SAND2009-5600P

Sophisticated DSMC

Michael A. Gallis

Engineering Sciences Center
Sandia National Laboratories
Albuquerque, New Mexico, USA

DSMC: Fundamentals through Advanced Concepts
Short Course

Direct Simulation Monte Carlo: Theory, Methods, and Applications
Santa Fe, New Mexico; September 13-16, 2009

Sandia is a multiprogram laboratory operated by Sandia Corporation, a Lockheed Martin Company, for the United States Department of Energy's National Nuclear Security Administration under contract DE-AC04-94AL85000.

Sandia National Laboratories

Outline

- Characteristics
- Implementation
- Convergence
- Efficiency
- Accuracy

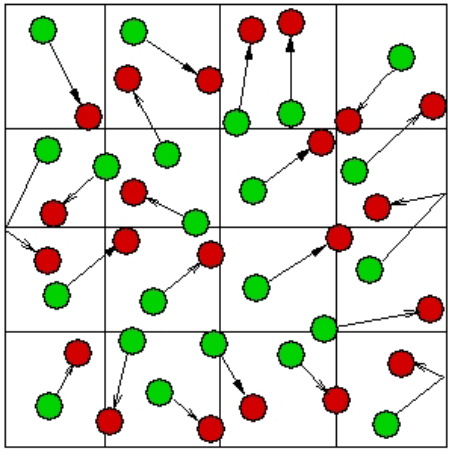
Sandia National Laboratories

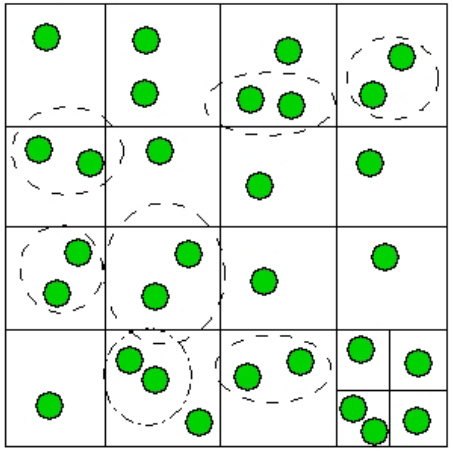
DSMC Procedures

- Since the inception of the original 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.
- Bird's new DSMC algorithm (DSMC07) addresses these concerns while maintaining the accuracy of the method.

Overview of Sophisticated DSMC

- Basic features of DSMC algorithm retained
  - Move (ballistic at molecular velocity)
  - Collisions (binary, molecular chaos)
  - Molecular models (VSS, VHS)
  - Collision frequency calculation
  - Sampling
- Changes in collide
  - Nearest neighbor collisions
  - Virtual collision cells (VCS): nearest-neighbor (*NN*) collisions, N^2 operation (N<30)
  - Adaptive transient collision cells (TASC) based on a background grid (*N*>30)
  - Exclusion of latest collision partner: physically realistic requirement for *NN* schemes
- Changes in temporal advection
  - Two time-steps used
  - Global time step
  - Cell-based time step
- Changes in time-tracking
  - Global time
  - Cell time
  - Molecule time
- Separate sampling and collision cells





Sandia National Laboratories

DSMC94 Collision Partner Selection

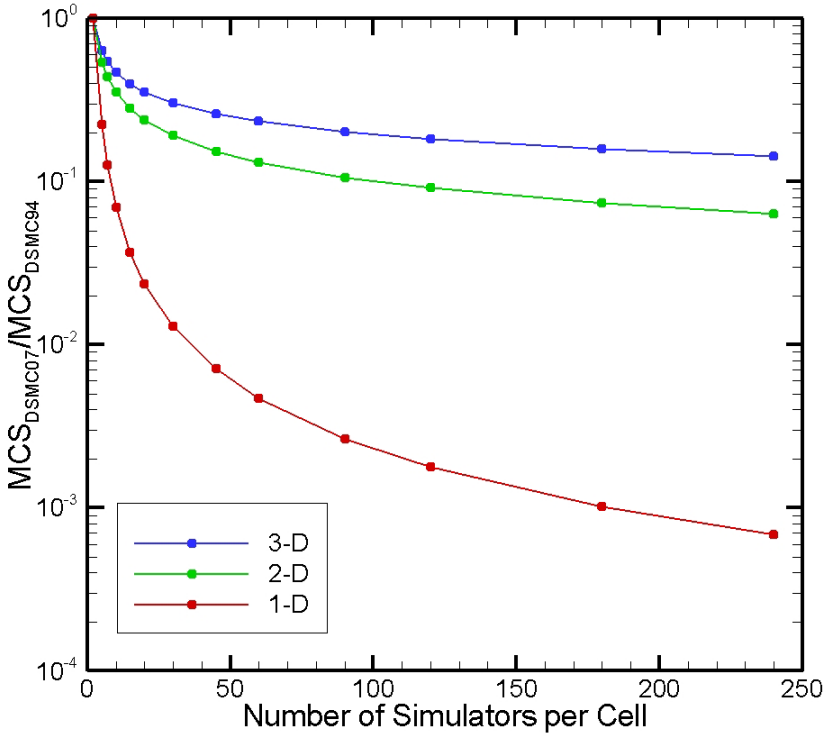
- **DSMC94 randomly selects collision partners from a cell**
- Average distance between two randomly selected points in an n-D cell:
  - 1-D = 0.333…
  - 2-D = 0.521…
  - 3-D = 0.662…
- Independent of number of points per cell.
- Increasing the number of simulators per cell (N_c) will not reduce mean distance between randomly selected molecules.

VSC and TASC

- Virtual Sub Cells (LeBeau 2003)
  - Deterministically determines the nearest neighbor
  - More accurate
  - More expensive than TASC for large N, $O(N^2)$
- Transient Adaptive Sub Cells (Bird 2000)
  - Stochastically determines the nearest neighbor
  - Creates Cartesian sub-cell structure for each collision phase
  - Number simulators in each sub-cell ~ 1-2
  - Less expensive for large N, O(N)

VSC, TASC Spatial Discretization

- **With VSC, TASC the average distance between nearest-neighbor points in a cell is a function of:**
  - Dimensionality
  - Cell Size
  - Number of Simulators
- **Effect plateaus after about**
  - **50 sims/cell for 3-D**
  - **100 sims/cell for 2-D**
  - **250 sims/cell for 1-D**



Sandia National Laboratories

VSC, TASC Result in Better Spatial Discretization

- **The way potential collision partners are selected affects the average distance between collision partners.**
- **The spatial discretization error is a function of the MCS/MFP ratio.**
  - "MCS" is Mean Collision Separation, "MFP" is Mean Free Path

Effect on Mean Collision Separation (MCS)		
	DSMC94	DSMC07
Simulators/cell	no	yes
Cell Size	yes	yes
Dimensionality	yes	yes

DSMC94 achieves only cell-size resolution

- Collisions between random simulators

DSMC07 achieves sub-cell resolution

- Collisions between nearest neighbors

Sandia National Laboratories

Nearest Neighbor Procedures

- This improvement comes at a cost.
- VSC and TASC are computationally more expensive than random selection.
- However, MCS will be smaller and the accuracy better.
- Same pair cannot have sequential collisions.
  - Physically unlikely collision.
- Coarse, reduced-dimensionality implementations can introduce stress-tensor anisotropy.
  - Molecular motion is always 3-D even in 1-D codes.
  - Periodic boundary conditions on degenerate dimensions.

Temporal Discretization
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 average 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 collision cell
  Move is considered for a particular molecule

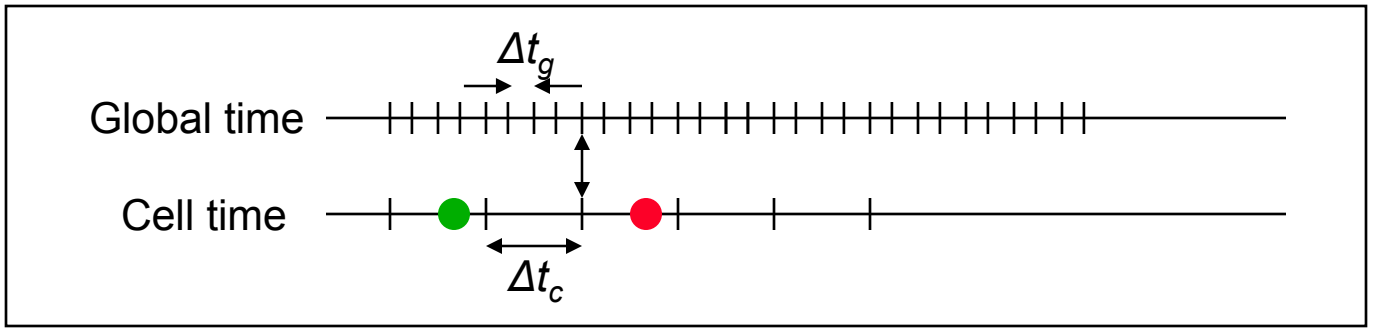
Sandia National Laboratories

DSMC07 Advection and Collision

- 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 for $2\Delta t_c$ only when their "time" (cell time) falls more than Δt_c behind global time
  - Molecules move $2\Delta t_c$ only when their "time" (molecule time) falls more than Δt_c behind global time



Sandia National Laboratories

Calculation of Δt_c

- 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*)
- Cells are examined at frequent intervals to calculated new values for the time step.
- MTT is based on both thermal and average molecular velocities.
  - Typical values: MCT=3~5, MTT=2~4

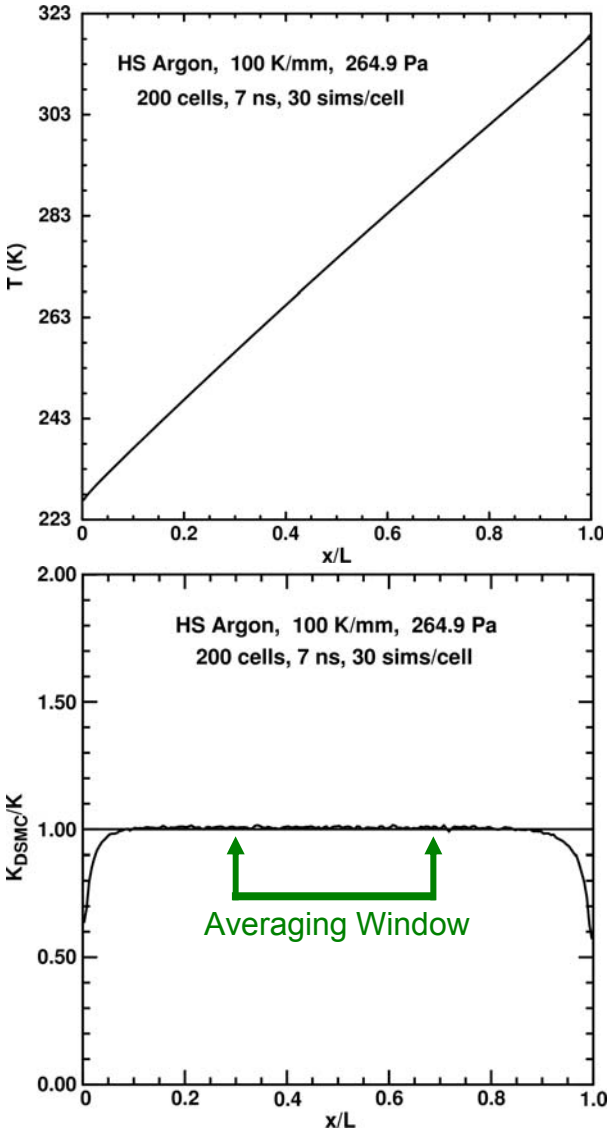
Calculation of Δt_g

- The global time step is calculated as a function of (Δt_c)
- When all cells have updated their (Δt_c), the minimum, average, and maximum (Δt_c) are calculated.
- Δt_g is a user-specified function of the average Δt_c
  - *Typical value* $\Delta t_g = 0.2\ \Delta t_{c,average}$
- Smaller values of Δt_g lead to more accurate simulations.

Move-Collide: A Closer Coupling

- Molecules cannot travel across a sampling cell in one move without considering collisions.
- DSMC07 is more sensitive to time step.
- It is physically inconsistent to allow molecules to ignore collision partners during long advection phases.
- Similar to DSMC94 sub-cells. Time step should conform to sub-cell structure.

Assessing DSMC 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

Sandia National Laboratories

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 sub-cells were used for any N_c
- To eliminate statistical noise, 100 simulations were performed for each data point (ensemble averaging)

Sandia National Laboratories

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)

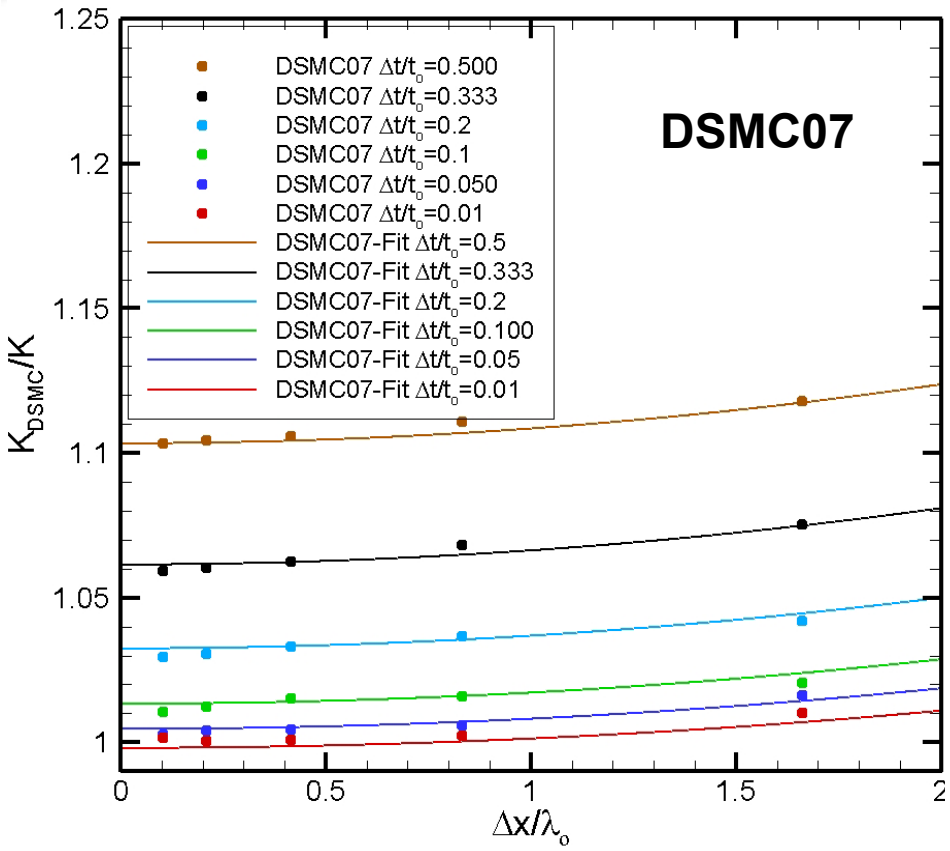
Error related to cell width, Δx

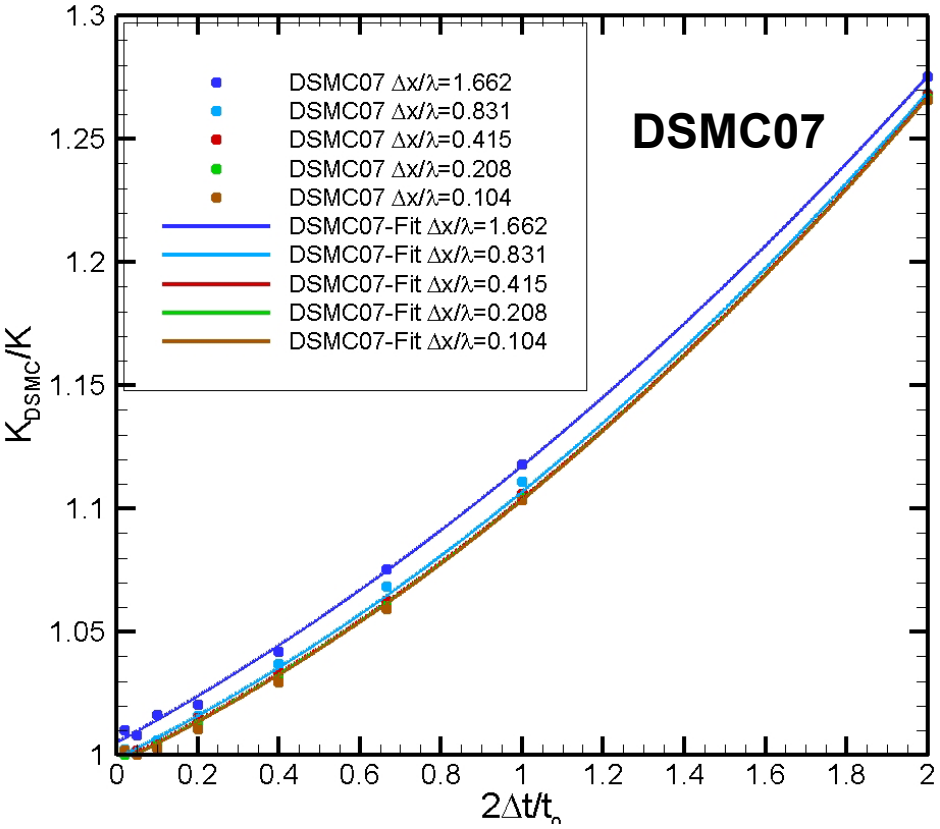
- Collision partners selected from anywhere in same cell
- Some potential partners move into adjacent cells
- Some invalid partners move into the same cell

Error related to time step, Δt

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

Convergence Behavior for $N_c \rightarrow \infty$

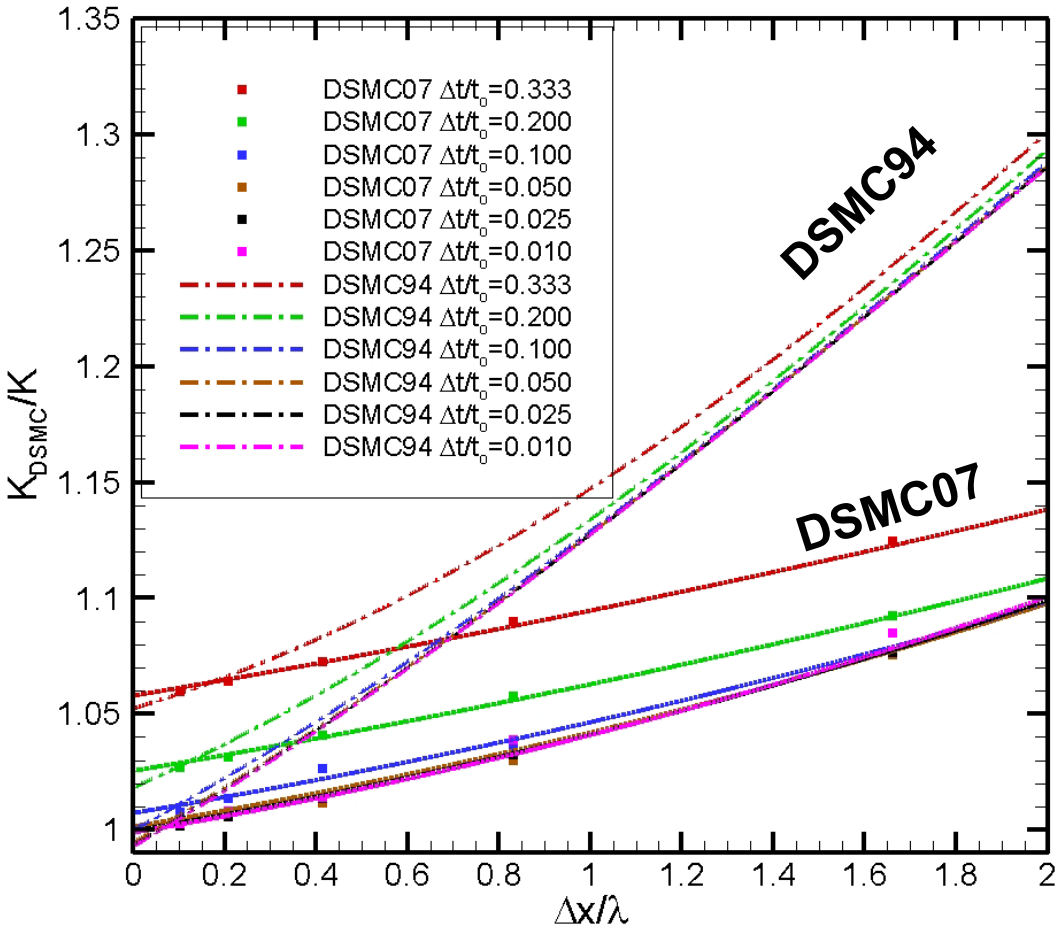




- The algorithm is
  - Insensitive to spatial resolution
  - Spatial resolution constraint: $\Delta x \leq \lambda$
  - Almost linearly dependent on time step

Sandia National Laboratories

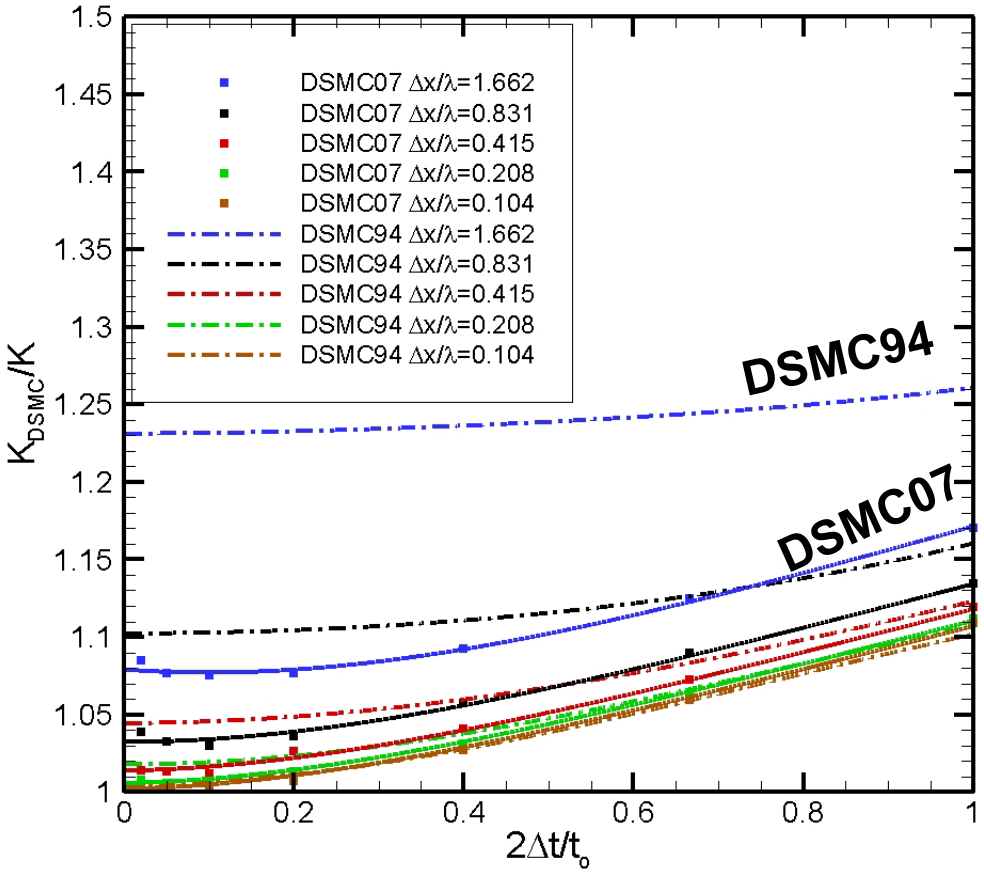
Convergence Behavior for $N_c = 10$ Effect of Cell Size



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

Sandia National Laboratories

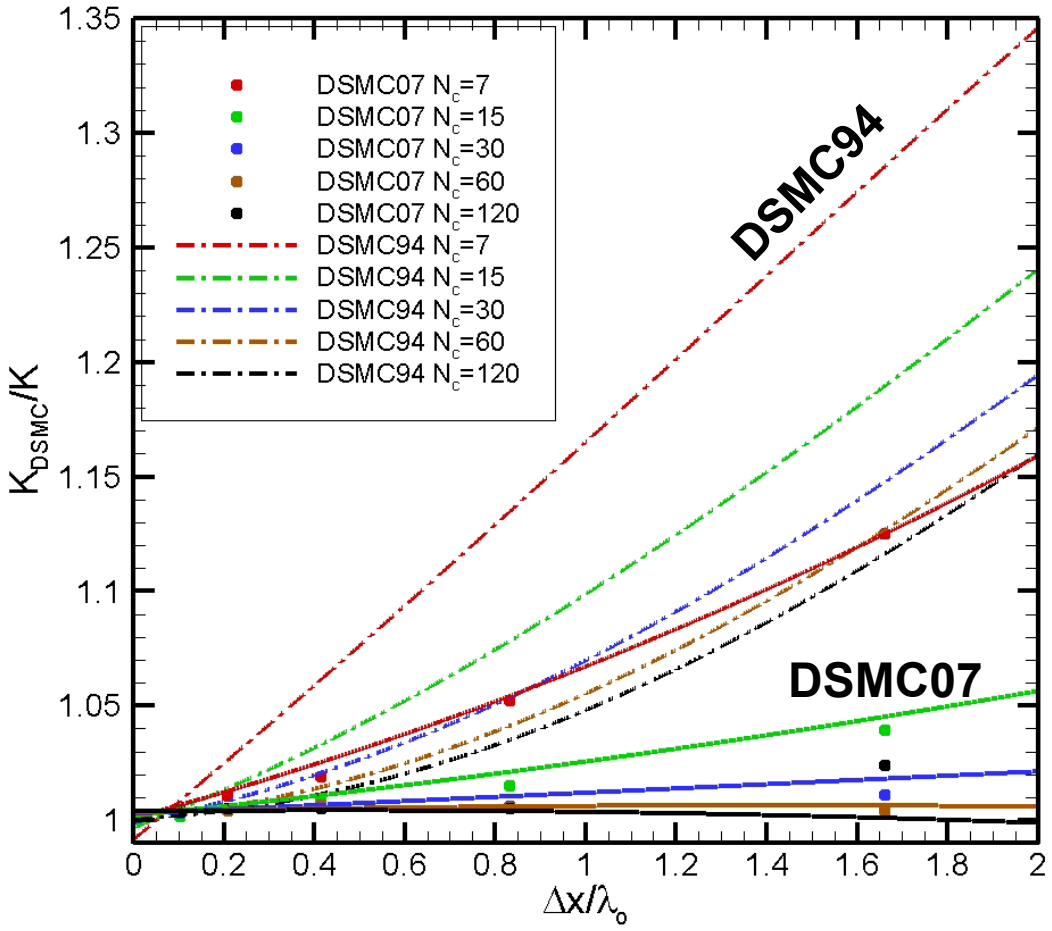
Convergence Behavior for $N_c = 10$ Effect of Time Step



- The algorithm exhibits a near-linear dependence on time step
- For nearest-neighbor schemes, time-step should conform to effective spatial resolution.

Sandia National Laboratories

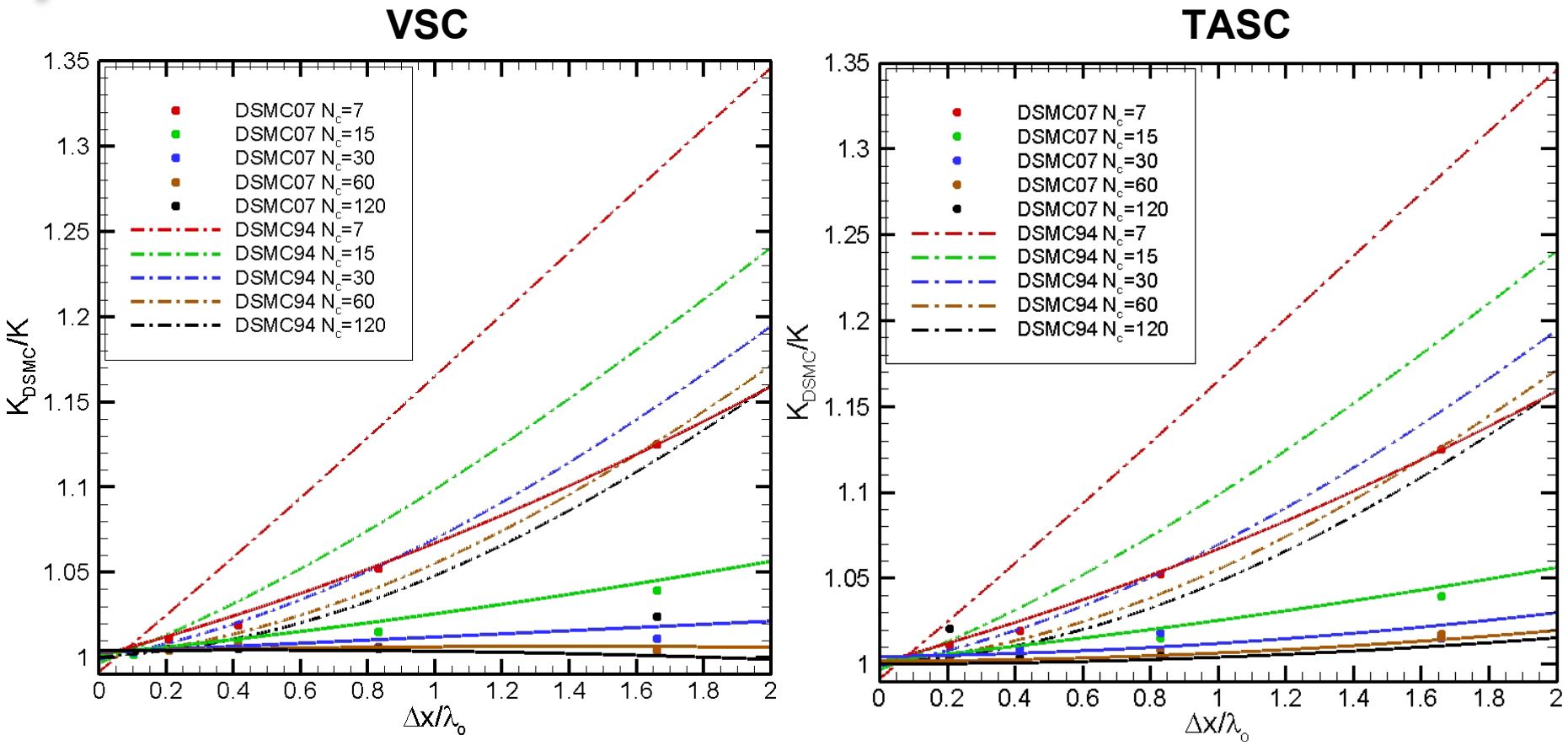
Effect of Simulators Per Cell N_c at $\Delta t/t_o$=10



- By following DS2V guidelines error can be limited to ~2%

Sandia National Laboratories

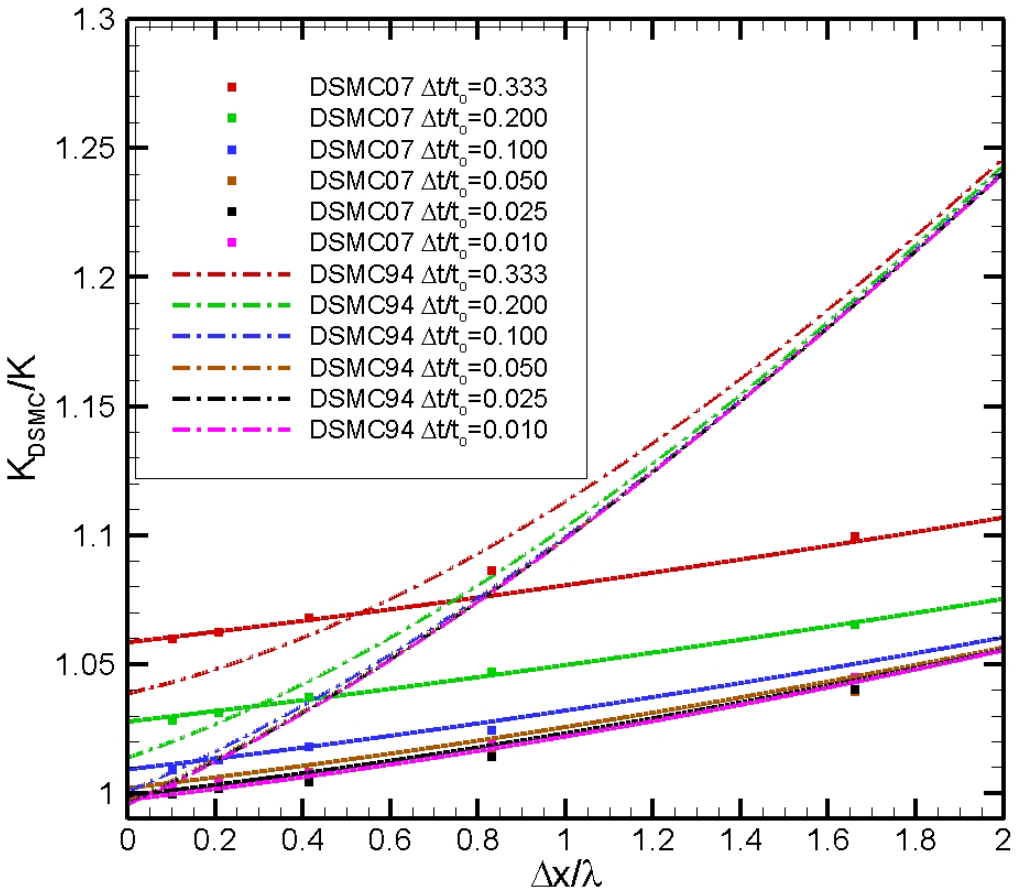
Effect Search Scheme ($\Delta t/t_o$=10)



- VSC and TASC give similar results for small N_c.
- For large N_c TASC may not always pick the nearest neighbor.

Sandia National Laboratories

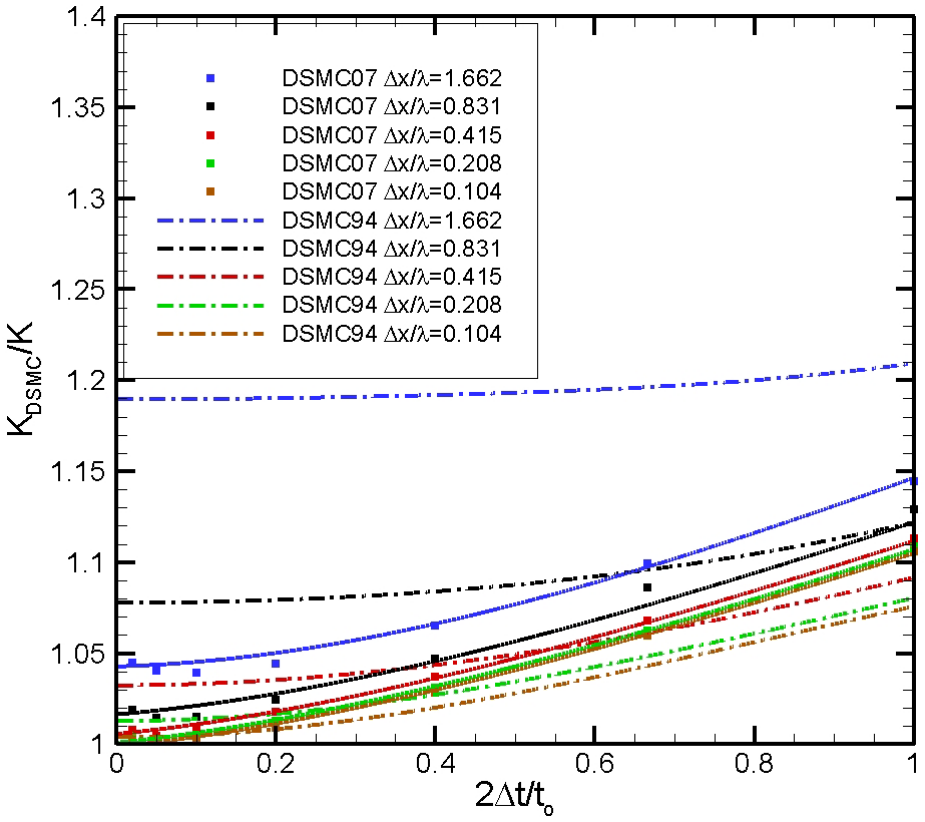
Convergence Behavior for $N_c = 15$ Effect of Time Step

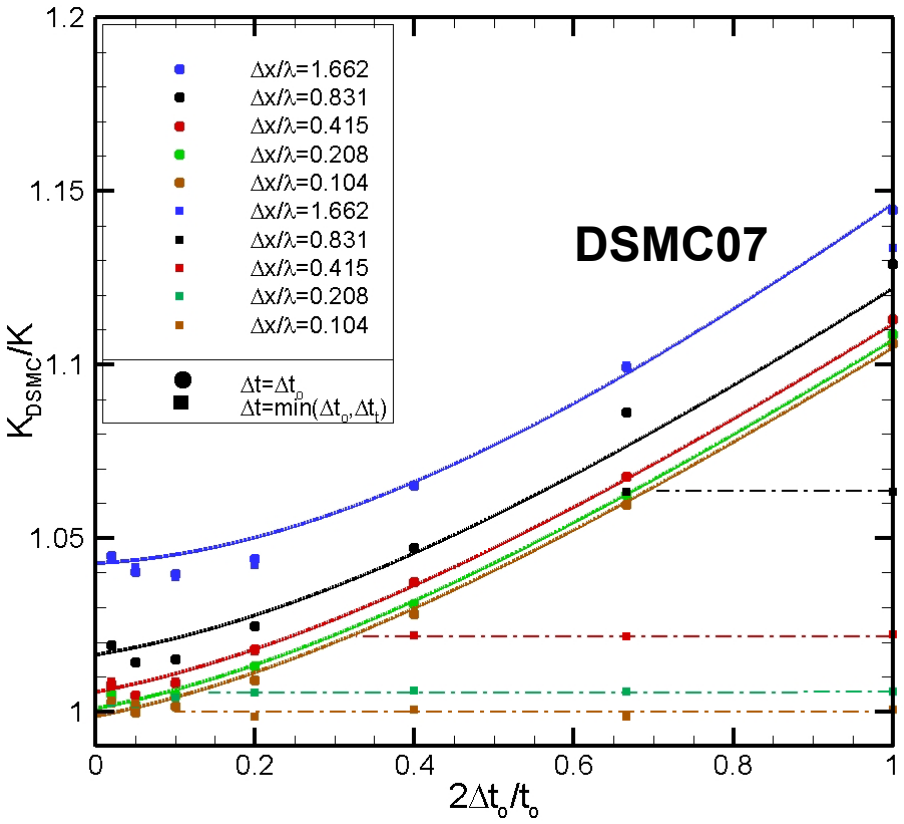


For large $\Delta t/t_o$ and fine $\Delta x/\lambda$, the error of DSMC07 can be greater than DSMC94!

Sandia National Laboratories

Convergence Behavior for $N_c = 15$
Limiting the Time Step error





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 $\Delta t_t \propto t_t$

Sandia National Laboratories

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

Sandia National Laboratories

DSMC07
Functional Form of Error

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

$$\frac{K_{DSMC}}{K} = 0.99508 + 0.06289\left(\frac{2\cdot\Delta t}{t_o}\right) + 0.04780\left(\frac{2\cdot\Delta t}{t_o}\right)^2 - 0.00267\left(\frac{\Delta x}{\lambda}\right)^2$$
$$- 0.00193\left(\frac{2\cdot\Delta t}{t_o}\right)^2\left(\frac{\Delta x}{\lambda}\right)^2 + 0.09216\frac{1}{N_c} + \frac{1}{N_c}F\left[\frac{2\cdot\Delta t}{t_o}, \frac{\Delta x}{\lambda}, \left(\frac{2\cdot\Delta t}{t_o}\right)^2\right]$$

DSMC limiting convergence differs from Green-Kubo (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)

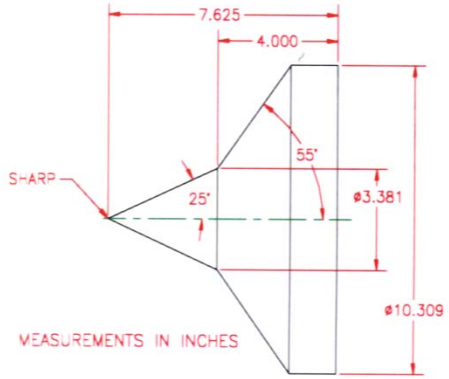
Sandia National Laboratories

Assessing Efficiency

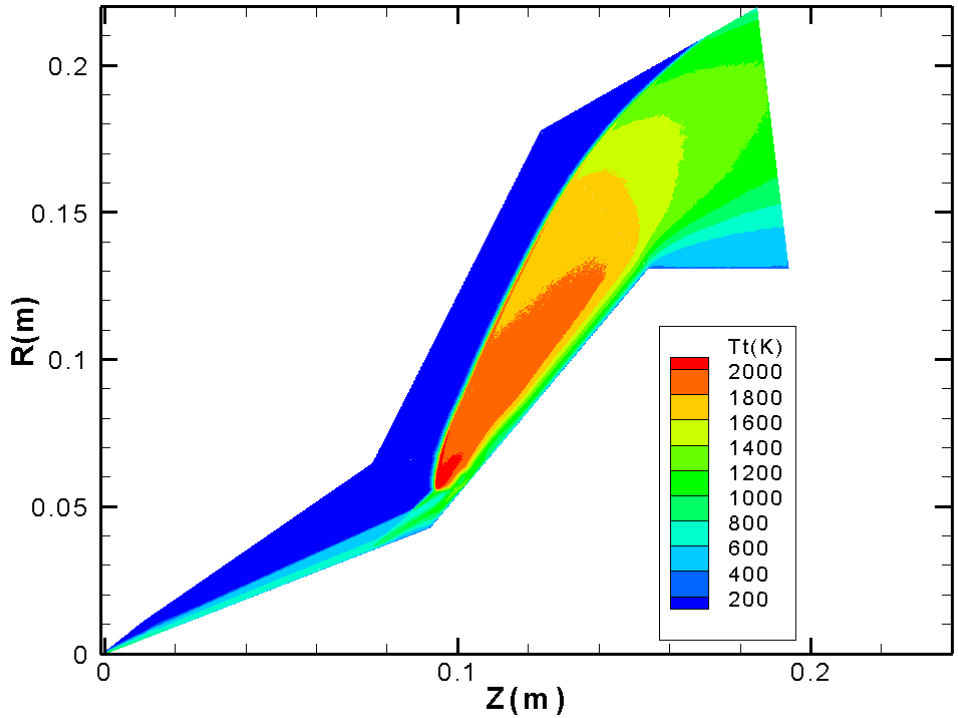
- Is the new method computationally more efficient than the old one?

- "Efficiency" is essentially the amount of time that can be simulated with a prescribed accuracy on the same computational platform.

Hypersonics Simulation



Mach 11, 25°-55° blunt biconic

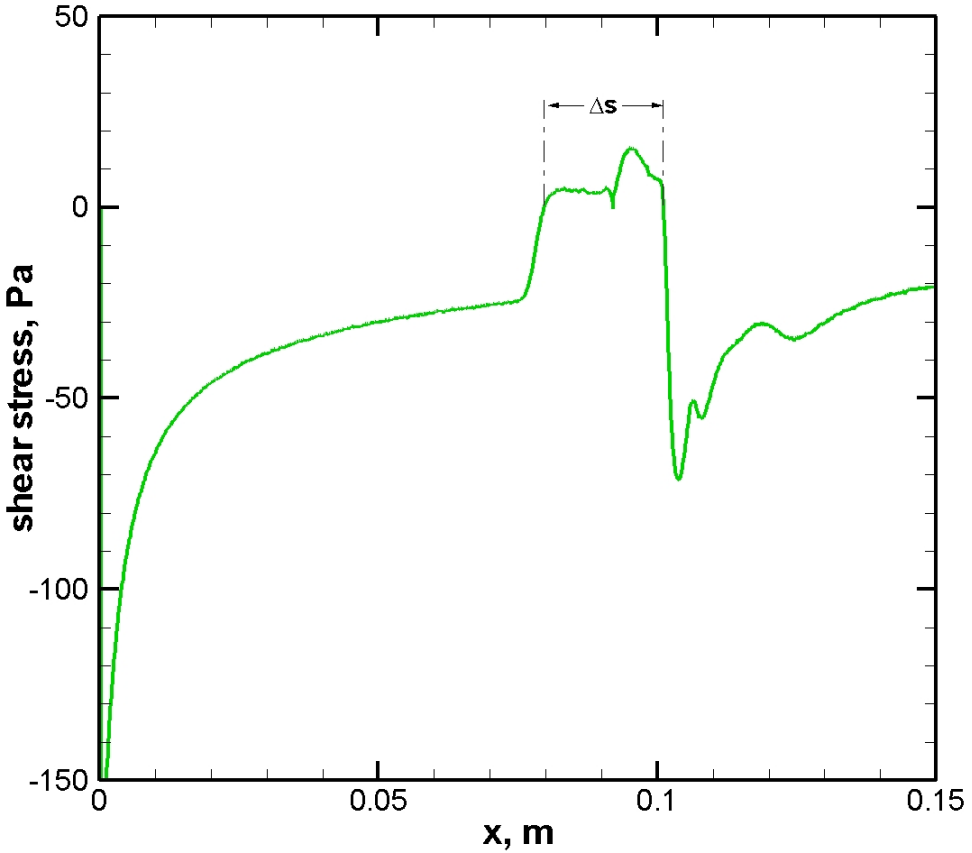


Flow Conditions

- Nitrogen gas
- *Re* = 140,000/m
- T_0 = 3280 K
- *V* = 2072 m/s
- *Kn* = 0.02
- *M* = 11.3
- *T* = 42 K
- T_{vib} = 1983 K

Sandia National Laboratories

Recirculation Zone

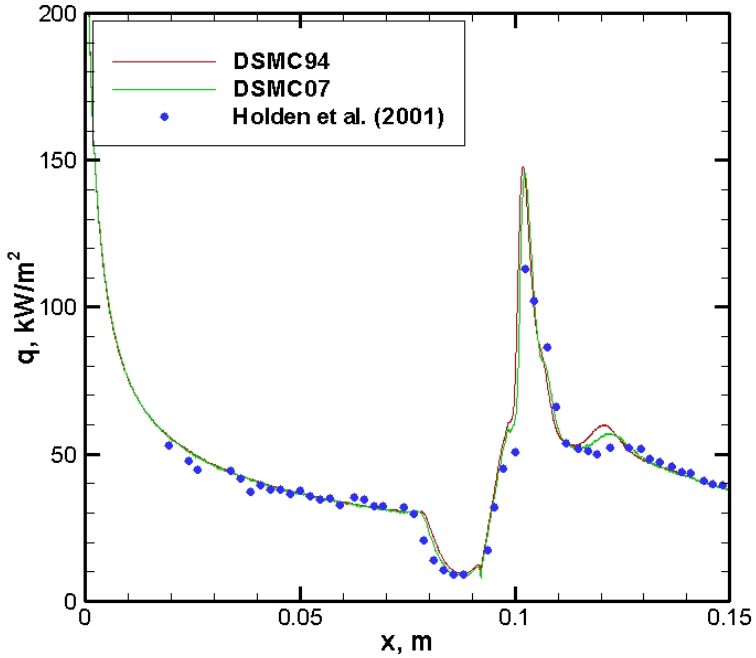


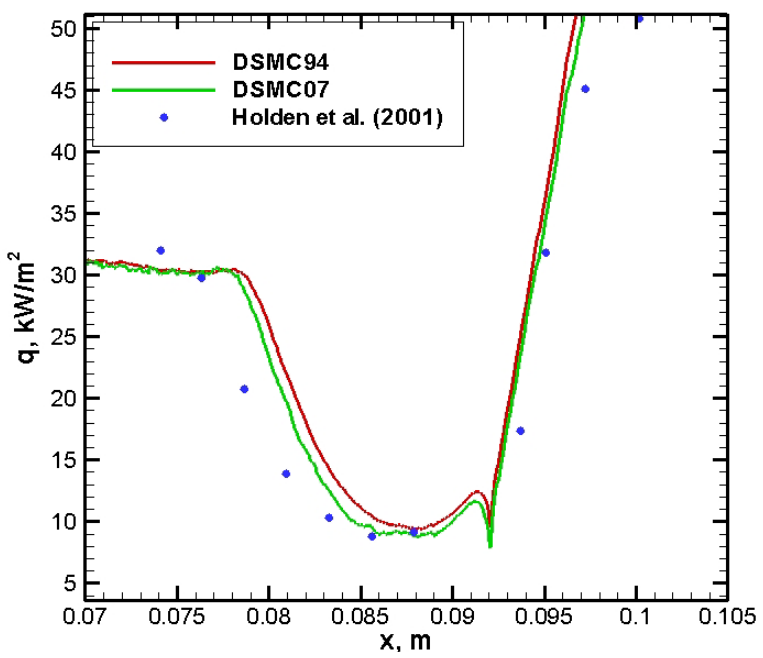
Extensive studies, (Moss, Markelov) indicate that the extend of the recirculation zone is $\Delta_{s,o}$=21.5mm.

Δs is sensitive to discretization parameters and is used as a convergence criterion.

Sandia National Laboratories

DSMC94 & DSMC07 Simulation Speed when Achieving Equal Accuracy

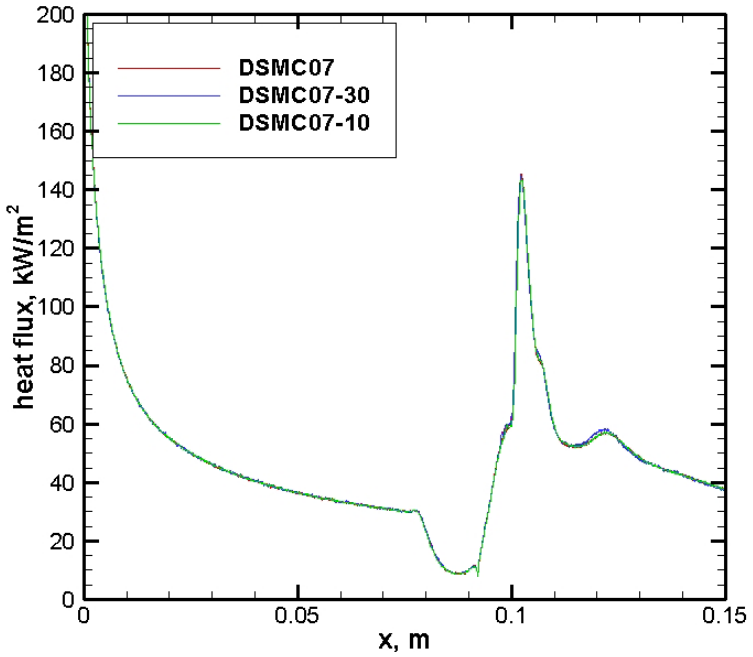


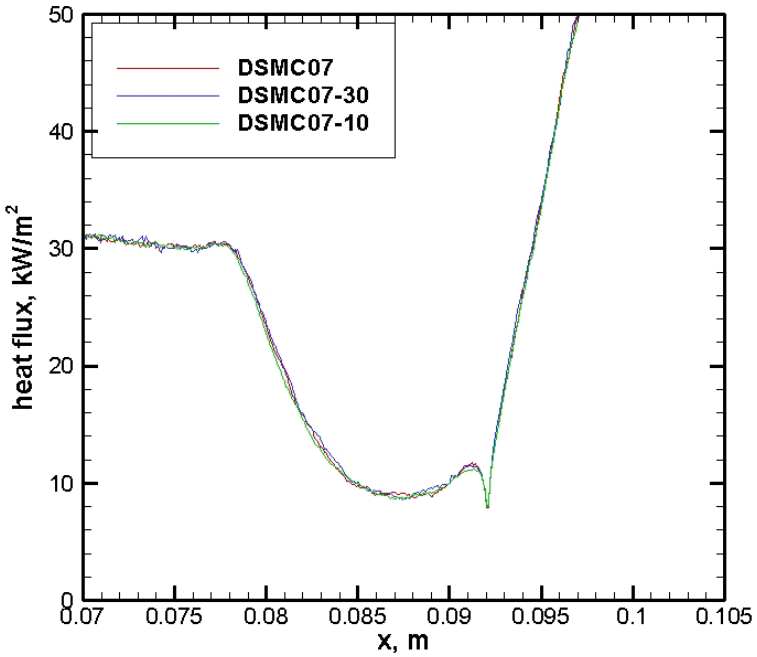


DSMC94 MCS = DSMC07 MCS							
DSMC94				DSMC07			
# Cells	Sims/cell	$\Delta s/\Delta_{s,o}$	ns/proc-min	# Cells	Sims/cell	$\Delta s/\Delta_{s,o}$	ns/proc-min
250,000	10	76%	8.72	250,000	10	94%	5.61
1,000,000	10	94%	1.48	1,000,000	10	100%	1.01

Sandia National Laboratories

DSMC07 Simulation Speed
Limited Collision Partner Search

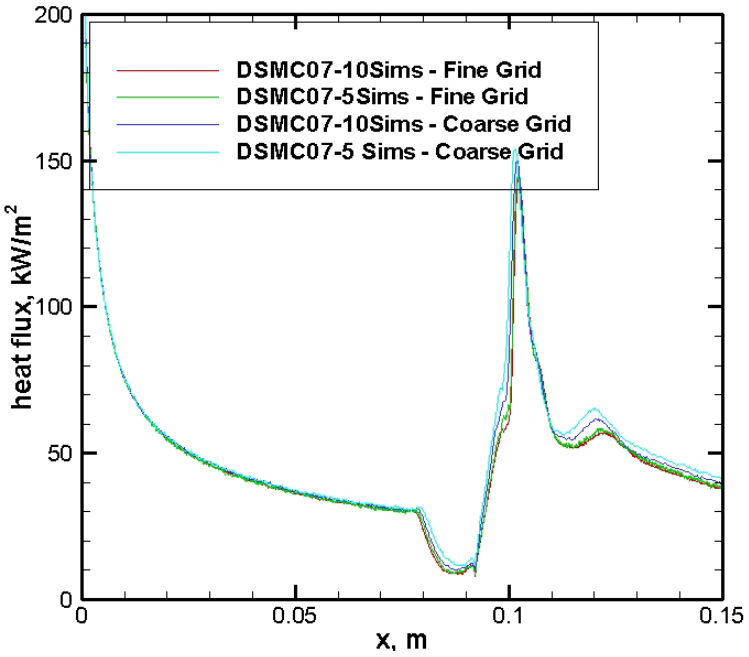


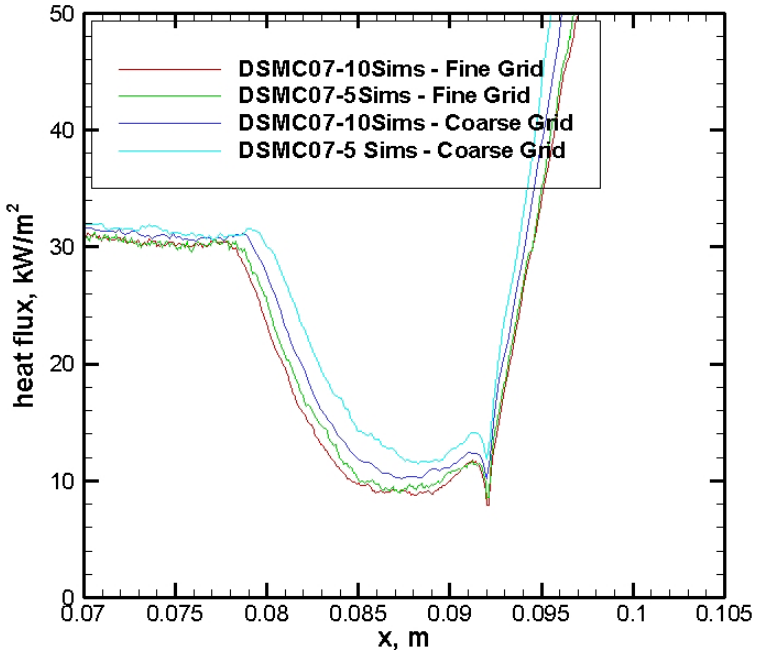


Algorithm	$\Delta s/\Delta_{s,o}$	ns/proc-min
DSMC07	99.5%	1.01
DSMC07-30	100%	1.19
DSMC07-10	99.0%	1.33
DSMC94	94.4%	1.48

Sandia National Laboratories

DSMC07 Simulation Speed
Simulators or Cells?





Algorithm	$\Delta s/\Delta_{s,o}$	ns/proc-min
10 Sims & Fine Grid	99.5%	1.01
5 Sims & Fine Grid	97.2%	1.16
10 Sims & Coarse Grid	94.4%	5.61
5 Sims & Coarse Grid	86.5%	9.51

Sandia National Laboratories

DSMC Guidelines

DSMC94 rule-of-thumb guidelines

- Sample enough to drive statistical error down
- Keep time step smaller than ~1/4 mean collision time
- Keep cell size smaller than ~1/3 mean free path
- Use a minimum of ~20 simulators per cell

DSMC07 rule-of-thumb guidelines

- Sample enough to drive statistical error down
- Keep time step smaller than ~1/3 mean collision time and ~1/2 mean cell transit time
- Keep cell size ~1/2 mean free path
- Use ~10 simulators per cell

Following these simple guidelines will lead to a discretization error ~2%

Summary

- DSMC07 can achieve the same accuracy as DSMC94 using less resources.
- VSC/TASC is the main contributor.
- Dynamic time-stepping offers significant advantages.
- For nearest-neighbor schemes, time-step should conform to effective spatial resolution.

Sandia National Laboratories

Assessing the Accuracy of DSMC

- Comparison of DSMC predictions to measured flow field quantities is the ultimate criterion
- Simple, 0-D or 1-D problems can be very efficient in assessing the accuracy of the DSMC algorithm (or its implementation)
- Analytical solutions exists for flows in:
  - Equilibrium
  - Local thermodynamic equilibrium
  - Near-equilibrium (Chapman-Enskog regime, Kn~0.01)
  - Thermodynamic non-equilibrium (Kn>0.01)

Collision Frequency in an Equilibrium Bath

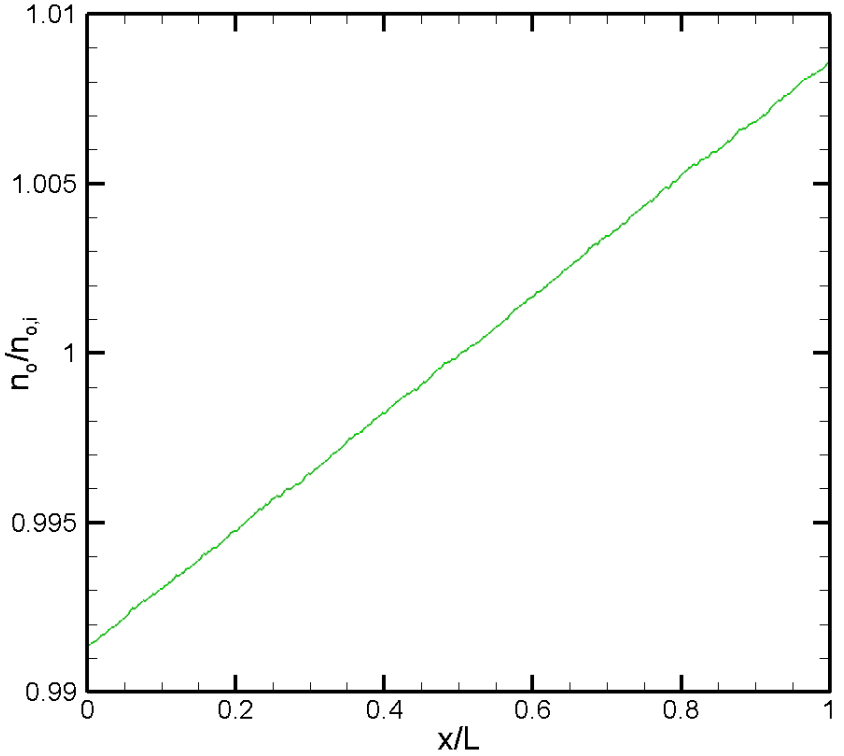
Simulators per cell	ν_{DSMC07} / ν_{th}
2	0.9969
5	1.0004
10	0.9994
30	1.0007
60	0.9970
120	1.0001

- Molecules HS “argon”
- Walls fully accommodating
- Width 0.001 m (1 mm)
- Pressure 264.9 Pa (~2 torr)

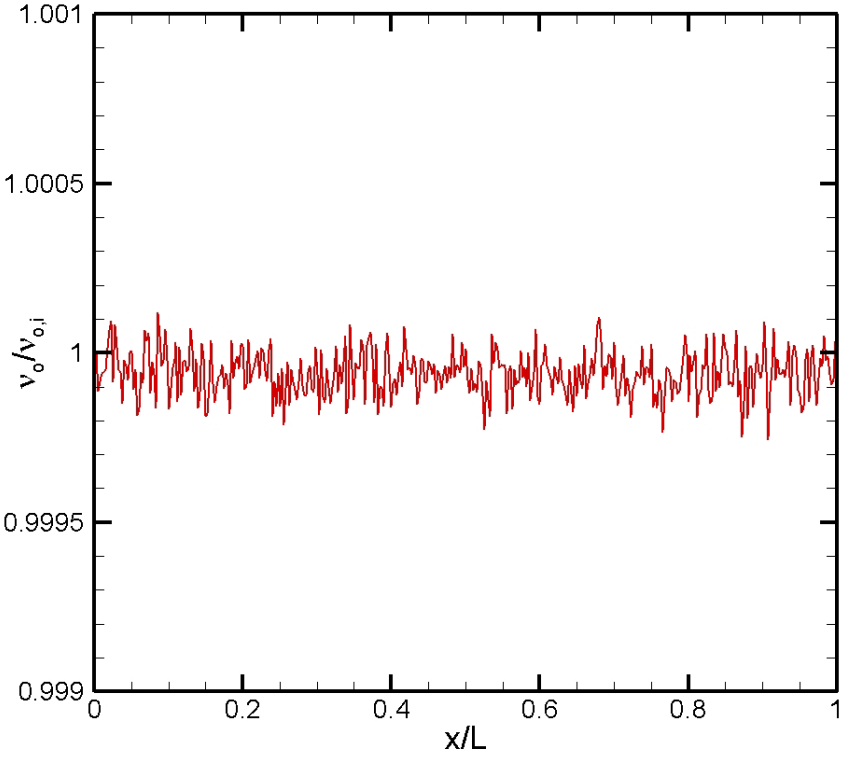
Sandia National Laboratories

Collision Frequency in an Equilibrium Bath with Gravity

Normalized Density



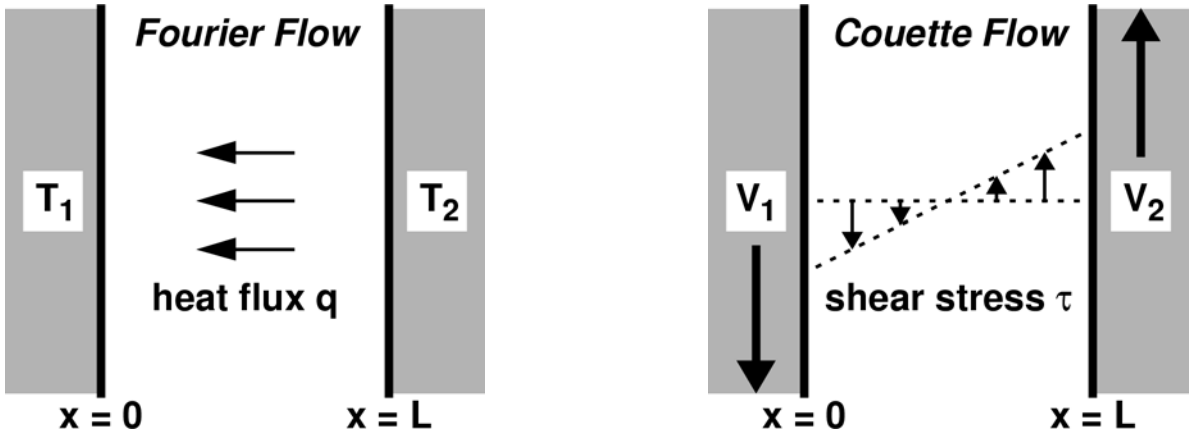
Collision Frequency Ratio



- Molecules HS “argon”
- Walls fully accommodating
- Width 0.001 m (1 mm)
- Pressure 264.9 Pa (~2 torr)
- Gravity 9.81×10^4 m/s^2 (10^4 g)

Sandia National Laboratories

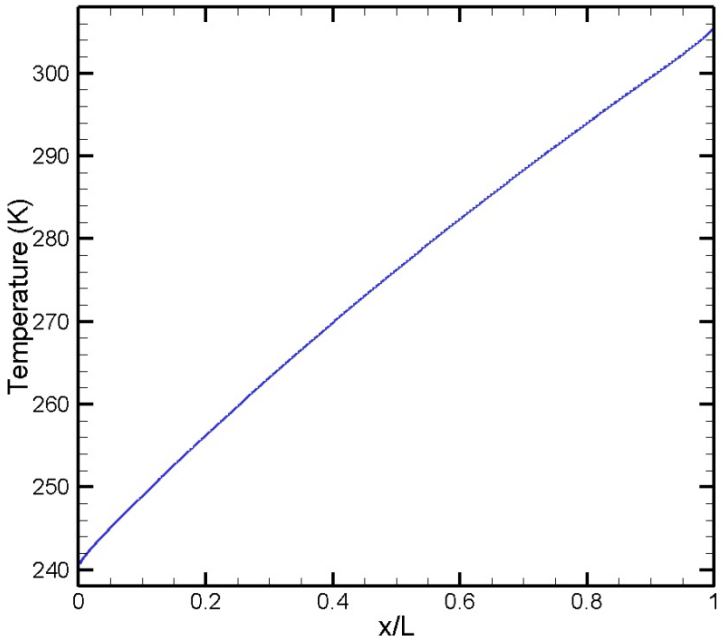
Fourier-Couette Benchmark Flow



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

Sandia National Laboratories

Comparing DSMC to Near-Equilibrium Theory



Temperature profile (velocity profile is similar)

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

Chapman-Enskog and Moment Hierarchy theory
DSMC results

- Thermal conductivity, viscosity: K, μ

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

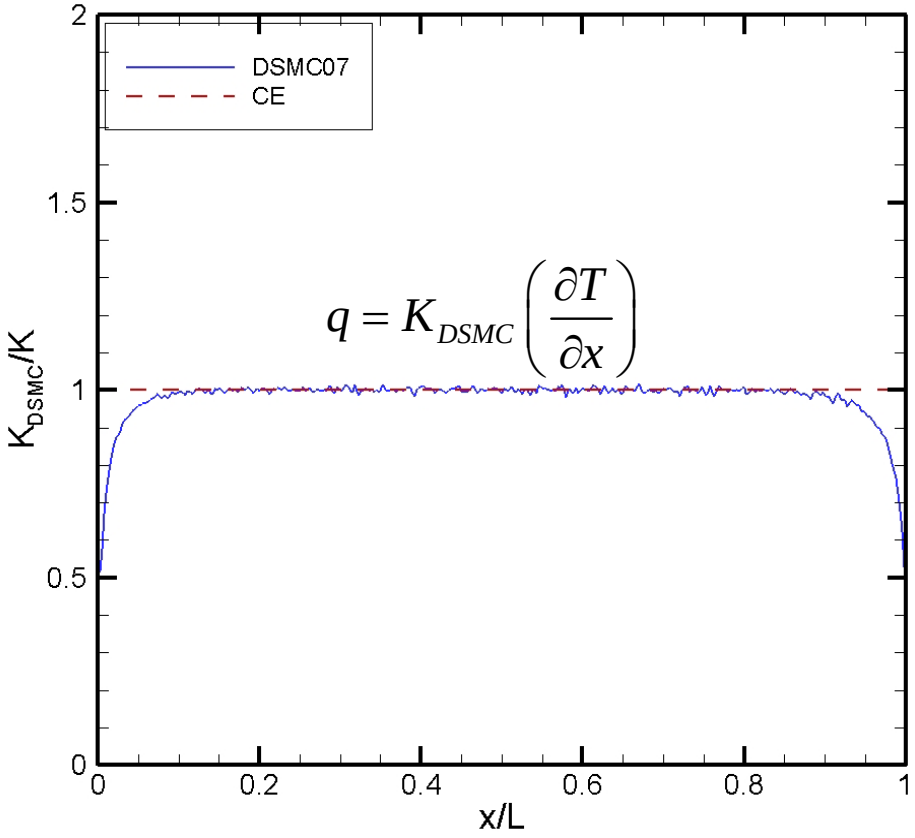
- Sonine polynomial coefficients: a_k/a_1, b_k/b_1

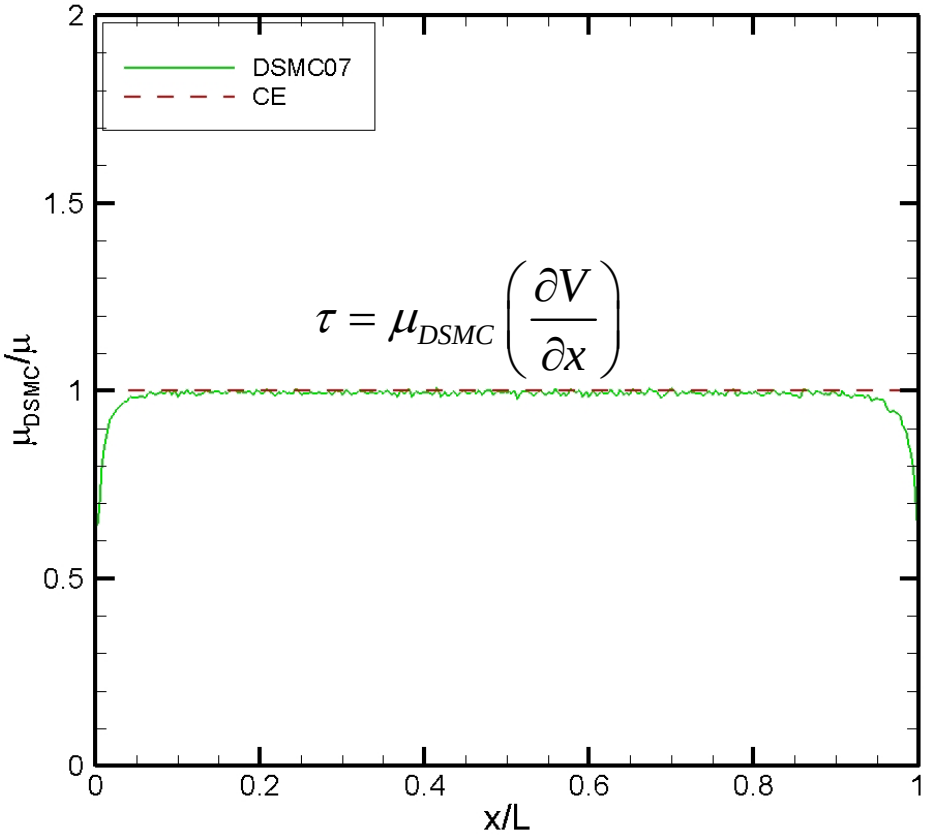
$$\left(\frac{a_k}{a_1}\right)_{DSMC} = \sum_{i=1}^{k}\left(\frac{(-1)^{i-1}k!(5/2)!}{(k-i)!i!(i+(3/2))!}\right)\left(\frac{\left\langle \tilde{c}^{2i}\tilde{c}_x\right\rangle}{\left\langle \tilde{c}^{2}\tilde{c}_x\right\rangle}\right)$$

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

Sandia National Laboratories

DSMC07: Hard-Sphere Transport Coefficient Profiles

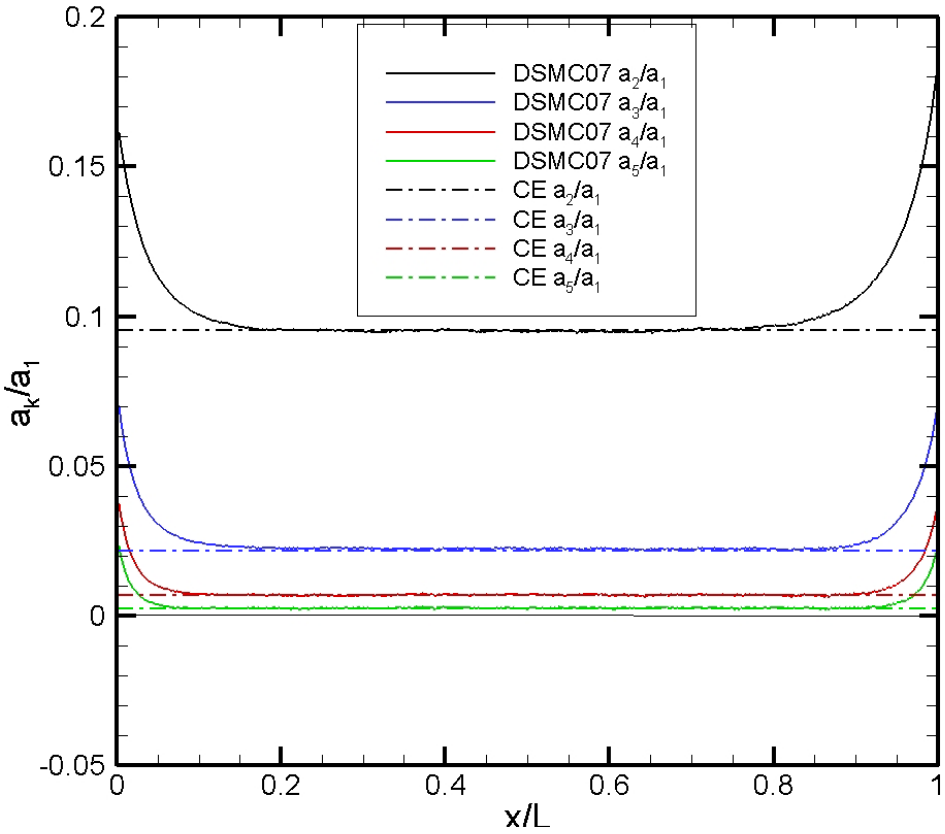


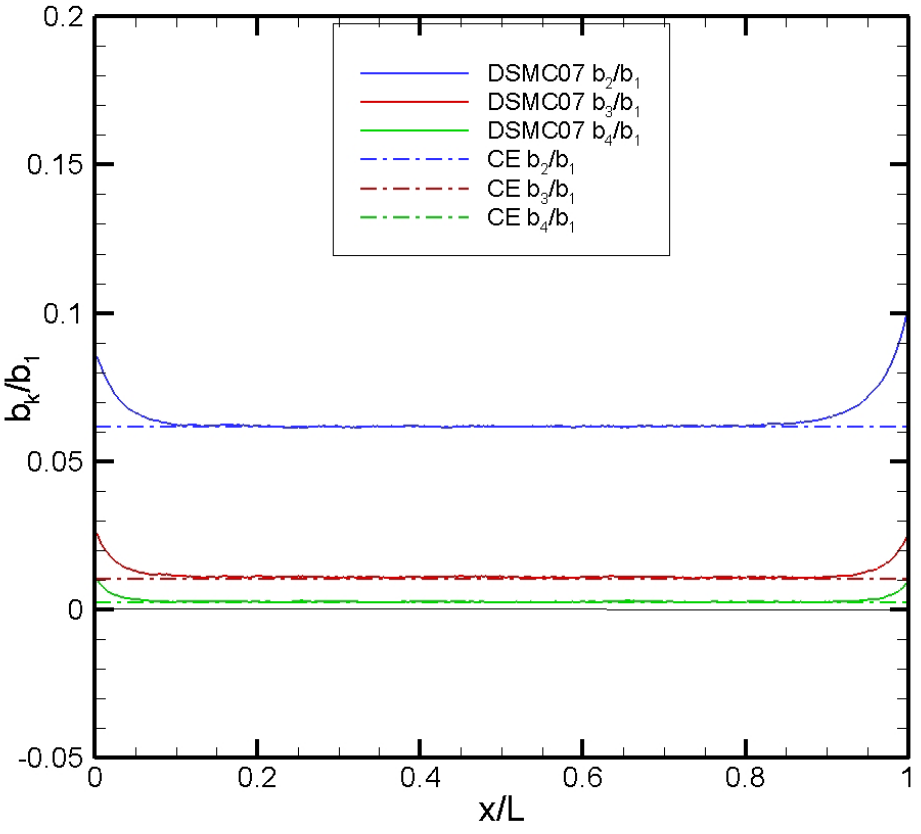


- DSMC07 and CE thermal conductivity and viscosity
  - Low heat flux, low shear stress: $Kn_q = 0.006$, $Kn_\tau = 0.003$
  - Agreement in central region: normal solution
  - Demonstrates accuracy in capturing transport properties and non-equilibrium effects

Sandia National Laboratories

DSMC07: Hard-Sphere Sonine-Coefficient Profiles

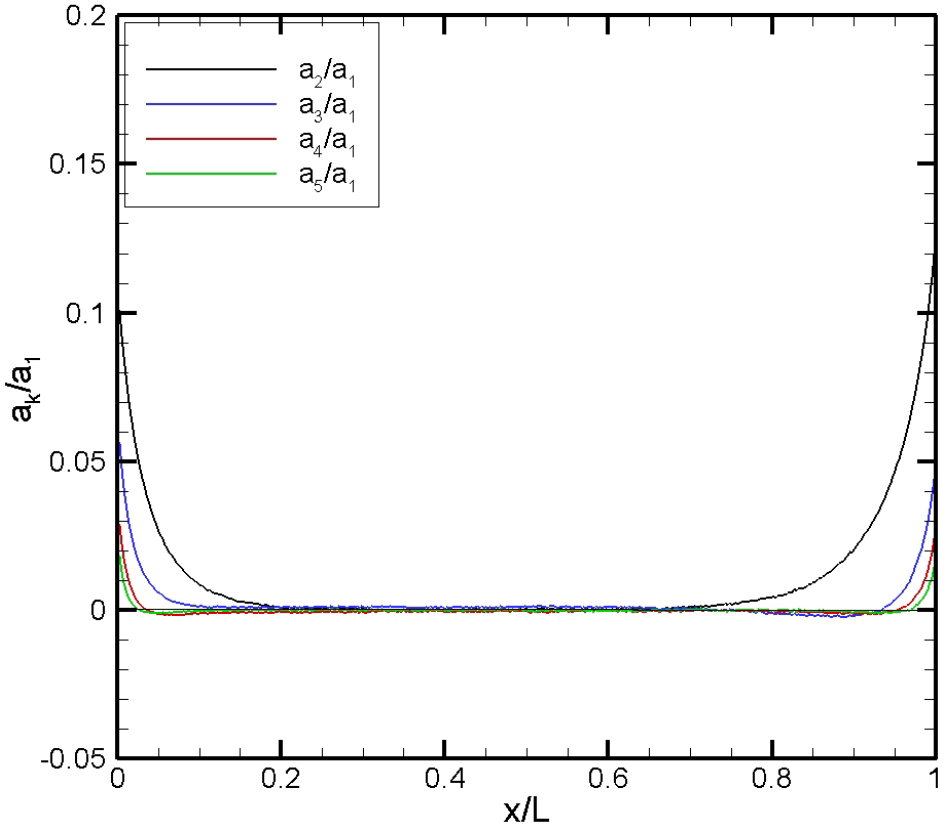


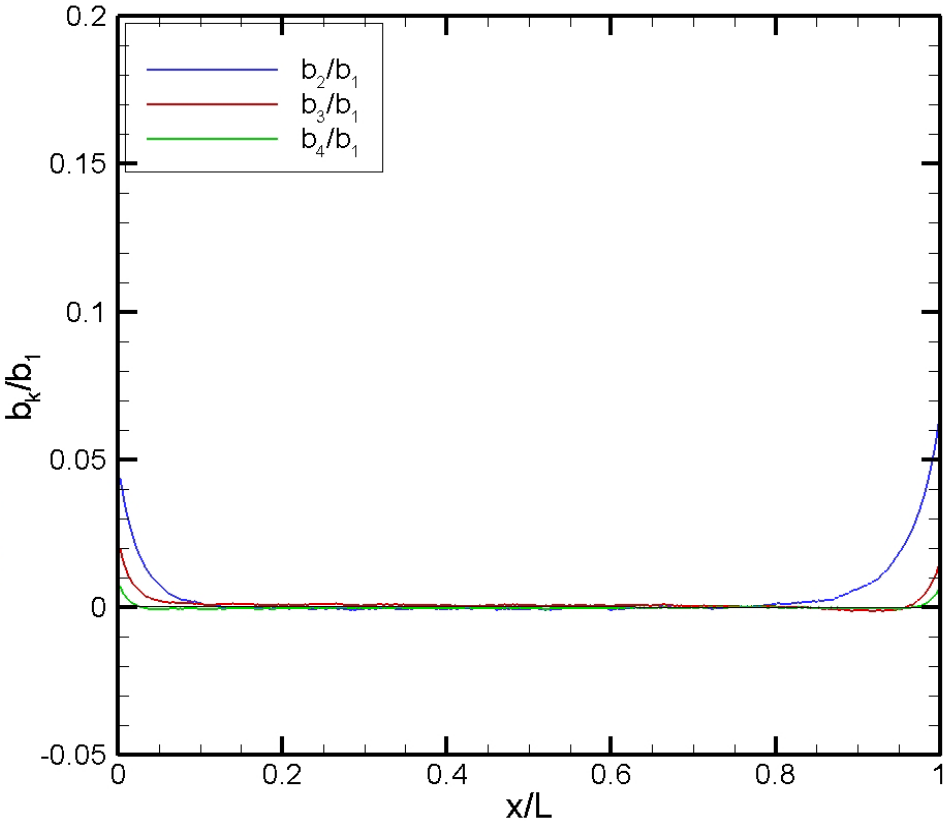


- DSMC07 and CE Hard-Sphere Sonine polynomial coefficients a_k/a_1 and b_k/b_1
  - Low heat flux, low shear stress: $Kn_q = 0.006$, $Kn_\tau = 0.003$
  - Good agreement in central region: normal solution
  - Demonstrates accuracy of molecular velocity distribution

Sandia National Laboratories

DSMC07: Maxwell Sonine-Coefficient Profiles

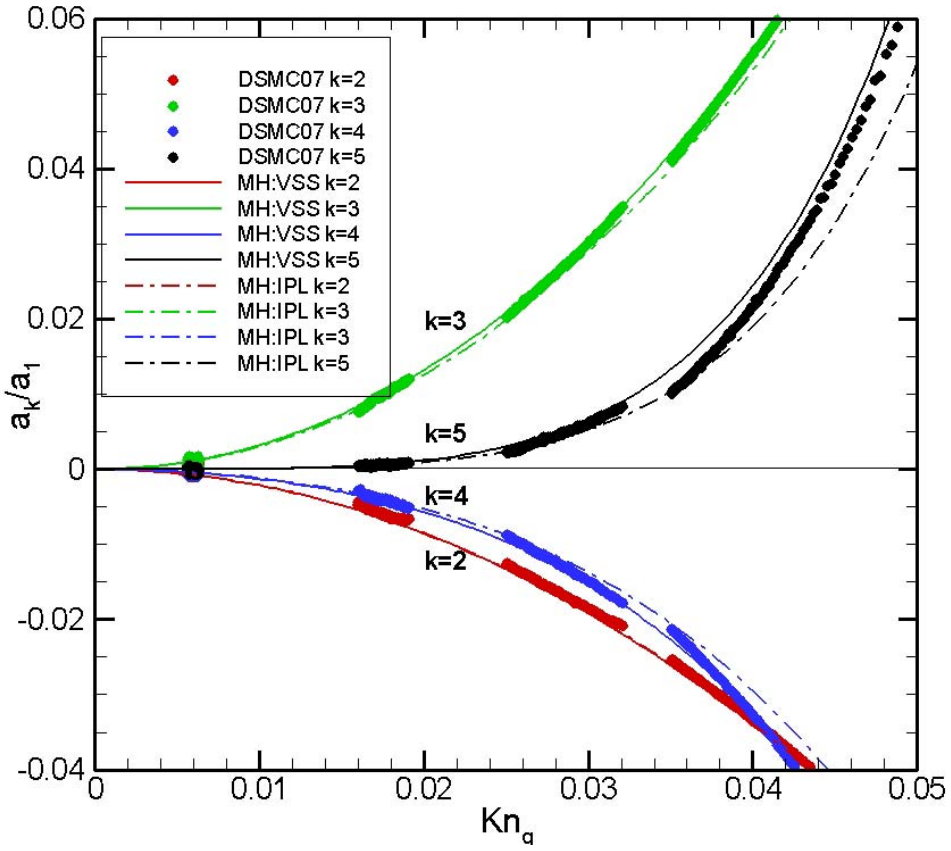


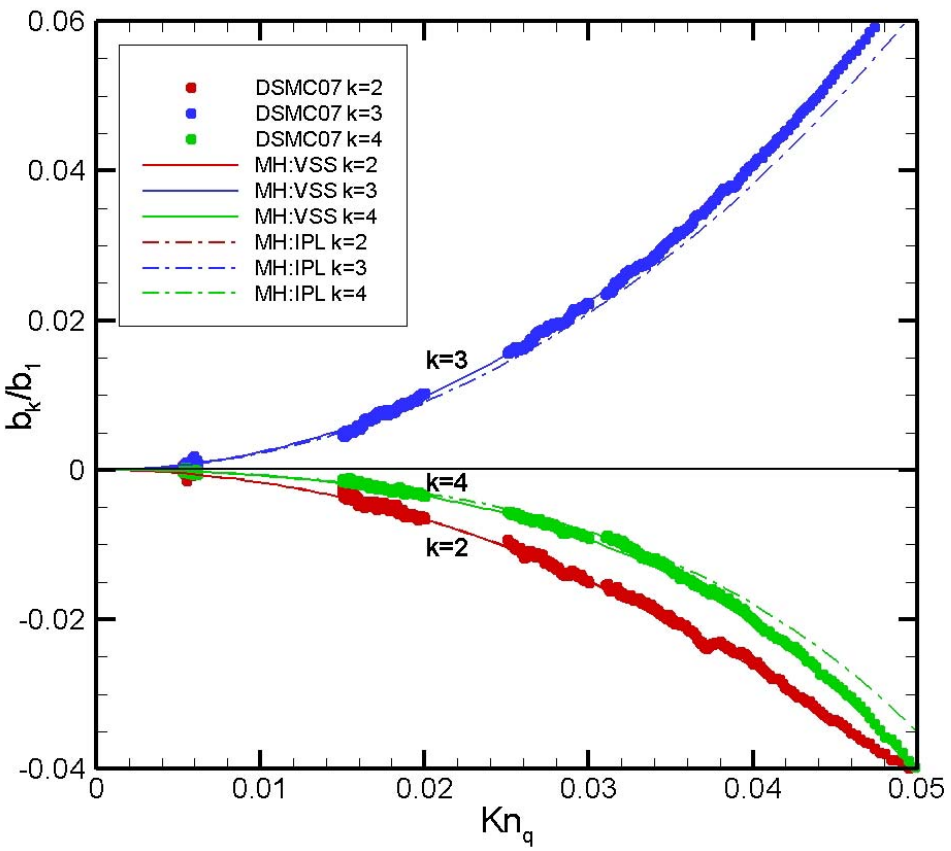


- DSMC07 and CE Maxwell Sonine polynomial coefficients a_k/a_1 and b_k/b_1
  - Low heat flux, low shear stress: $Kn_q = 0.006$, $Kn_\tau = 0.003$
  - Good agreement in central region: normal solution
  - Demonstrates accuracy of molecular velocity distribution

Sandia National Laboratories

DSMC07: Maxwell
Normal Sonine Coefficients

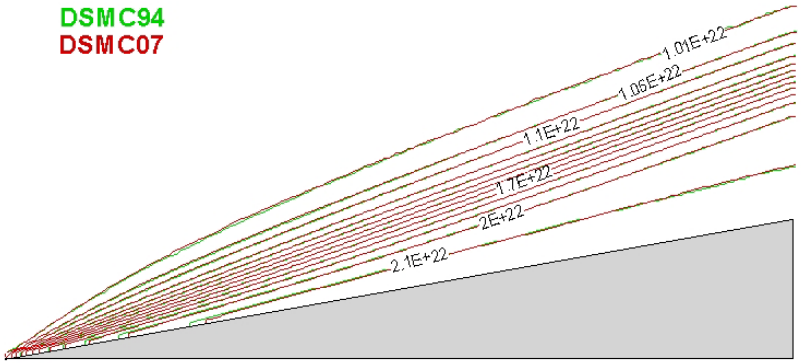




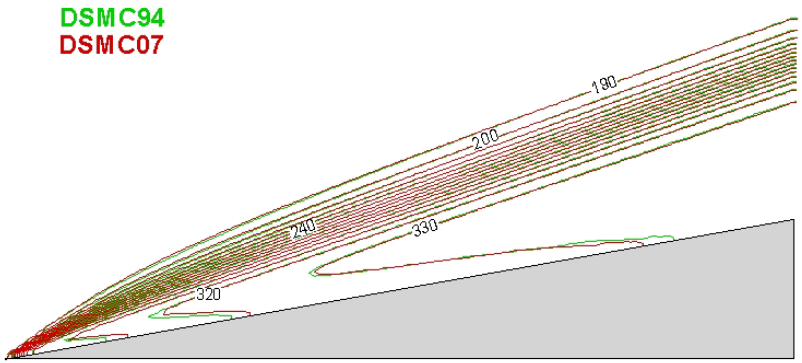
- DSMC07 and MH Maxwell normal solutions for a_k/a_1 and b_k/b_1
  - Four DSMC07 simulations: ΔT = 70, 200, 300, 400 K
  - MH: VSS-Maxwell (solid) and IPL-Maxwell (dashed) differ
  - DSMC07 and MH VSS-Maxwell normal solutions agree

Sandia National Laboratories

2-D Problem
Hypersonic Flow over a Wedge



Number Density



Temperature

Gas	Argon
Flow Speed	Mach 5.463
Pressure	25 Pa
Wedge Angle	10º
Shock Angle	19.6º

DSMC94 and DSMC07 are in agreement when the same simulation parameters are used

Downstream properties are in agreement with shock theory

Sandia National Laboratories

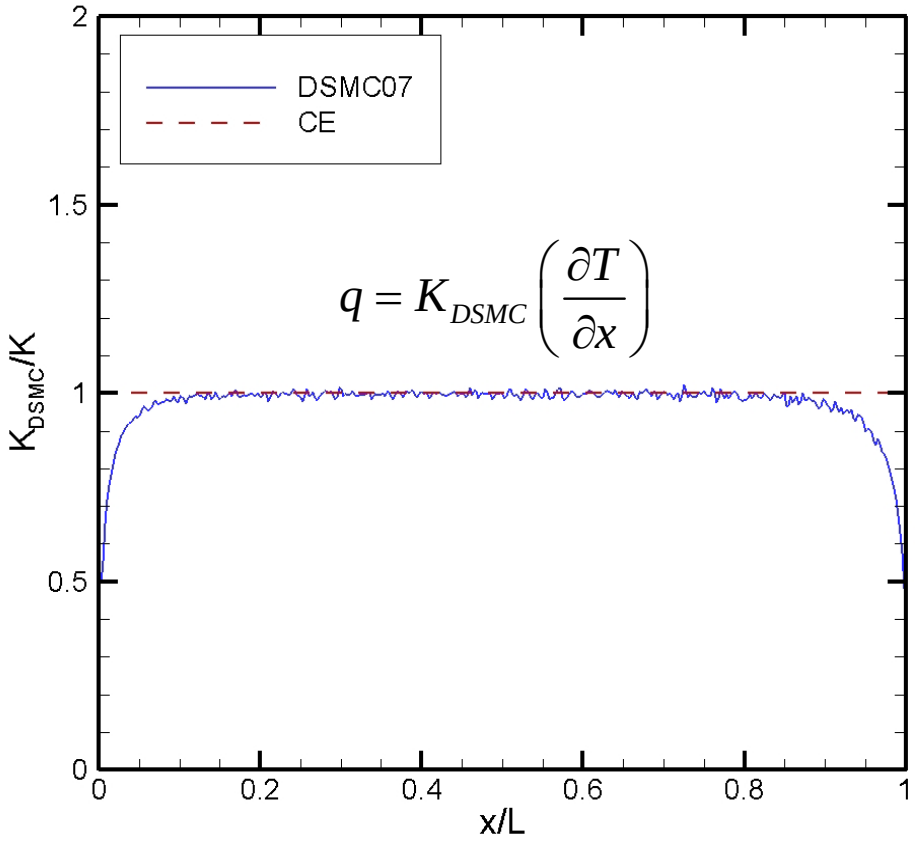
Summary

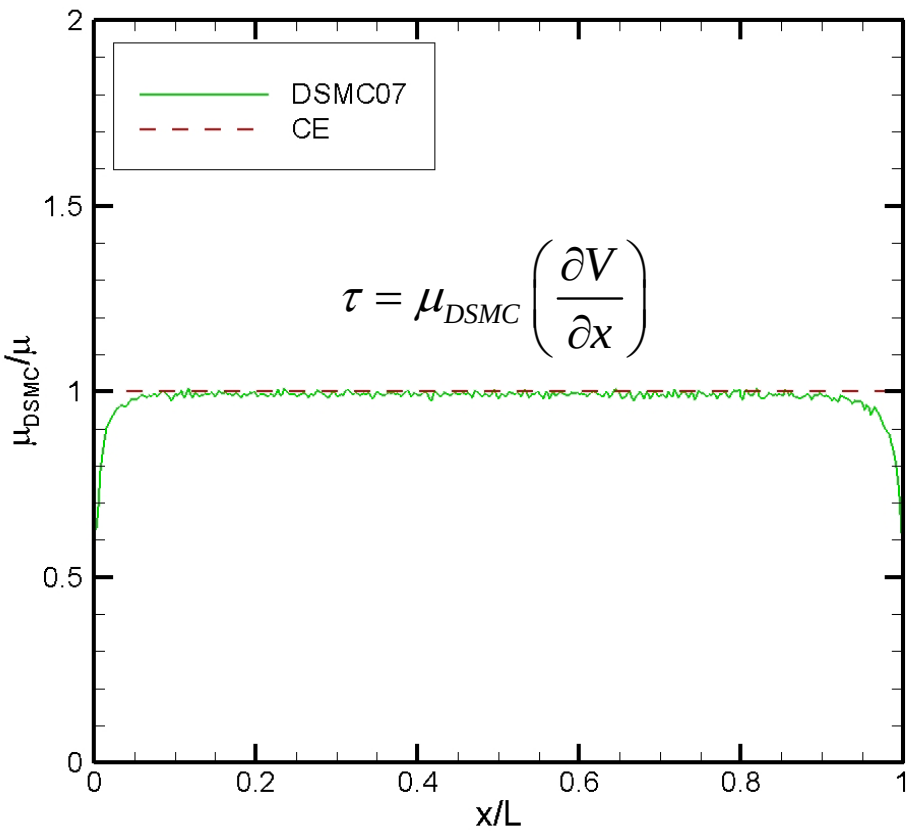
DSMC can reproduce the infinite-order solution to the Boltzmann equation.

There is a number of DSMC benchmark problems where analytical solutions exist.

Higher-order moments are progressively more difficult to capture.

DSMC07: 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

Sandia National Laboratories