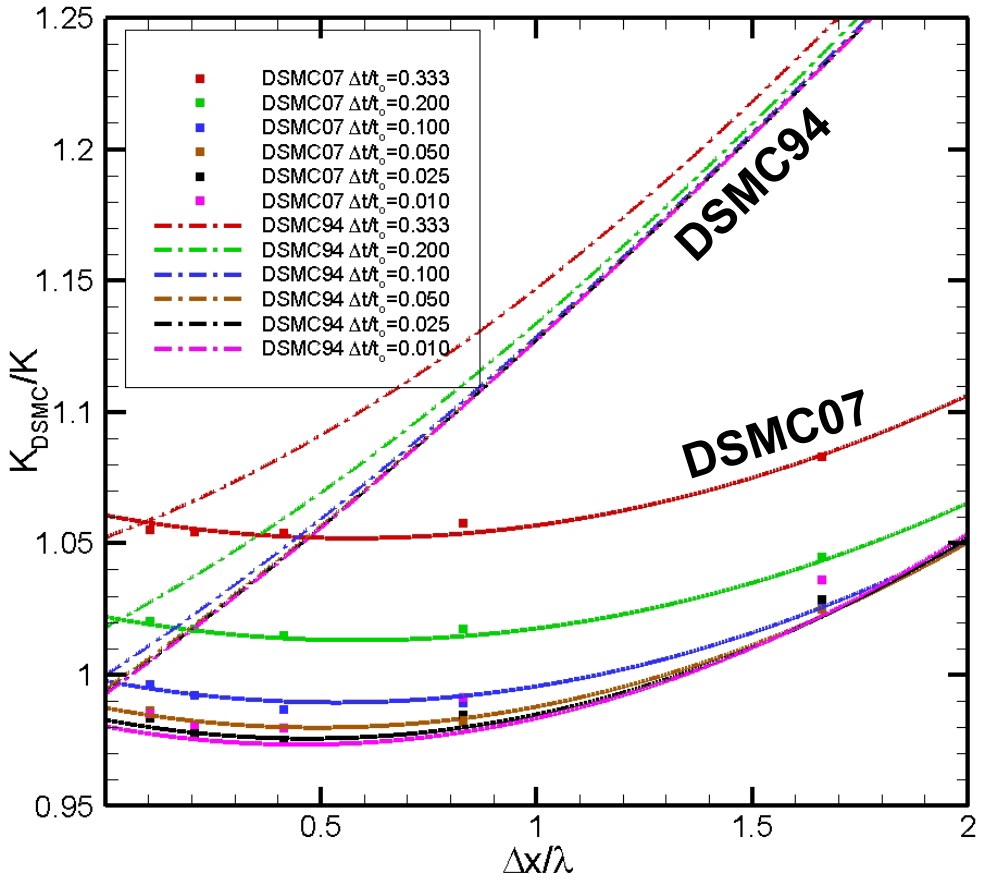
Convergence Behavior for $N_c = 10$ Effect of Cell Size



- For finite number of simulators, the algorithm is
  - Insensitive to spatial resolution
  - With error below 2% for all cases as long as $\Delta t/t_o \leq 0.2$

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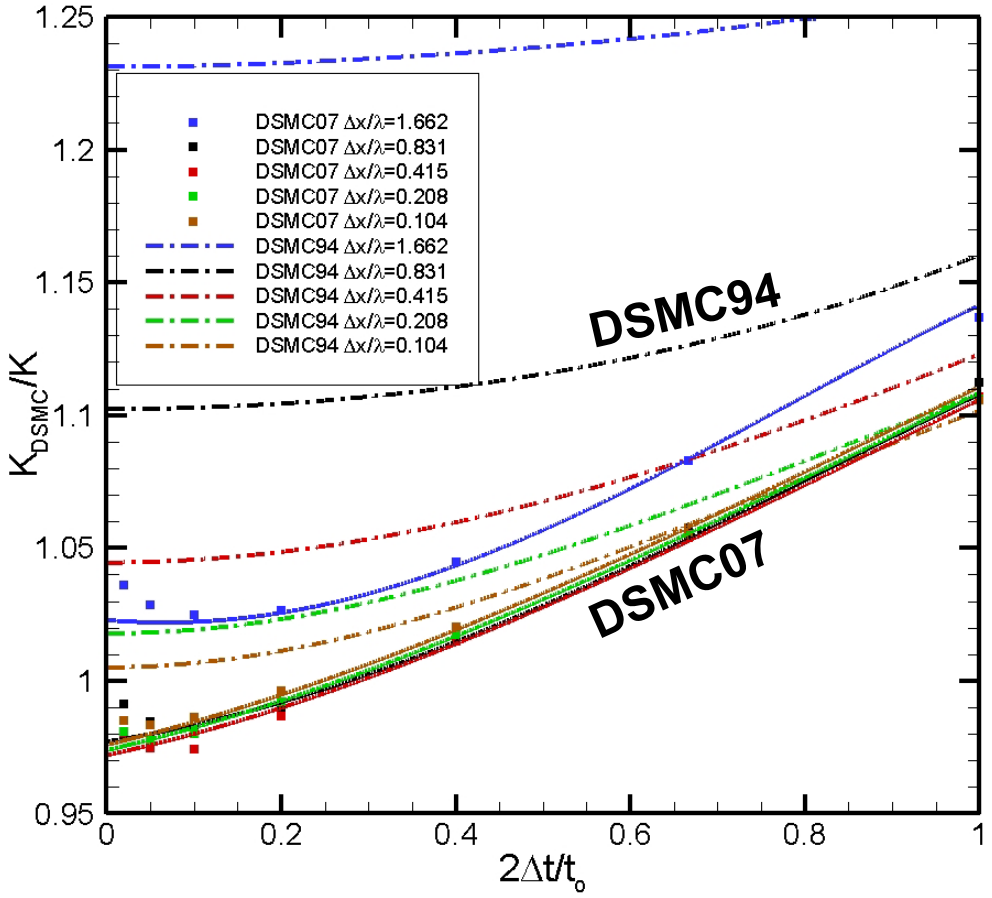
Convergence Behavior for $N_c = 10$ Effect of Time Step



- The algorithm exhibits a near-linear dependence on time step
- For very small time steps ($\Delta t/t_o \leq 0.1$), under-prediction is possible (due to nearest-neighbor scheme)

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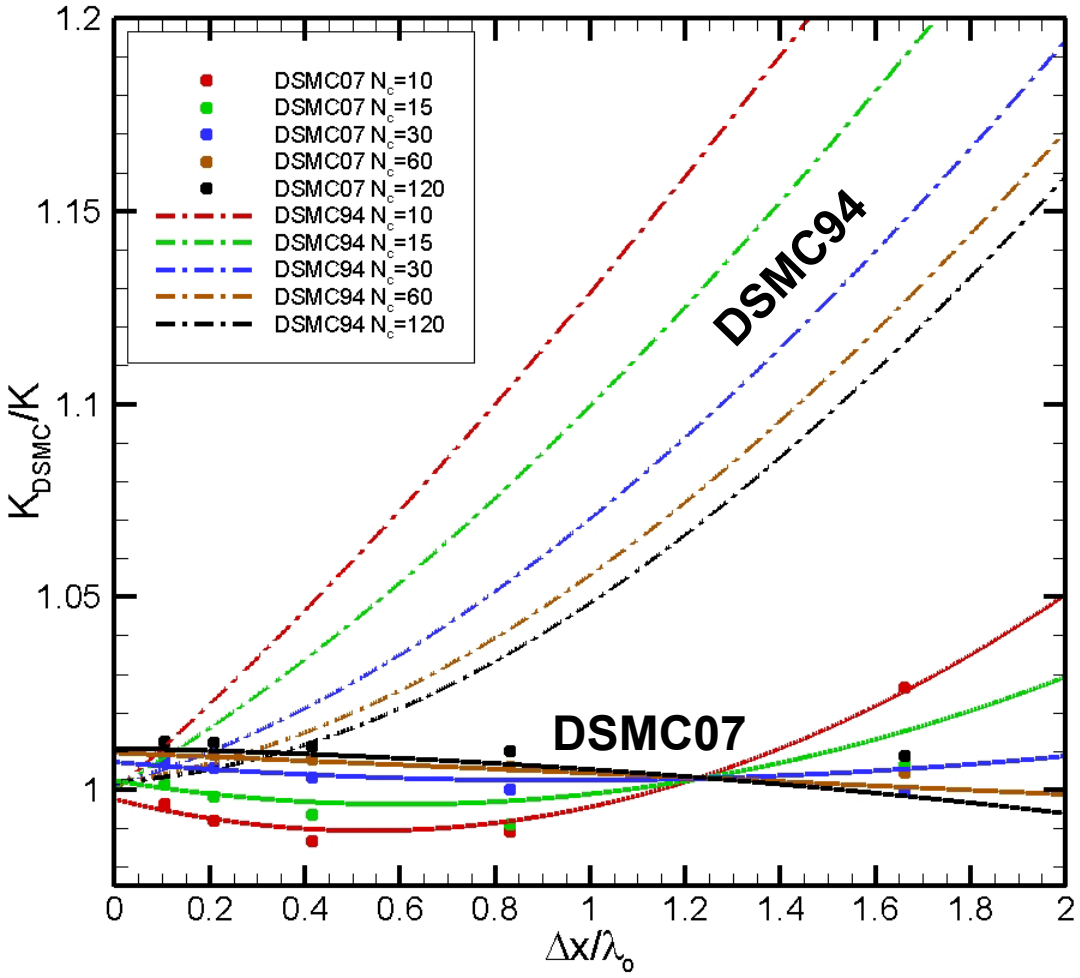
Effect of Simulators Per Cell N_c at $\Delta t/t_o$=10



- Small effect on error (2% maximum)
- Maximum error does not exceed 2%

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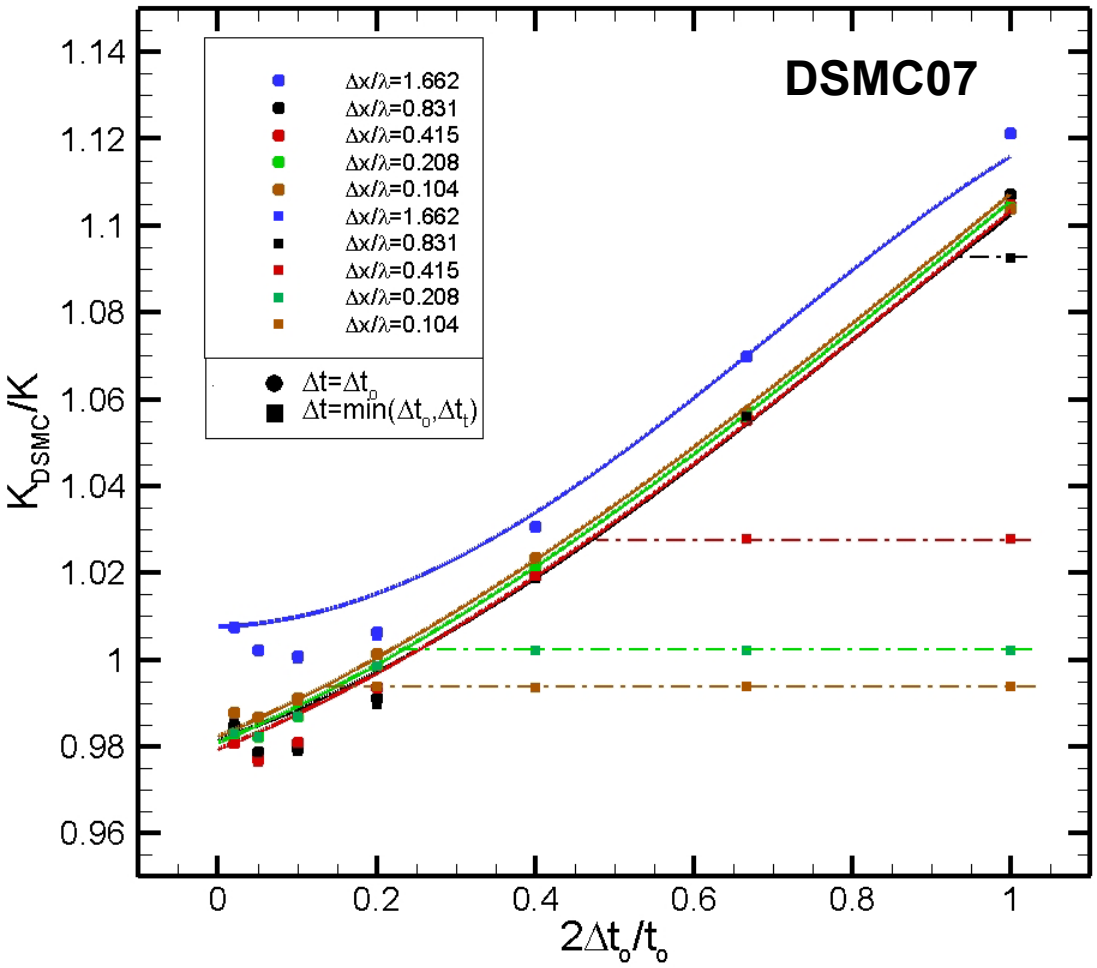
Convergence Behavior for $N_c = 15$ Effect of Time Step



The DSMC07 time step Δt is based on both

- mean collision time t_o, via $\Delta t_o \propto t_o$
- mean cell-transit time t_t, via $\Delta t_t \propto t_t$

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DSMC07
Functional Form of Error

Best-fit correlation function for sophisticated DSMC with $\Delta t = \Delta t_o$

$$\frac{K_{DSMC}}{K} = 0.9953 + 0.07773\left(\frac{2\cdot\Delta t}{t_o}\right) + 0.02795\left(\frac{2\cdot\Delta t}{t_o}\right)^2 - 0.0066\left(\frac{\Delta x}{\lambda}\right)^2$$
$$-0.0234\left(\frac{2\cdot\Delta t}{t_o}\right)^2\left(\frac{\Delta x}{\lambda}\right)^2 + 0.60375\frac{1}{N_c} + \frac{1}{N_c}F\left[\frac{2\cdot\Delta t}{t_o}, \frac{\Delta x}{\lambda}, \left(\frac{2\cdot\Delta t}{t_o}\right)^2\right]$$

DSMC limiting convergence differs from GK behavior

- Linear convergence in time step ($\Delta x/\lambda \to 0$, $N_c \to \infty$)
- Weak quadratic convergence in cell size ($\Delta t/t_o \to 0$, $N_c \to \infty$)
- Linear convergence in $1/N_c$ for $N_c \geq 30$ simulators/cell
- Cross terms needed for finite discretization (but in general smaller than for DSMC94)

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Conclusions

Accuracy and convergence of a new DSMC algorithm investigated

The sophisticated DSMC algorithm reproduces the near-equilibrium CE and non-equilibrium MH solutions to 0.1%

- Error has weak dependence on cell size (~10% of GK theory)
- Error has strong linear dependence on time step

The time-step selection criteria of DS2V contain error to within 2%

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