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DSMC Convergence Behavior for Transient Flows

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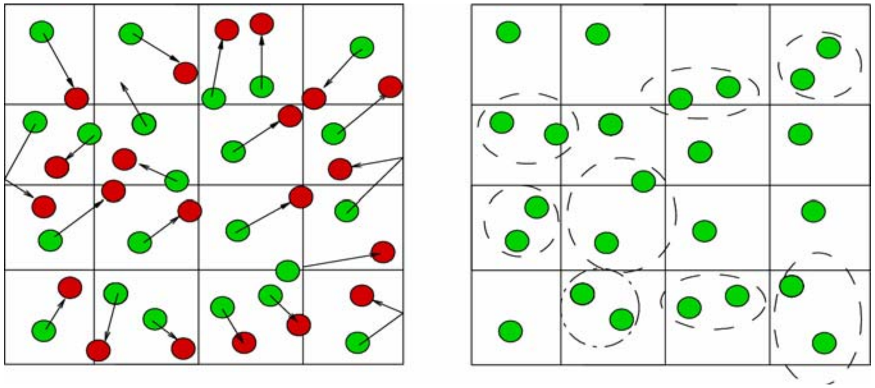
Convergence of Transient DSMC



ballistic move **stochastic collide**

Reasons to investigate convergence of transient DSMC

- DSMC is standard to judge other noncontinuum methods
- Investigators starting to do transient DSMC simulations
- Although inherently transient, only steady flows studied

Systematic study of transient convergence is needed

- Focus on generic flows
- Converge to “right answer”?
- How does it converge?

Goal: extract maximum accuracy with minimum effort

- Identify major parameters controlling DSMC accuracy
- Perform systematic convergence study

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DSMC Numerical Error

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)

Early DSMC users followed 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

Cell-Size Error

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

Green-Kubo theoretical analysis (Alexander *et al*., 1998)

- Thermal conductivity for hard-sphere gas ($\Delta t \to 0$, $N_c \to \infty$)

$$\frac{K_{DSMC}}{K} = 1 + \frac{32}{225\pi}\left(\frac{\Delta x}{\lambda}\right)^2 = 1 + 0.04527\left(\frac{\Delta x}{\lambda}\right)^2$$

- Where the hard-sphere mean free path is $\lambda = \frac{1}{\sqrt{2}\pi d_{ref}^2 n}$
- Supporting DSMC calculations provided
- *More data needed for* $\Delta x/\lambda < 1$

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Time-Step Error

Error related to time step, Δt

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

Green-Kubo theoretical analysis (Hadjiconstantinou, 2000)

- Thermal conductivity for hard-sphere gas ($\Delta x \to 0$, $N_c \to \infty$)

$$\frac{K_{DSMC}}{K} = 1 + \frac{64}{675\pi}\left(\frac{\Delta t}{t_o}\right)^2 = 1 + 0.03018\left(\frac{\Delta t}{t_o}\right)^2$$

- With the hard-sphere mean collision time $t_o = \frac{\lambda}{c_o} = \frac{\lambda}{\sqrt{2k_B T / m}}$
- Supporting DSMC calculations (Garcia & Wagner, 2000)
- *More data needed for* $\Delta t/t_o < 1$

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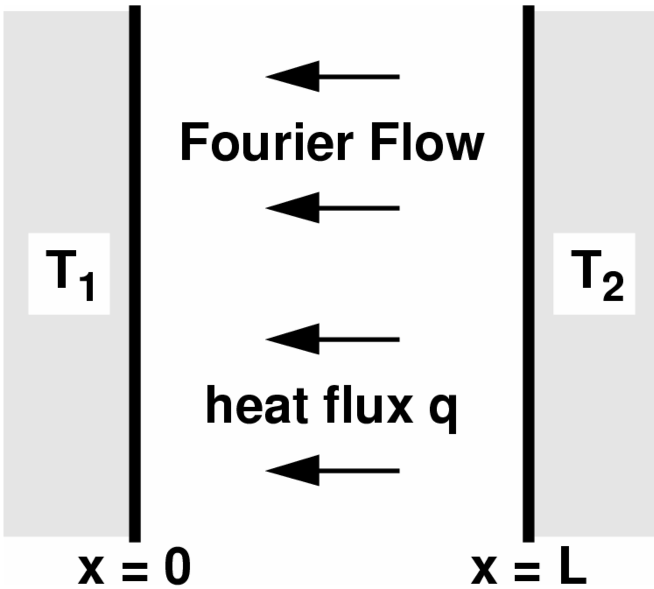
Rader et al. Convergence Analysis for Fourier Flow



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

K = thermal conductivity
T = gas temperature

One-dimensional gas-phase conduction

Temperature, heat flux calculated from DSMC molecular velocity distribution

- Knudsen layers at walls (*not* of interest here)
- If continuum, *Chapman-Enskog* in interior

Conditions:

- Molecules Hard-sphere "argon"
- Walls 223.15 and 323.15 K
- Width 0.001 m (1 mm)
- Pressure 264.9 Pa (~2 torr)
- L/λ ~42
- t_o 71 ns (273.15 K)

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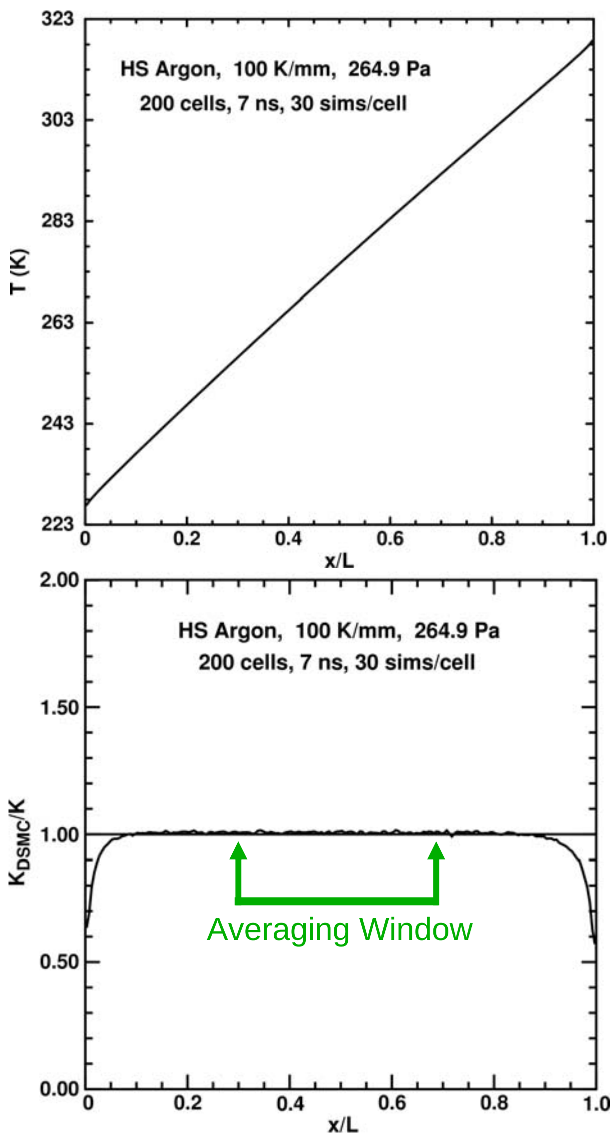
DSMC Calculations



Temperature Profile

- Nearly linear
- Small jumps near walls
- Low level of statistical scatter

Thermal Conductivity Ratio Profile

- Calculated from CE theory & DSMC values

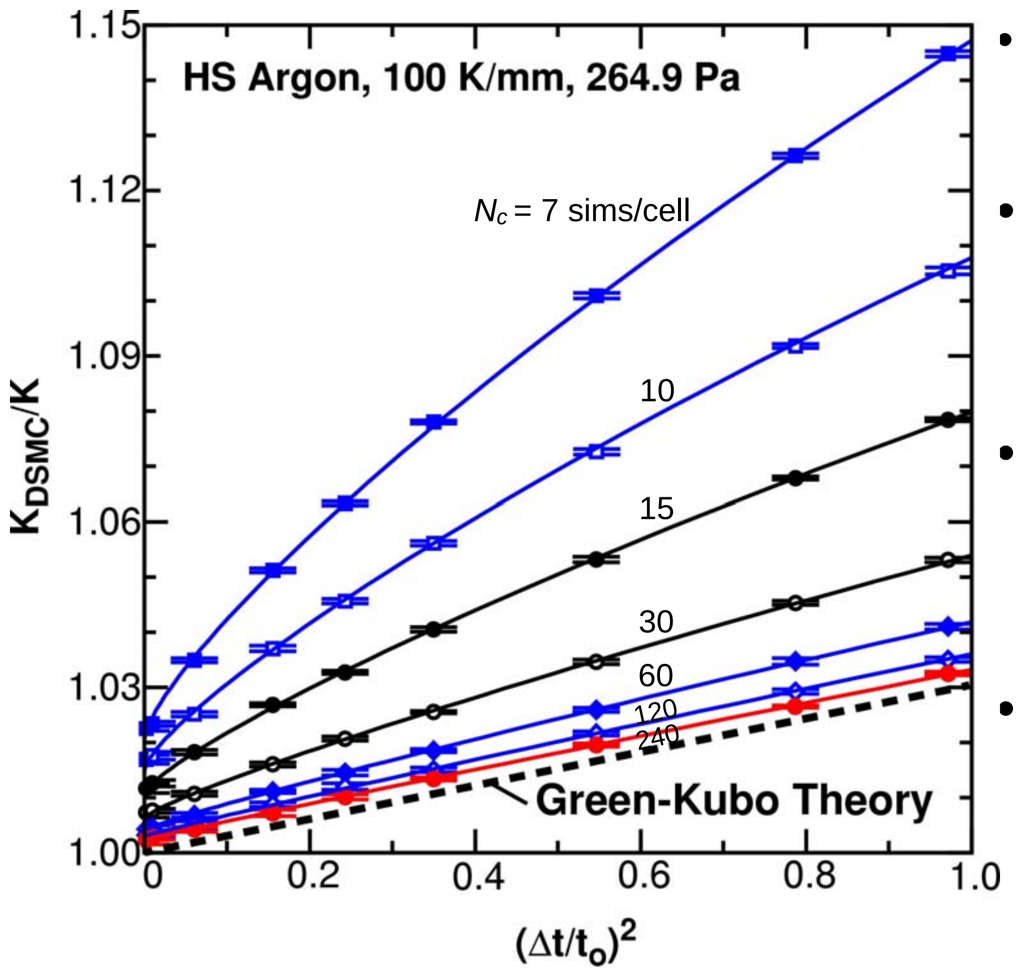
$$\frac{K_{DSMC}}{K} = \frac{T_{ref}^{1/2}}{K_{ref}} \frac{|q_{wall}|}{T^{1/2}} \left(\frac{dT}{dx} \right)^{-1}$$

- Knudsen layers apparent near walls
- Good agreement with theory in center

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

Time-Step Convergence

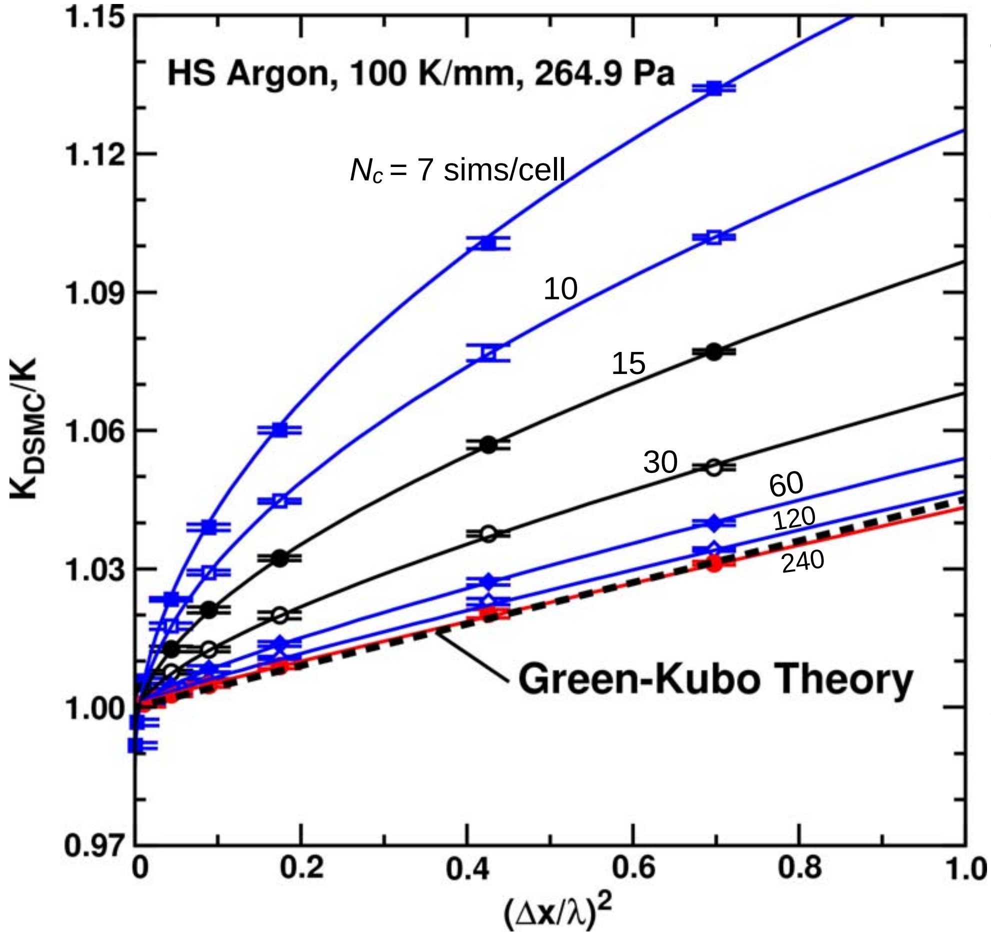
200 cells, $\Delta x/\lambda = 0.209$



- Complicated behavior of error with time step
- Quadratic dependence on time step observed only for large N_c
- Quadratic coefficient (0.029) agrees with G-K theory (0.0302) in the limit $N_c \to \infty$
- Curves through data from least squares fitting

Cell-Size Convergence

$\Delta t = 7$ ns, $\Delta t/t_o = 0.1$



- Complicated behavior of error with cell size
- Quadratic dependence on cell size observed only for large N_c
- Quadratic coefficient (0.041) agrees with G-K theory (0.0453) in the limit $N_c \rightarrow \infty$
- Curves through data from least squares fitting

Functional Form of Error

Goal: find a functional form that represents DSMC data

Taylor series expansion in Δx, Δt, and 1/Nc

Perform least-squares fitting of entire data set

Retain statistically significant terms:

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

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

Key results:

DSMC reproduces CE conductivity to within fitting uncertainty

Quadratic terms $(\Delta x)^2$ and $(\Delta t)^2$ agree with Green-Kubo theory

Other terms have not been reported previously

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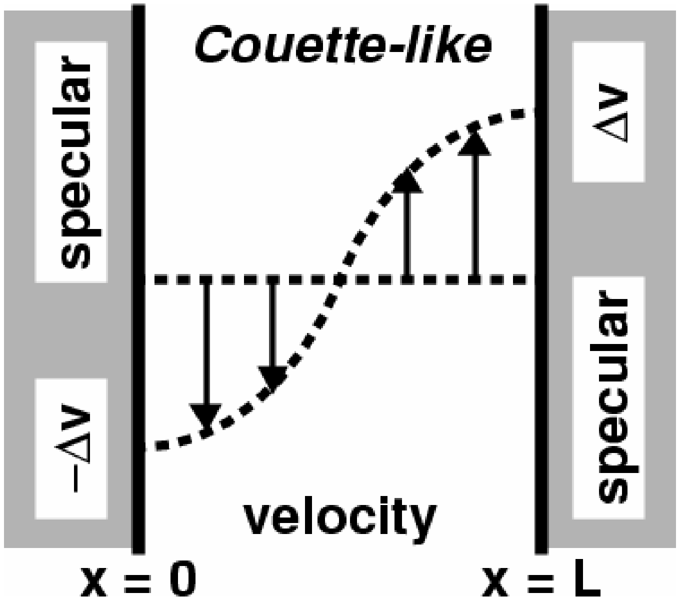
DSMC Convergence for Steady State Problems

- DSMC reproduces CE conductivity to within 0.01%
- DSMC limiting convergence behavior matches 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 available theory
- For finite values of parameters, convergence behavior is a complicated function of higher-order cross terms
- Problem: How does DSMC converge for transient problems

Couette-like Transient Flow



Decaying shear flow with slippery walls

– Initial conditions: half-cosine v velocity; zero u, w velocities; uniform pressure, temperature, density.
– Boundary conditions: specular walls (symmetry)
  - No Knudsen layers, investigate bulk flow behavior
– Long times: motionless; conserve mass, energy

Couette-like Transient Convergence Study

Parameters from steady convergence investigations

- Follow Rader, Gallis, Torczynski, and Wagner (2006)
- Domain: $0 < x < L$, $L = 1$ mm
- Gas: hard-sphere argon (Bird, App A, STP)
- Temperature: 273.15 K

Quantities varied in simulations

- Velocity: $v = -\Delta v \cdot \cos[\pi x / L]$, Δv = 50-500 m/s, c = 381 m/s
- Pressure: p = 4, 2, 1, 0.5, 0.25, 0.125 torr (focus on 2 torr)

  Kn = λ/L = 0.012, 0.024, 0.048, 0.095, 0.19, 0.38
- Cell size: $0.1 < \Delta x/\lambda < 1$ (MFP at 2 torr, λ = 0.024 mm)
- Time step: $0.1 < \Delta t/t_0 < 1$ (coll. time at 2 torr, t_0 = 70 ns)

Simulation specifics

- Algorithm: Bird (1994), move-sample-collide-sample
- Molecules: 10,000,000 (25,000-250,000 per cell)

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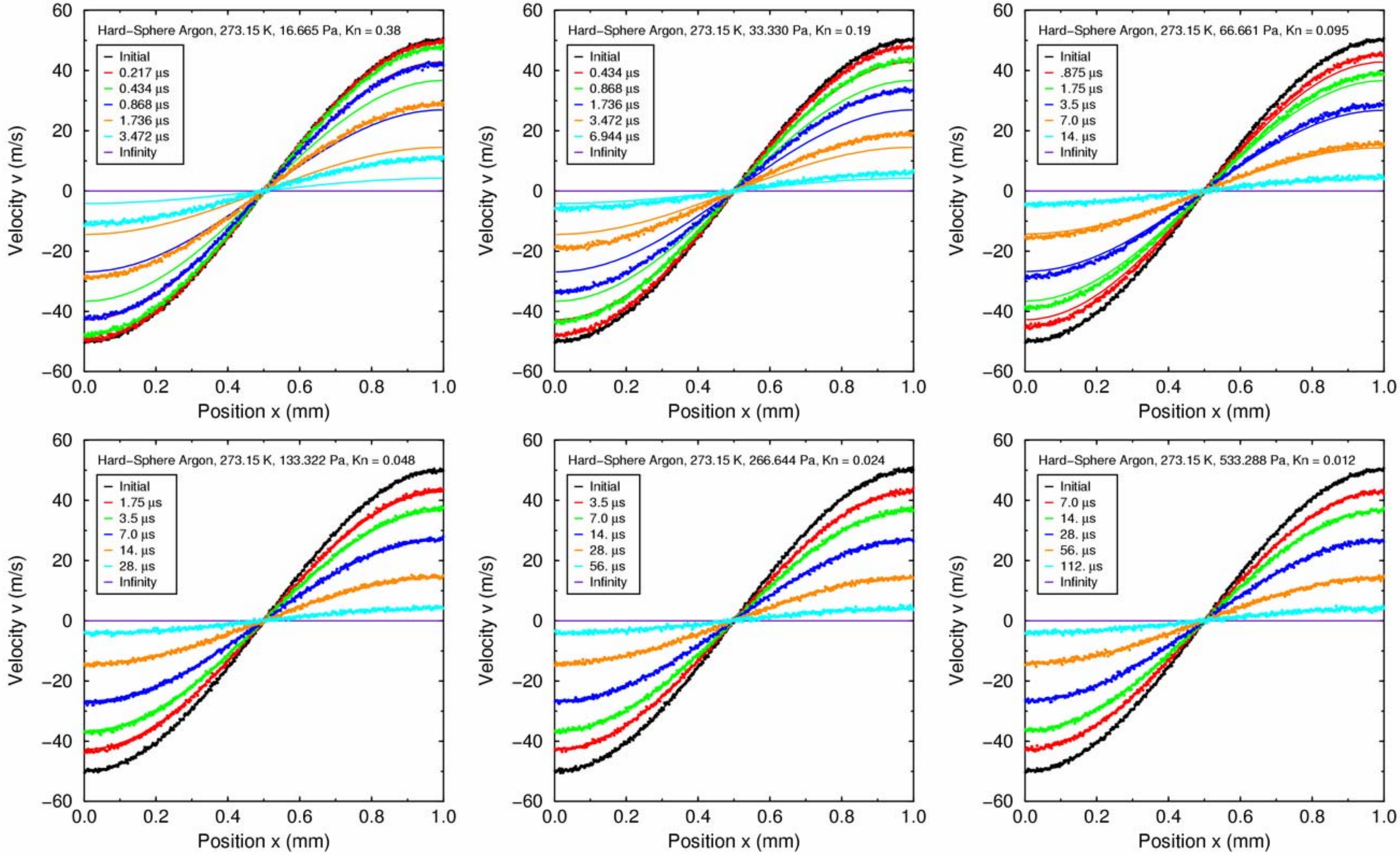
Pressure (Knudsen Number) Dependence



For Kn < 0.03, highly resolved DSMC (dots) and continuum (curves) agree closely

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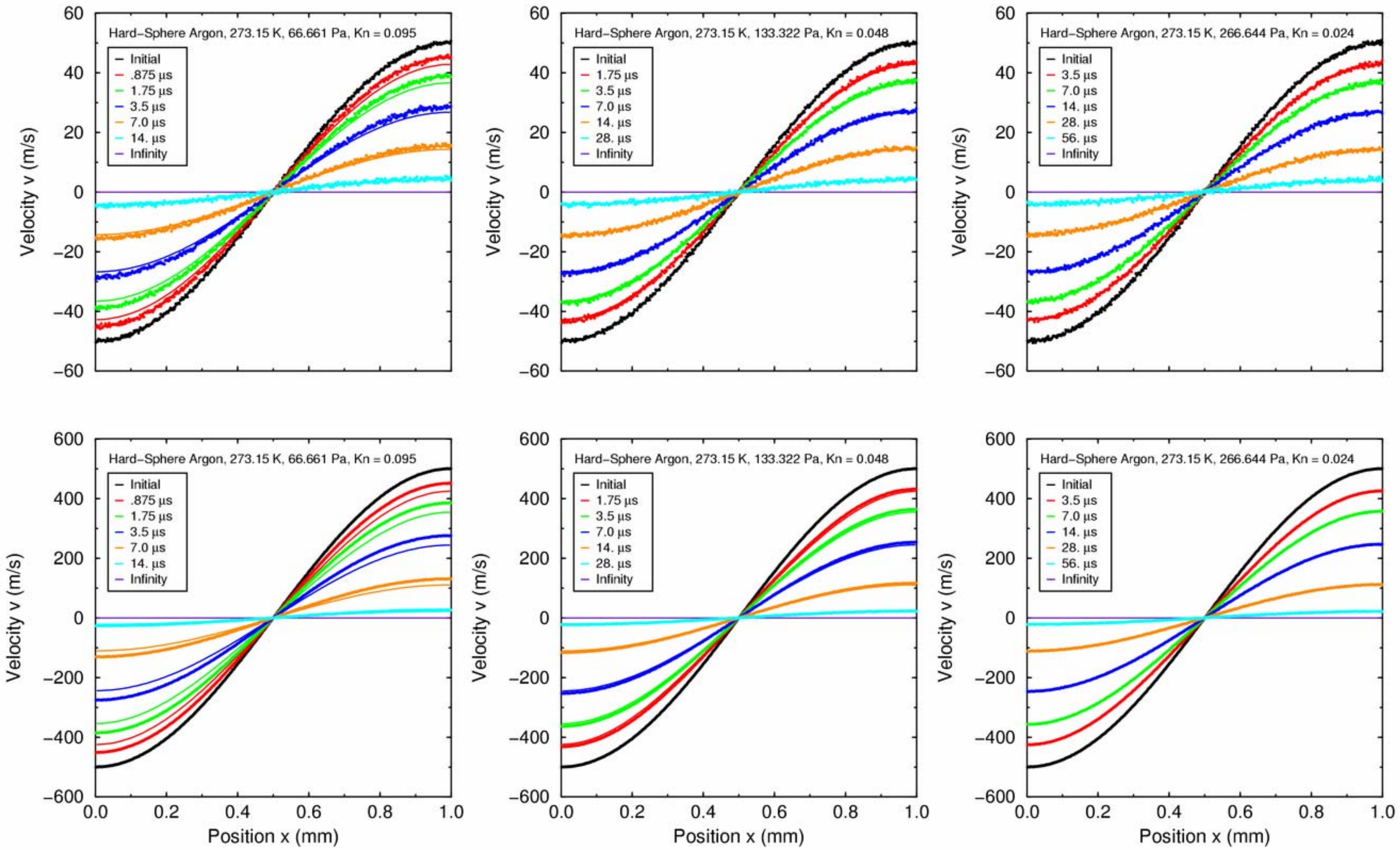
Velocity Dependence



Low-speed (top) and high-speed (bottom) DSMC behave similarly in approach to continuum

DSMC Effective Viscosity

$$v = -\Delta v \cos\left(\frac{\pi x}{L}\right) \exp\left(-\frac{\pi^2 \mu_{\text{eff}} t}{\rho L^2}\right)$$

Find DSMC effective viscosity at particular Δx and Δt

- Compare DSMC to continuum analytical solution
  - Appropriate for vanishing Knudsen numbers
  - Appropriate for constant uniform temperature
- Accurate for Δv = 50 m/s at 2 torr and 273.15 K
  - Small Knudsen numbers: system, 0.024; shear, 0.006
  - Small temperature rise: 2 K (viscosity increases 0.3%)
- Adjust continuum effective viscosity to match DSMC

Repeat for many different combinations of Δx and Δt

- Compare to predictions of Green-Kubo theory of Garcia & Wagner and Hadjiconstantinou (2000)

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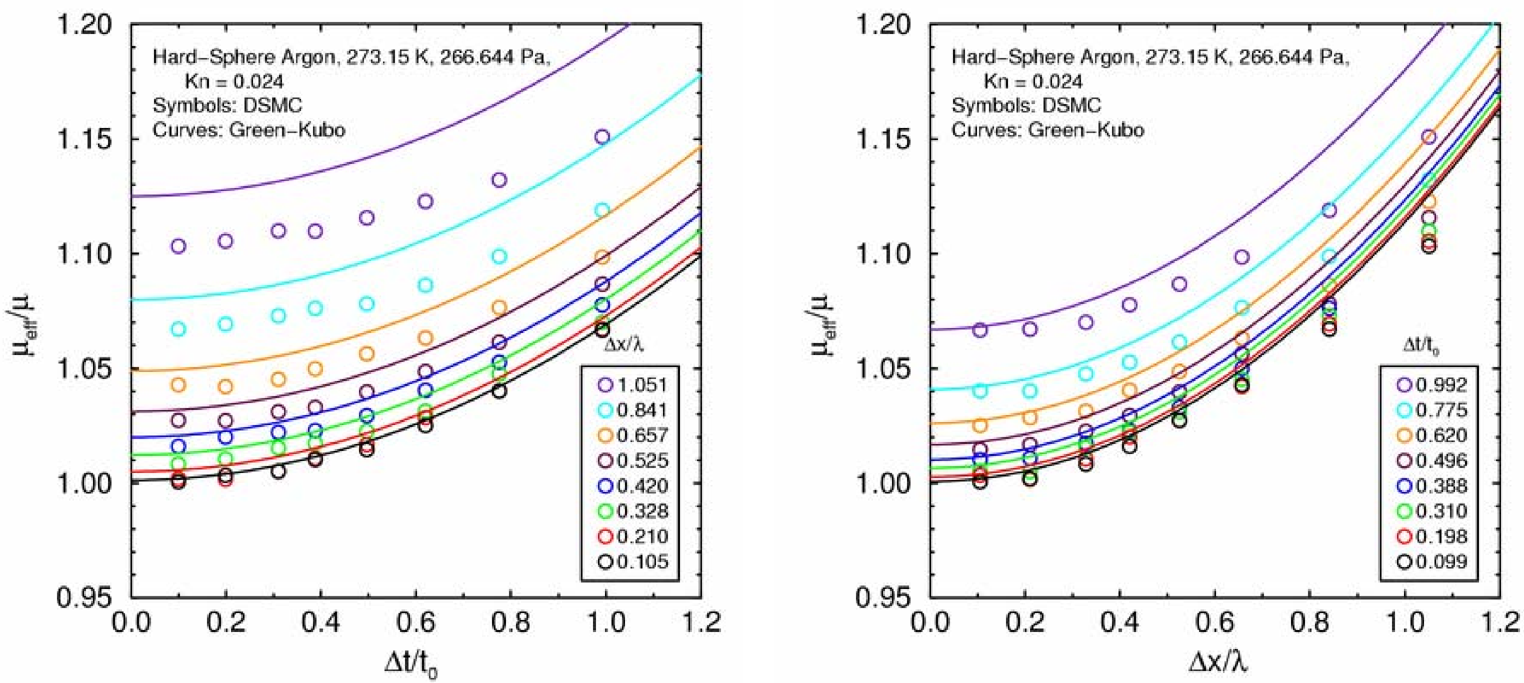
Comparison to Green-Kubo Theory

$$\frac{\mu_{\text{eff}}}{\mu} = 1 + \frac{16}{75\pi}\left(\frac{\Delta t}{t_0}\right)^2 + \frac{16}{45\pi}\left(\frac{\Delta x}{\lambda}\right)^2 = 1 + 0.0679\left(\Delta\tilde{t}\right)^2 + 0.1132\left(\Delta\tilde{x}\right)^2$$

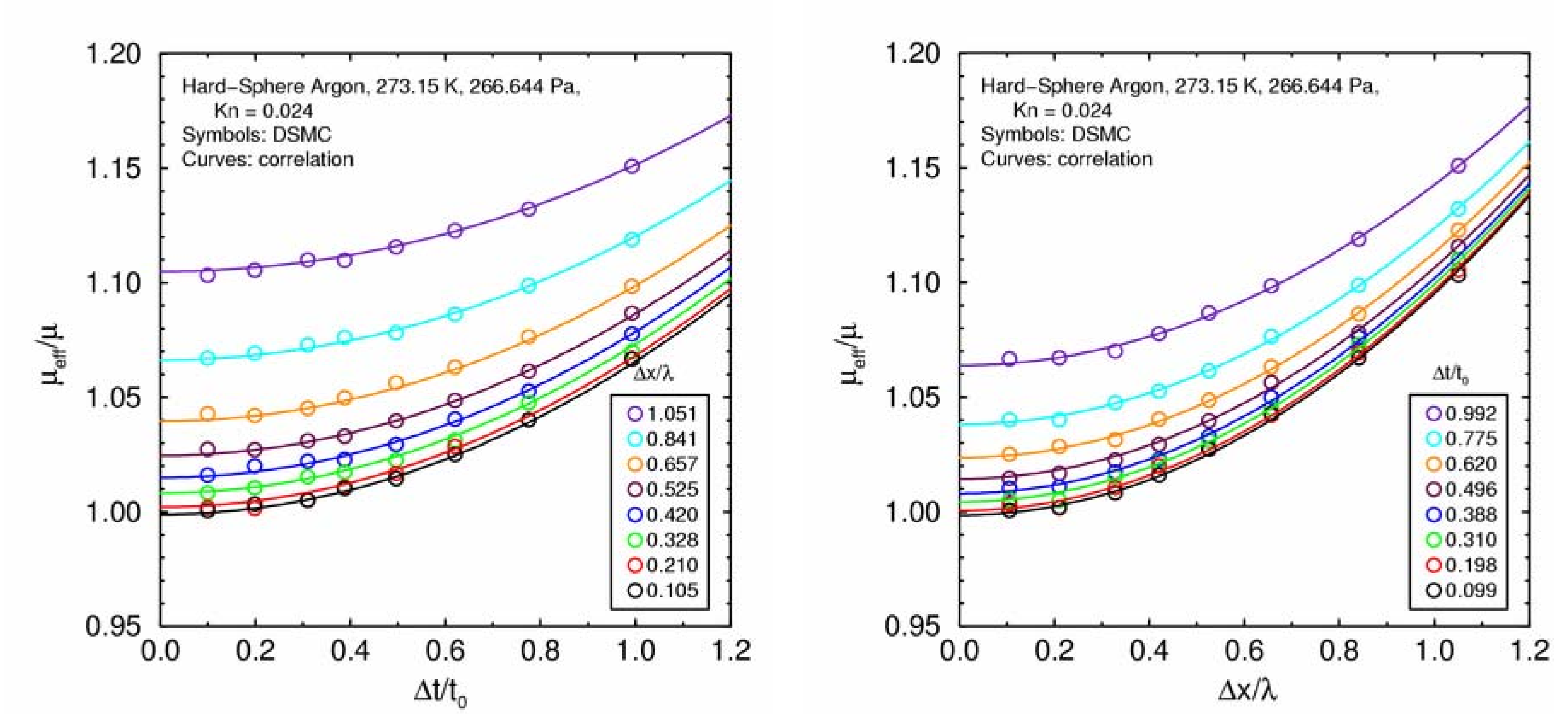


DSMC and Green-Kubo results agree reasonably

Green-Kubo error estimate is slightly conservative

Polynomial Correlation

$$\frac{\mu_{\text{eff}}}{\mu} = 0.9978 + 0.0670\left(\Delta\tilde{t}\right)^2 + 0.0969\left(\Delta\tilde{x}\right)^2 - 0.0209\left(\Delta\tilde{t}\right)^2\left(\Delta\tilde{x}\right)^2 + 0.0025\left(\Delta\tilde{t}\right)^3\left(\Delta\tilde{x}\right)^2$$



Viscosity differs by 0.3%, close to thermal variation

Pure terms agree reasonably with Green-Kubo

Cross terms are required to correlate values

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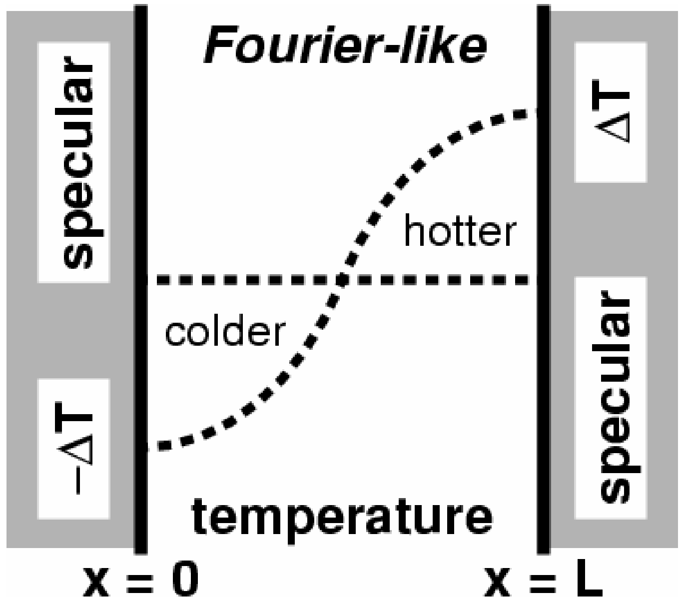
Fourier-like Transient Flow



Decaying heat flow with non-conductive walls

– Initial conditions: half-cosine T temperature; uniform pressure, density varies accordingly, quiescent gas
  Boundary conditions: specular walls (symmetry)
  - No Knudsen layers, investigate bulk flow behavior
– Long times: motionless; conserve mass, energy

Fourier-like Transient Convergence Study

Parameters from steady convergence investigations

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- Domain: $0 < x < L$, $L = 1$ mm
- Gas: hard-sphere argon (Bird, App A, STP)

Quantities varied in simulations

- Temperature: $T[x,0] = T_0 - \Delta T \cos[\pi x / L], \quad \Delta T = 50\text{K}$
- Pressure: p = 4, 2, 1, 0.5, 0.25, 0.125 torr (focus on 2 torr)

  Kn = λ/L = 0.012, 0.024, 0.048, 0.095, 0.19, 0.38
- Cell size: $0.1 < \Delta x/\lambda < 1$ (MFP at 2 torr, $\lambda = 0.024$ mm)
- Time step: $0.1 < \Delta t/t_0 < 1$ (coll. time at 2 torr, $t_0 = 70$ ns)

Simulation specifics

- Algorithm: Bird (1994), move-sample-collide-sample
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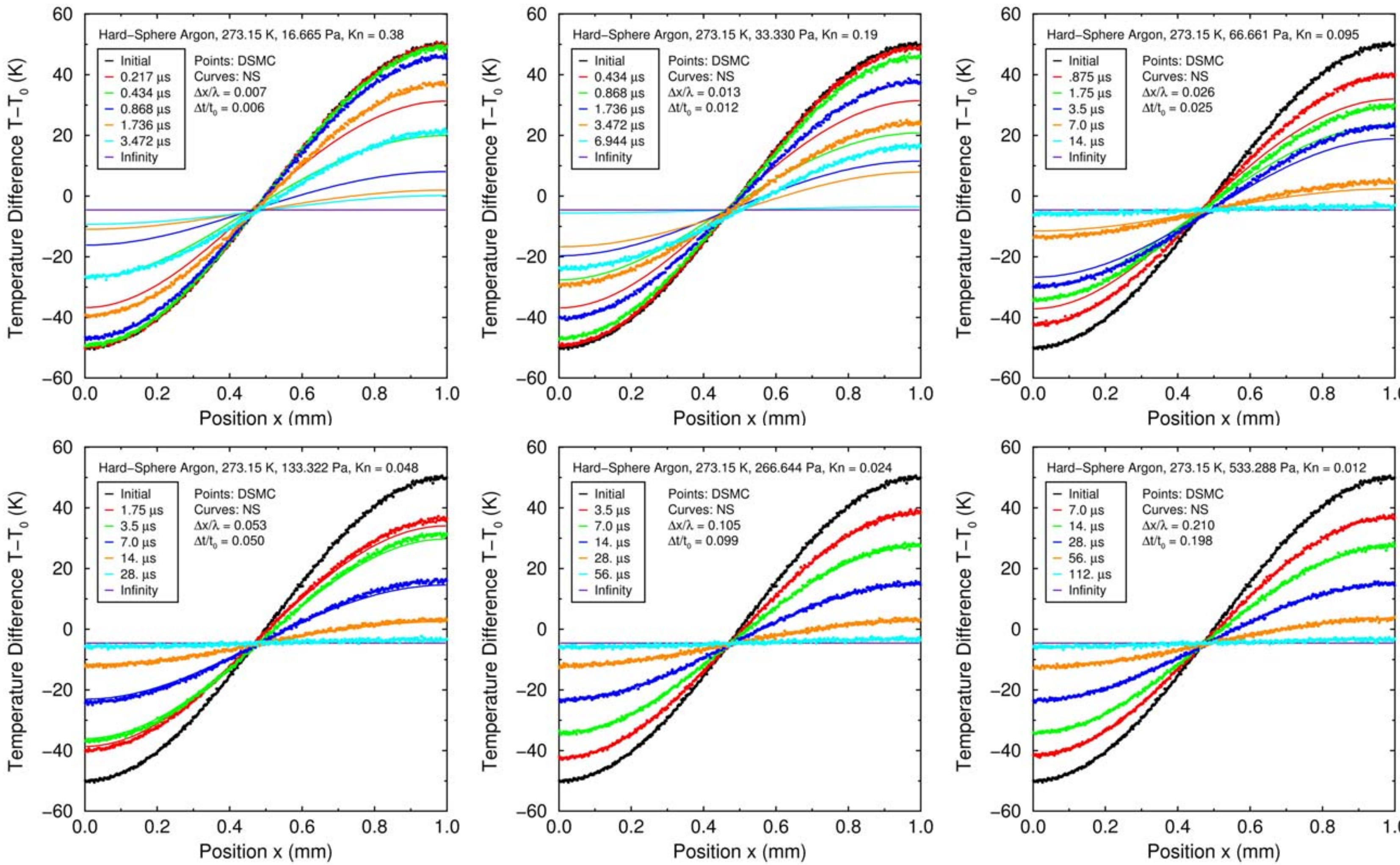
Pressure (Knudsen Number) Dependence



For Kn < 0.03, highly resolved DSMC (dots) and continuum (curves) agree closely

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Conclusions

Convergence of transient DSMC investigated for two flows without Knudsen layers

- Couette-like flow
  - DSMC in good agreement for Kn < 0.3
  - DSMC yields correct viscosity to within 0.3%
  - DSMC errors similar to Green-Kubo theory

- Fourier-like flow
  - DSMC in good agreement for Kn < 0.3
  - Convergence behavior more complicated to analyze