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Non-equilibrium Gas Modeling with DSMC

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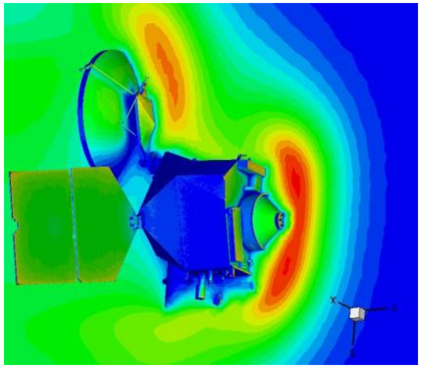
Non-equilibrium Gas Modeling Application Areas

Traditional

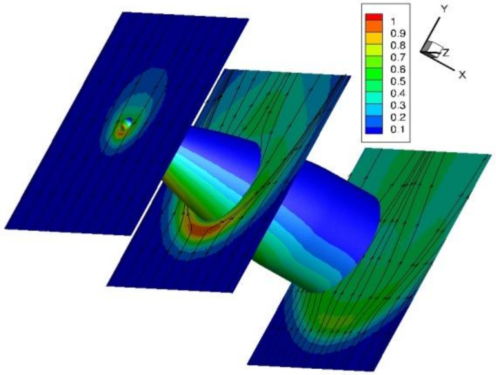
- Hypersonics and spacecraft
- Semiconductor equipment

Novel

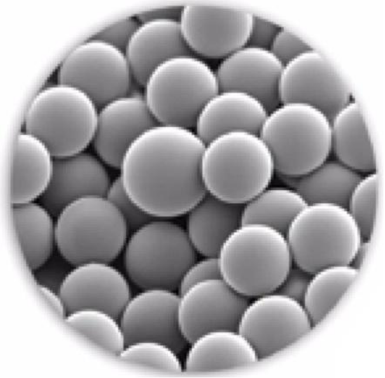
- MEMS damping, heat transfer
- Nanoparticle transport in gas



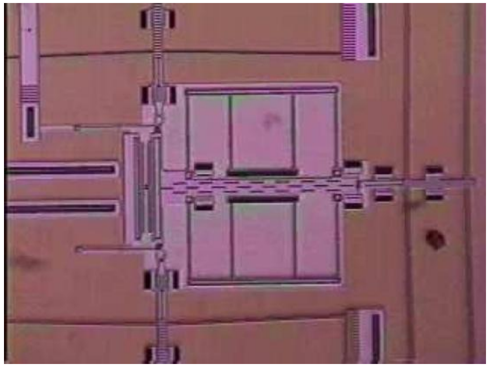
Satellites



Reentry Vehicles



PSL Nanoparticles



MEMS Devices

EUVL Equipment

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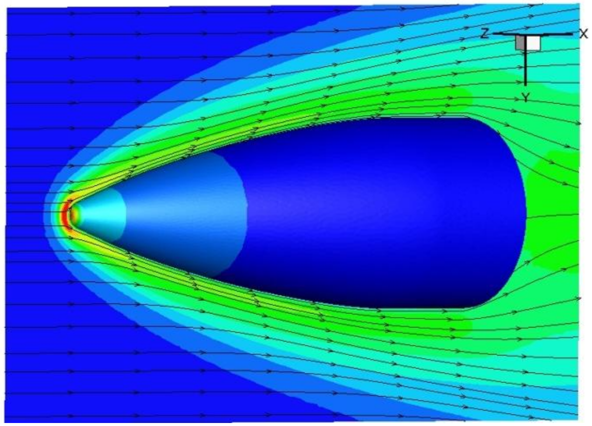
Modeling and Simulation

High-consequence applications require high-fidelity analysis

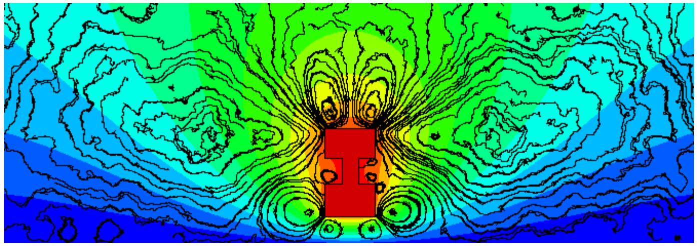
Two main simulation methods

- Navier-Stokes plus slip-jump: *NSSJ*
- Direct Simulation Monte Carlo: *DSMC*



Important issues

- How far can NSSJ approach be used
  - How do constitutive relations break down
  - Effect of thermo-chemical non-equilibrium
- Best accuracy/speed tradeoff for DSMC
- Transfer DSMC learning to NSSJ models
- Physical & chemical processes modeling



Better methods are needed

- Evolutionary improvements
- Revolutionary advances

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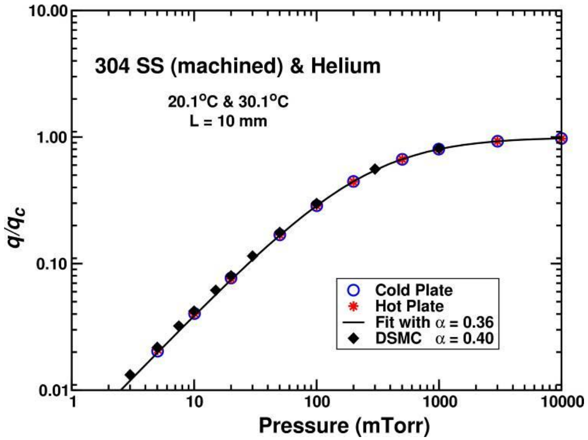
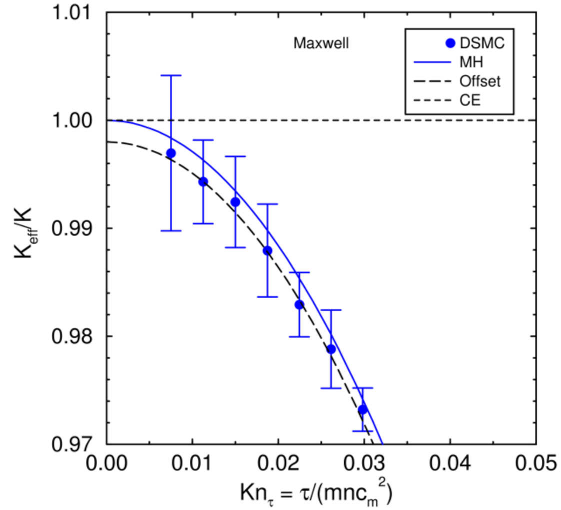
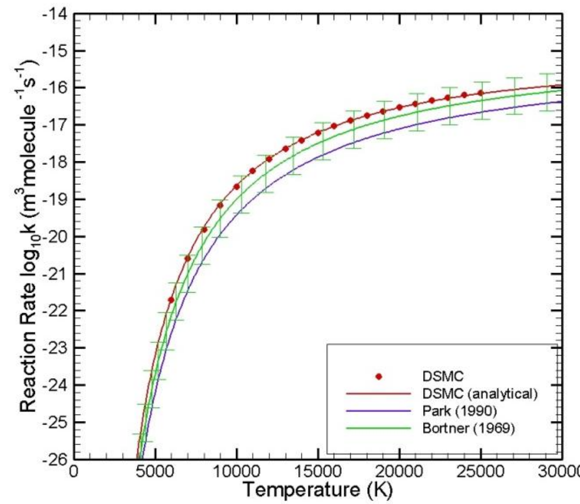
Thermophysical Properties

Acquiring critical modeling data and understanding physical behavior







Accommodation values

- "Known" surface properties need to be revisited
- New surfaces may offer significant advantages

Physical/chemical molecular data

- Energy-dependent cross sections, rate data
- Earth-atmosphere chemical reaction data
- Ionization and radiation cross sections

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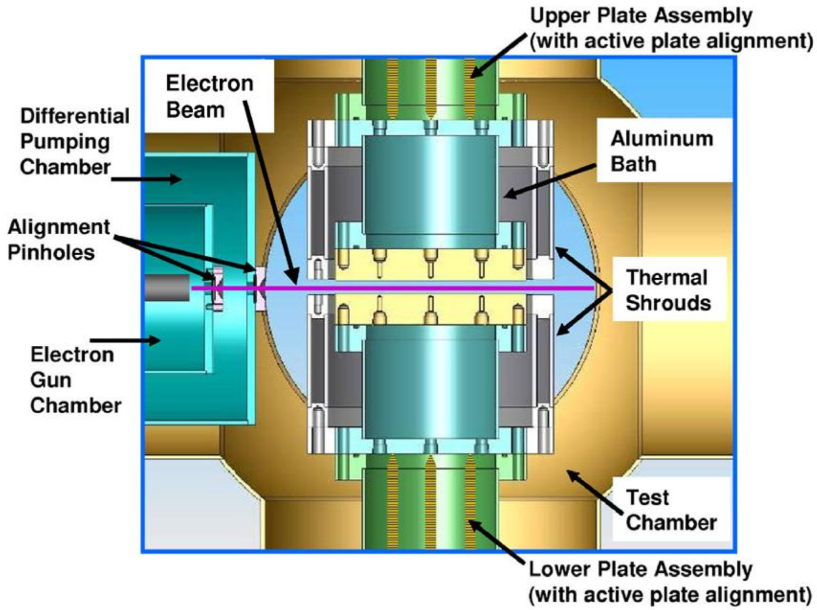
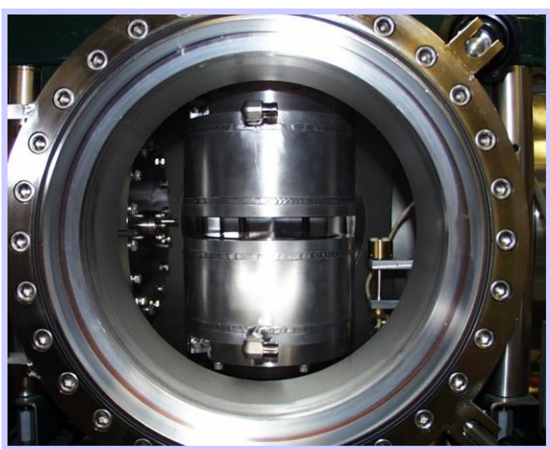
Measuring Accommodation Coefficients of Commonly used Materials





Effects examined

- RMS Roughness
- *Gas Composition*
- *Contamination*

304 Stainless Steel (machine finish)

- RMS Roughness ~ 2 µm
- Helium: $\alpha = 0.46 \pm 0.02$
- Nitrogen: $\alpha = 0.87 \pm 0.02$
- Argon: $\alpha = 0.95 \pm 0.02$

304 Stainless Steel (polished)

- Mirror finish
- RMS roughness ~ 20 nm
- Helium: $\alpha = 0.42 \pm 0.02$
- Nitrogen: $\alpha = 0.87 \pm 0.02$
- Argon: $\alpha = 0.96 \pm 0.02$

Gas	Untreated	Plasma-Treated
Argon	0.93 ± 0.02	0.85 ± 0.02
Nitrogen	0.83 ± 0.02	0.77 ± 0.02
Helium	0.41 ± 0.02	0.31 ± 0.02

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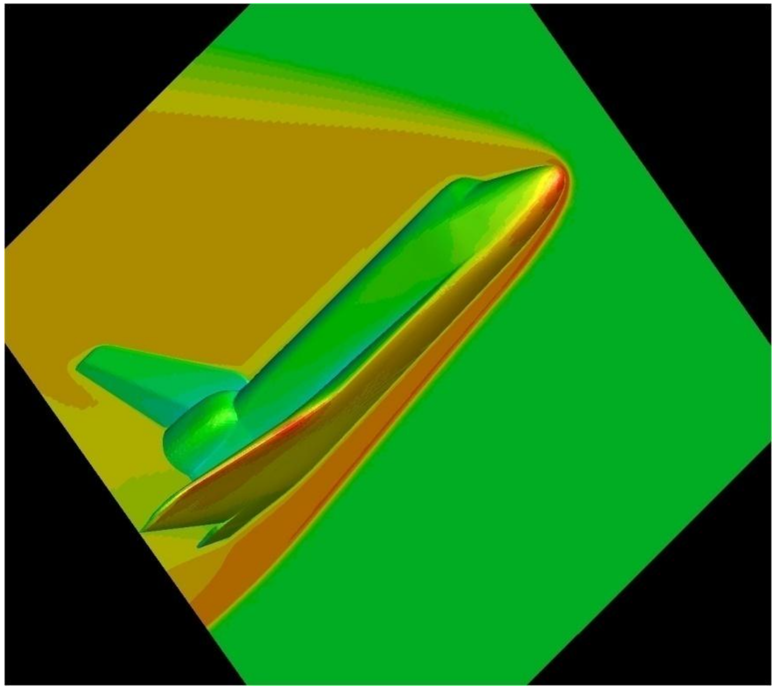
Simulation of Chemically Reacting Flow Fields

- DSMC model development has been hampered by the lack of appropriate data.
- Bird's Q-K models can predict non-equilibrium processes in a physically realistic and computationally efficient manner using only thermophysical properties of molecules.



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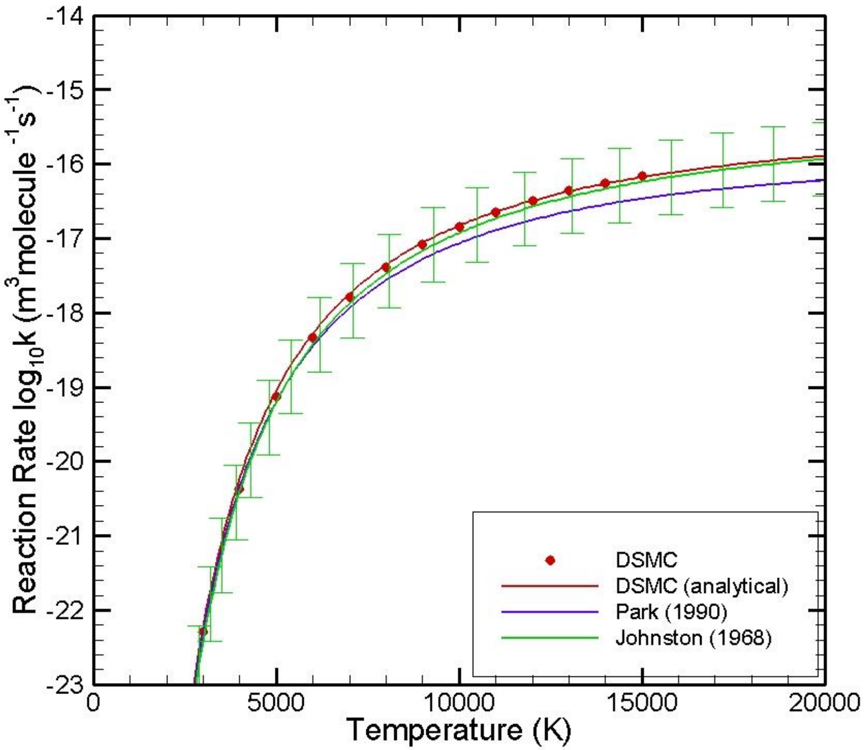
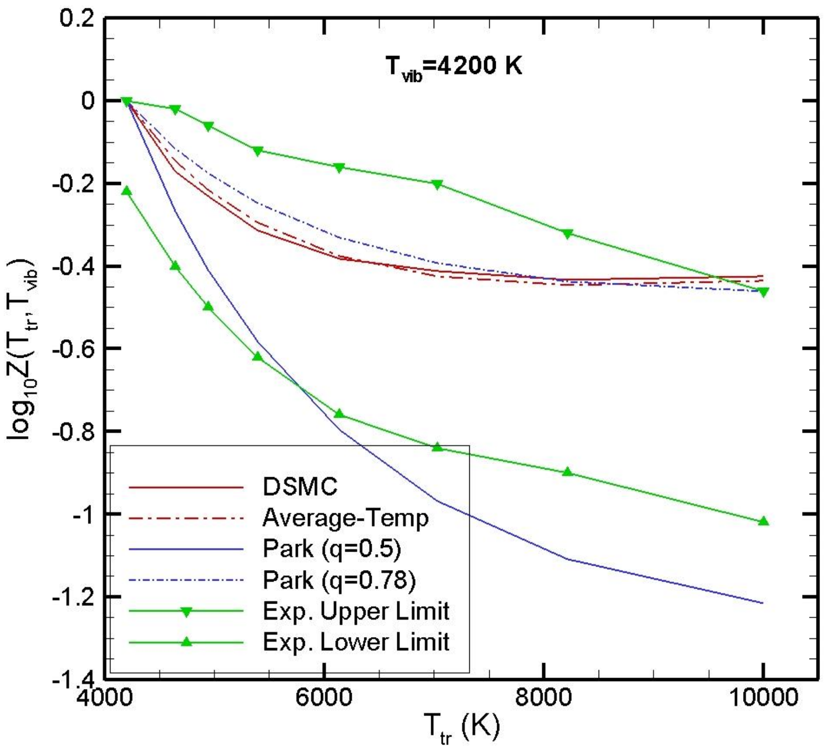
Dissociation Reactions

$$O_2 + O_2 \rightarrow O + O + O_2$$





DSMC models can predict equilibrium and non-equilibrium chemical reaction rates

- **Oxygen dissociation: equilibrium (left) and non-equilibrium (right)**

$$k(T_{tr}, T_{vib}) = \frac{2\sigma_{ref}}{\varepsilon\sqrt{\pi}}\left(\frac{T_{tr}}{T_{ref}}\right)^{1-\omega}\left(\frac{2k_B T_{ref}}{m_r}\right)^{1/2}\left\{\sum_{i=0}^{i_d} Q\left[\frac{5}{2}-\omega, \frac{\Theta_d-(i-1)\Theta_v}{T_{tr}}\right]\frac{\exp[-i\Theta_v/T_{vib}]}{z_{vib}(T_{vib})} + B\sum_{i=i_{d+1}}^{\infty}\frac{\exp[-i\Theta_v/T_{vib}]}{z_{vib}(T_{vib})}\right\}$$

Gallis M. A., Bond R. B., and Torczynski J. R., "A Kinetic-Theory Approach for Computing Chemical-Reaction Rates in Upper-Atmosphere Hypersonic Flows", *Journal of Chemical Physics,* 131, 124311, 2009.

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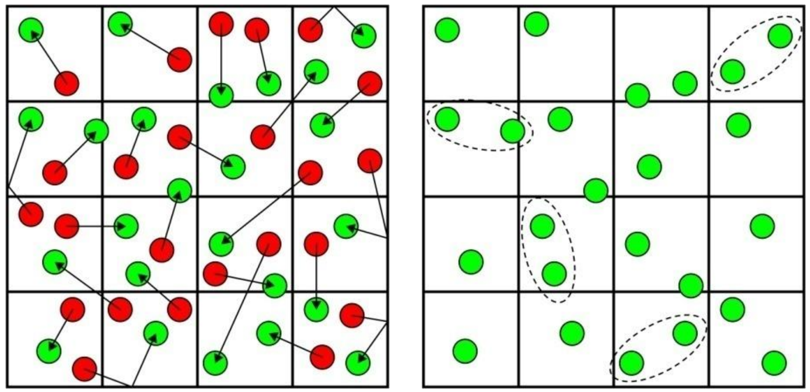
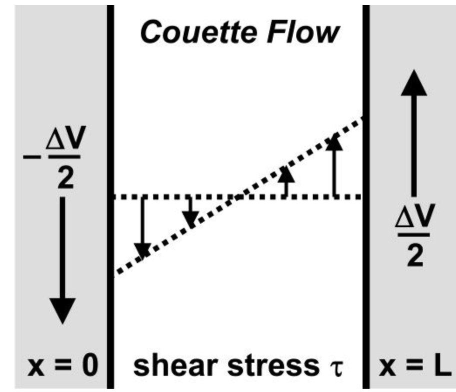
DSMC-Based Shear-Stress/Velocity-Slip Boundary Condition for Navier-Stokes

Use DSMC as a tool to obtain BC for NS





Develop shear-stress model for isothermal Couette flow

- Linear in gas-wall velocity difference
  - Low speeds relative to molecules, very small gaps
- Based on DSMC simulations
  - Wide ranges of pressures and accommodation coefficients
- Accurate in all flow regimes
  - Free-molecular, transitional, near-continuum, continuum
- Suitable for Navier-Stokes (NS) and dynamics simulations
  - Slip-jump (SJ) boundary conditions for NS equations

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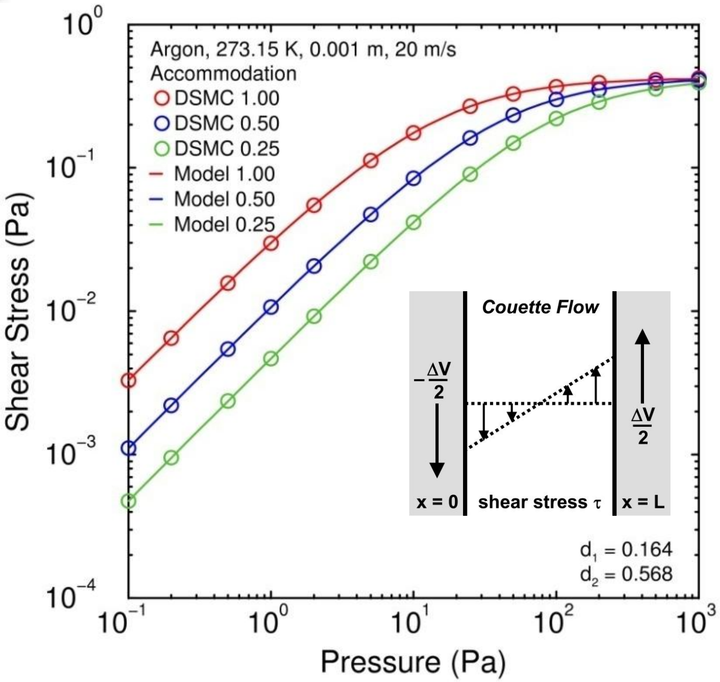
DSMC-Based Model



$$\tau_{\text{wall}} = \mu \frac{\partial v}{\partial n} = k\left(v - V_{\text{wall}}\right) \qquad k = \frac{\sigma \rho c_0}{S_1 S_2}$$

$$S_1 = 2 - \sigma \qquad S_2 = 1 + \frac{d_1 \sigma}{1 + d_2 \mathrm{Kn}} \qquad \mathrm{Kn} = \frac{\lambda}{L}$$

$$\lambda = \frac{\mu}{\rho c_0} \qquad c_0 = \frac{\bar{c}}{2} = \sqrt{\frac{2 k_B T}{\pi m}} \qquad \rho = \frac{mp}{k_B T}$$

DSMC-based shear-stress boundary condition developed

- Reproduces near-continuum and free-molecular limits
- Parameters depend only weakly on gas properties
- Agrees well with hard-sphere analytical approximations
- Suitable for Navier-Stokes and dynamics simulations

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Noncontinuum Modeling of Heat Conduction

Navier-Stokes Slip-Jump (NSSJ)

- **Continuum equations plus velocity slip and temperature jump**
- **Computationally less expensive, approximate for noncontinuum**

$$\text{Bulk gas:}\quad \mathbf{q} = -K\nabla T,\quad \rho C_p\left(\partial T/\partial t\right) = \nabla\cdot\left(K\nabla T\right) + S$$

$$\text{Jump BC:}\quad q = h\Delta T,\qquad h = \left(1+\frac{\varsigma}{4}\right)\left(\frac{\sigma}{2-\sigma}\right)\left(\frac{p\bar{c}}{T}\right)$$

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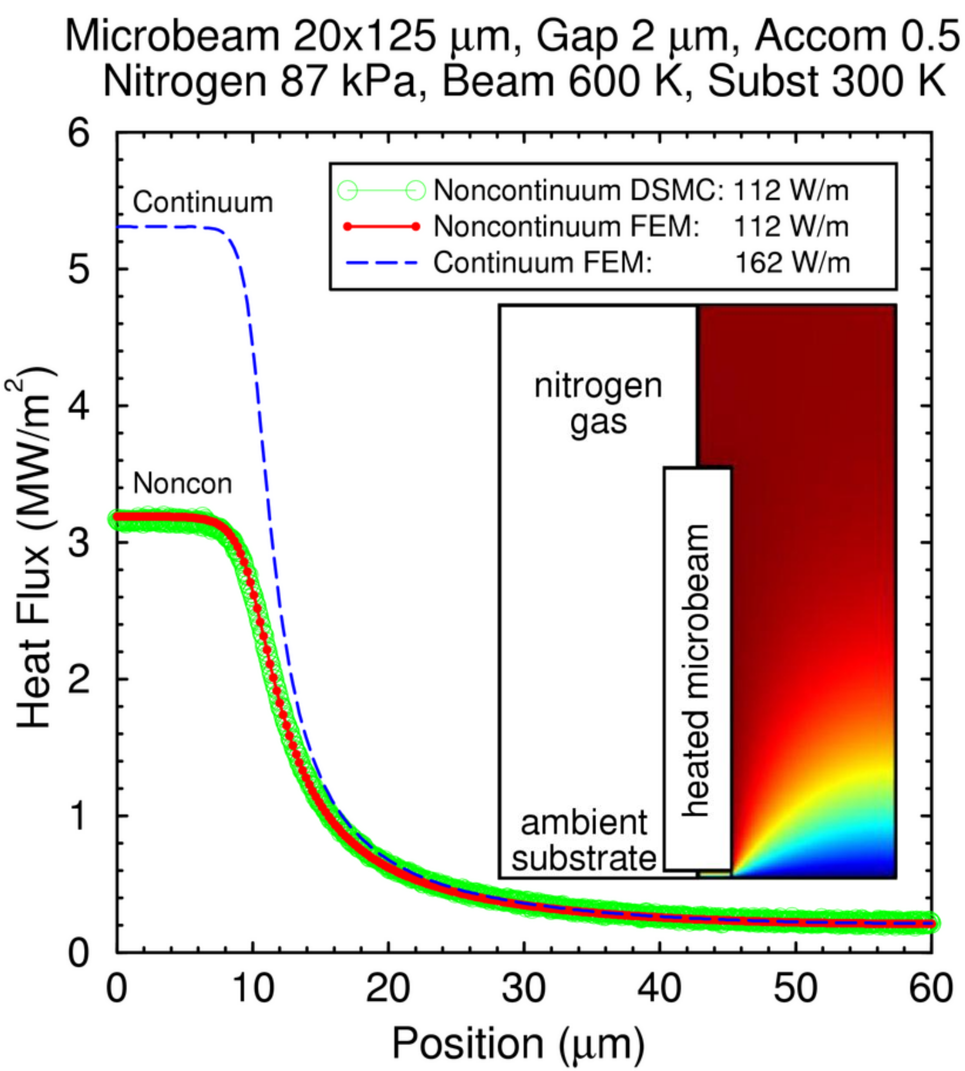
Microbeam Heat Flux to Substrate



NS alone overpredicts DSMC

- **Ignores large temperature jumps**

NSSJ accurately reproduces DSMC

- **Position-dependent heat flux**

NSSJ heat-transfer coefficient h

- **Obtained from DSMC simulations**
- **Applied at gas-solid boundaries**

$$\text{Jump BC:} \quad q = h\Delta T$$

$$h = \left(1 + \frac{\varsigma}{4}\right)\left(\frac{\sigma}{2-\sigma}\right)\left(\frac{p\bar{c}}{T}\right)$$

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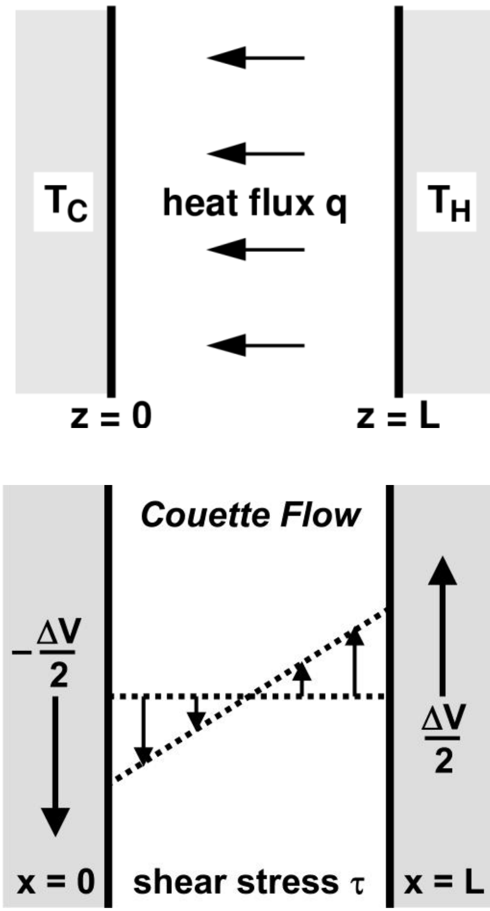
Accuracy of DSMC

Extract maximum accuracy with minimum effort

- **Identify major parameters controlling DSMC accuracy**
- **Perform systematic convergence study**
- **Develop tools to evaluate proposed modifications**
- **Improve DSMC accuracy**

Non-Equilibrium Gas Simulations

Detailed DSMC simulations of well-characterized problems demonstrate its ability to provide an infinite-approximation solution to the Boltzmann equation



Fourier Flow/Couette Flow

Monatomic gas confined between cold & hot walls moving with respect to each other

If near-equilibrium & continuum, Chapman-Enskog molecular velocity distribution in center (away from walls)

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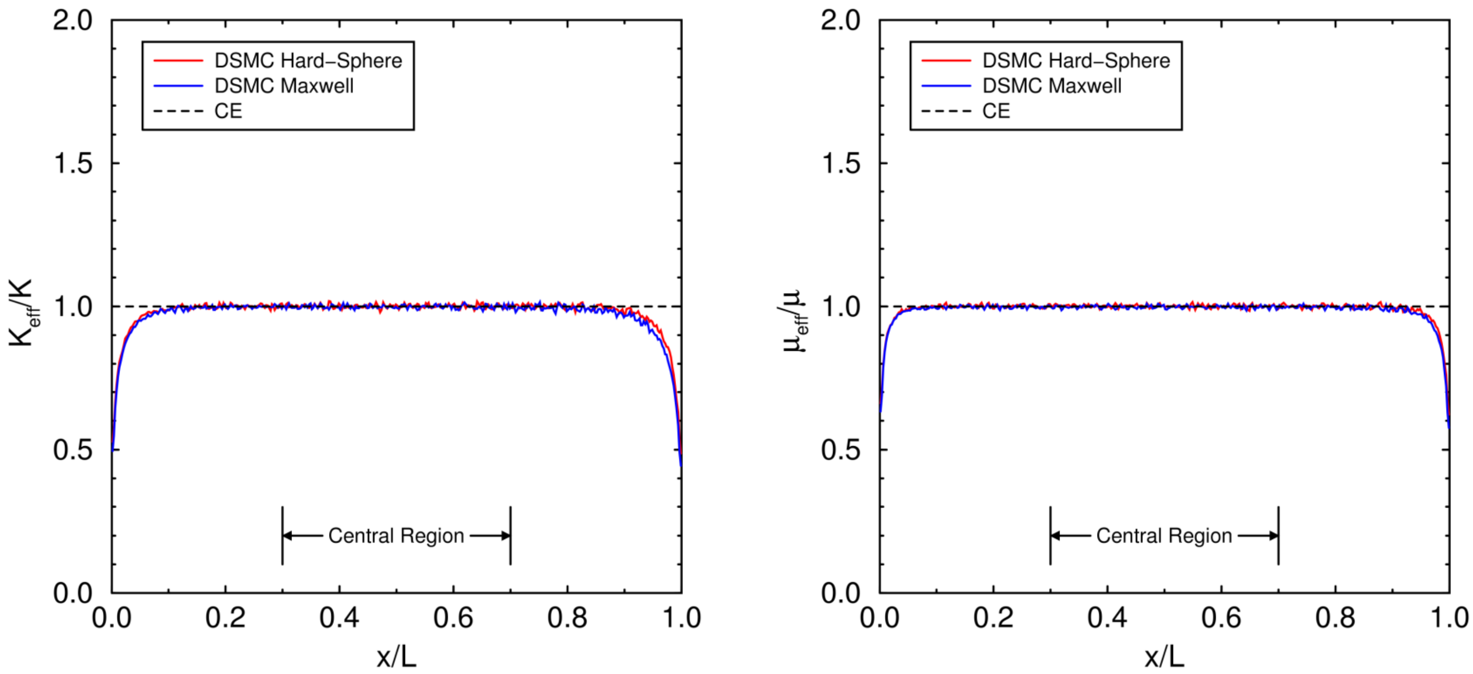
DSMC Reproduces Infinite-Approximation Chapman-Enskog Transport Coefficients



Thermal conductivity (left) and viscosity (right) away from walls

- **Maxwell and Hard-Sphere results bound most gases**
- **Agreement with Chapman-Enskog theory verifies DSMC**

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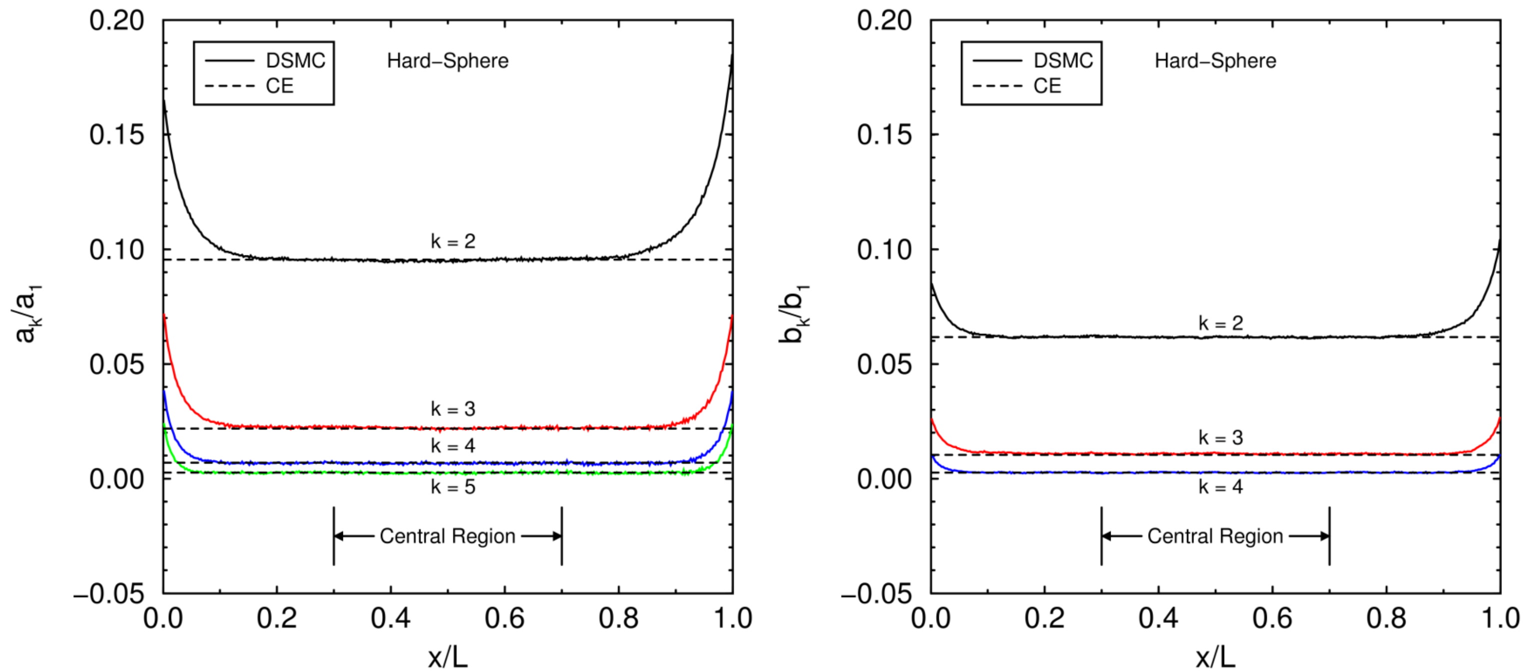
DSMC Reproduces Infinite-Approximation Chapman-Enskog Velocity Distribution



Sonine polynomial coefficients for temperature (left) & velocity (right) gradients

- **Hard-sphere values are shown, other interactions have similar agreement**
- **Higher-order (k > 5) coefficients (not shown) also have similar agreement**

Gallis, Torczynski, and Rader, "Molecular Gas Dynamics Observations of Chapman-Enskog Behavior and Departures Therefrom in Nonequilibrium Gases", *Physical Review E*, 69, 042201, 2004.

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DSMC Numerical Error

Four parameters control DSMC numerical error:

- Sample size per cell (M_c) → statistical error
  - *Statistical errors can be kept small by robust sampling*
- Simulators per cell (N_c)
- Cell size (Δx)
- Time step (Δt)

→ discretization error (simulators per cell, cell size, time step)

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

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Functional Form of Error

Find a functional form that represents DSMC data

- Taylor series expansion in Δx, Δt, and $1/N_c$
- 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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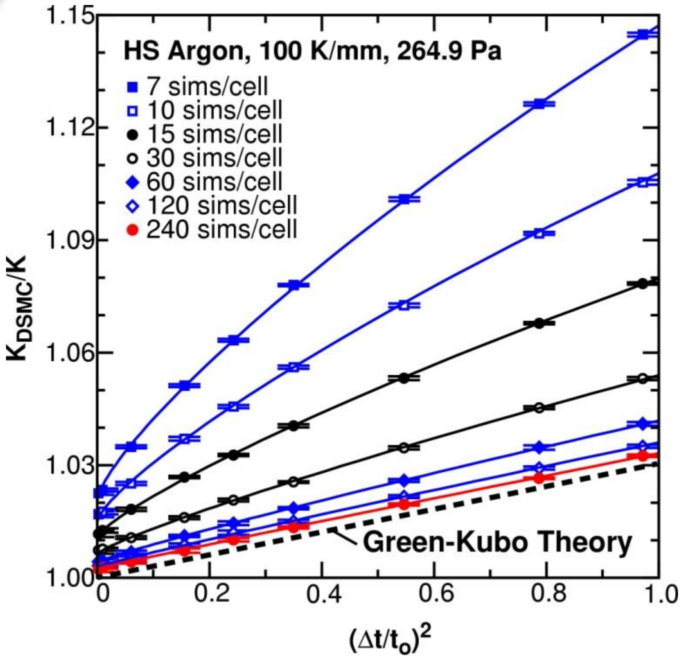
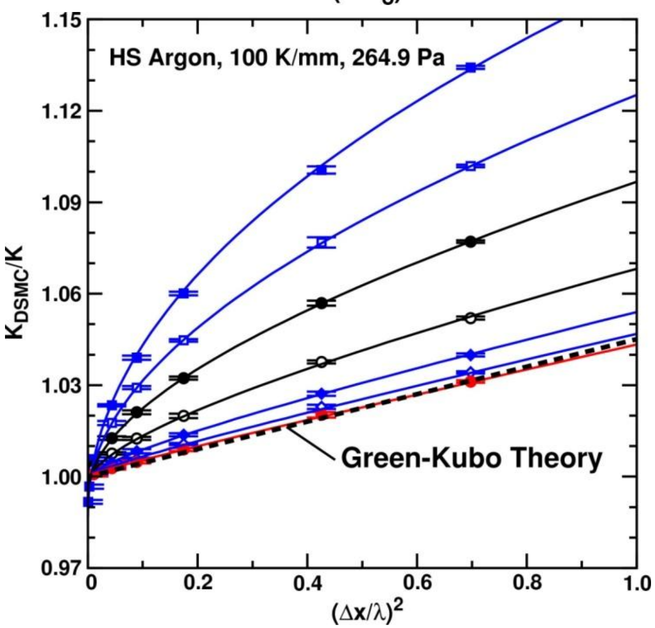
DSMC Convergence





DSMC limiting convergence behavior matches theory

- **Quadratic convergence in time step ($\Delta x/\lambda \rightarrow 0$, $N_c \rightarrow \infty$)**
- **Quadratic convergence in cell size ($\Delta t/t_o \rightarrow 0$, $N_c \rightarrow \infty$)**
- **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

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Sophisticated DSMC (DSMC07)

Basic features of DSMC algorithm retained

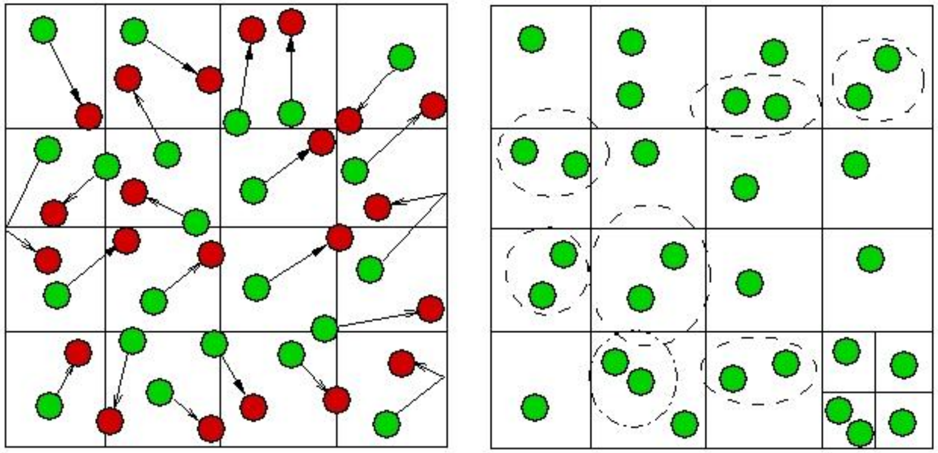
- Move-collide separation, molecular models, collision frequency calculation

Changes in collide

- Virtual sub-cells (VSC): nearest-neighbor collisions, N^2 search operation
- Adaptive transient sub-cells (TASC) based on a background grid (N>30)
- Exclusion of latest collision partner: physically realistic requirement for VSC/TASC schemes

Changes in temporal advection

- Global time step
- Cell-based time step

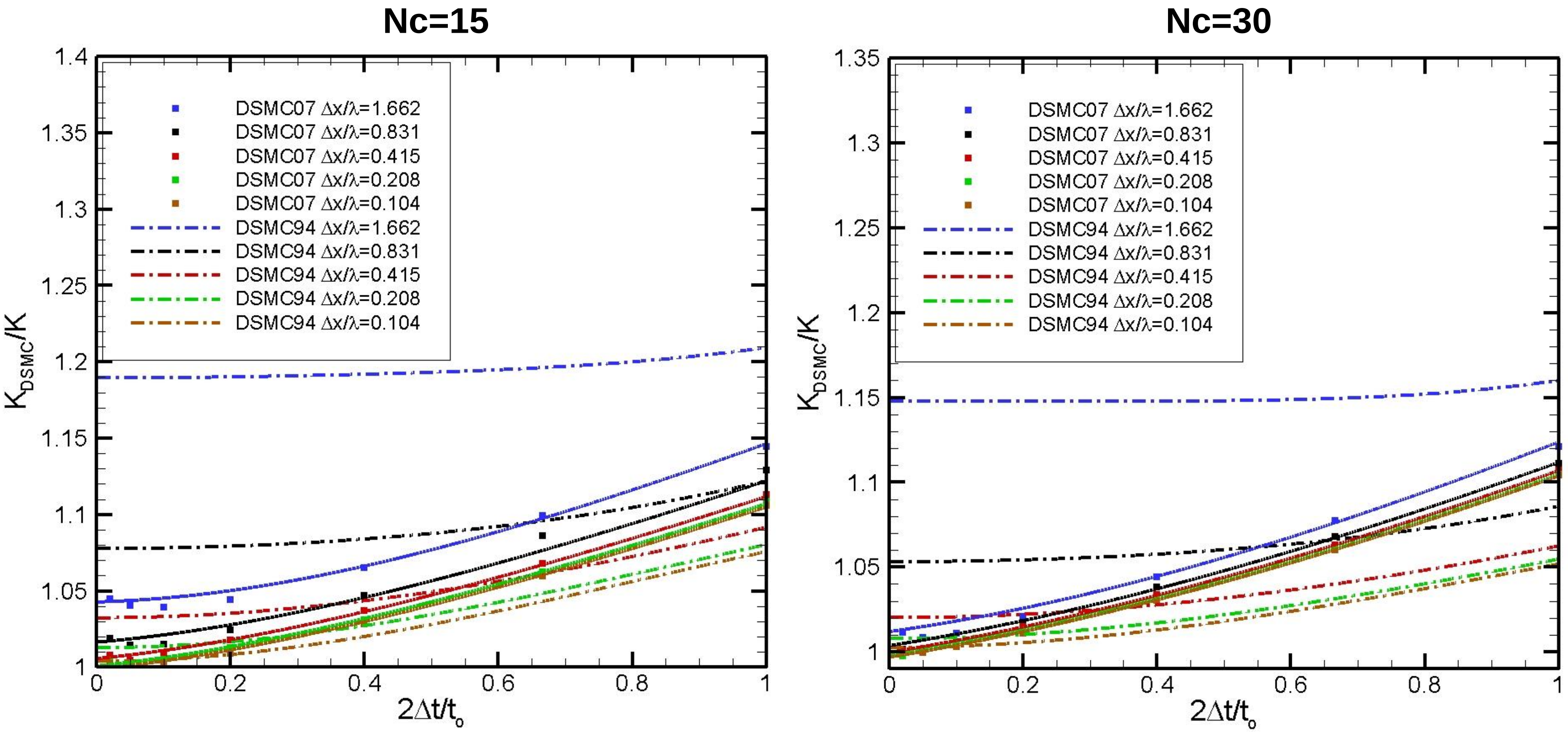


Changes in time-tracking

- Global time
- Cell time
- Molecule time

Separate sampling and collision cells

Convergence Behavior for N_c = 15,30
Effect of Time Step



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

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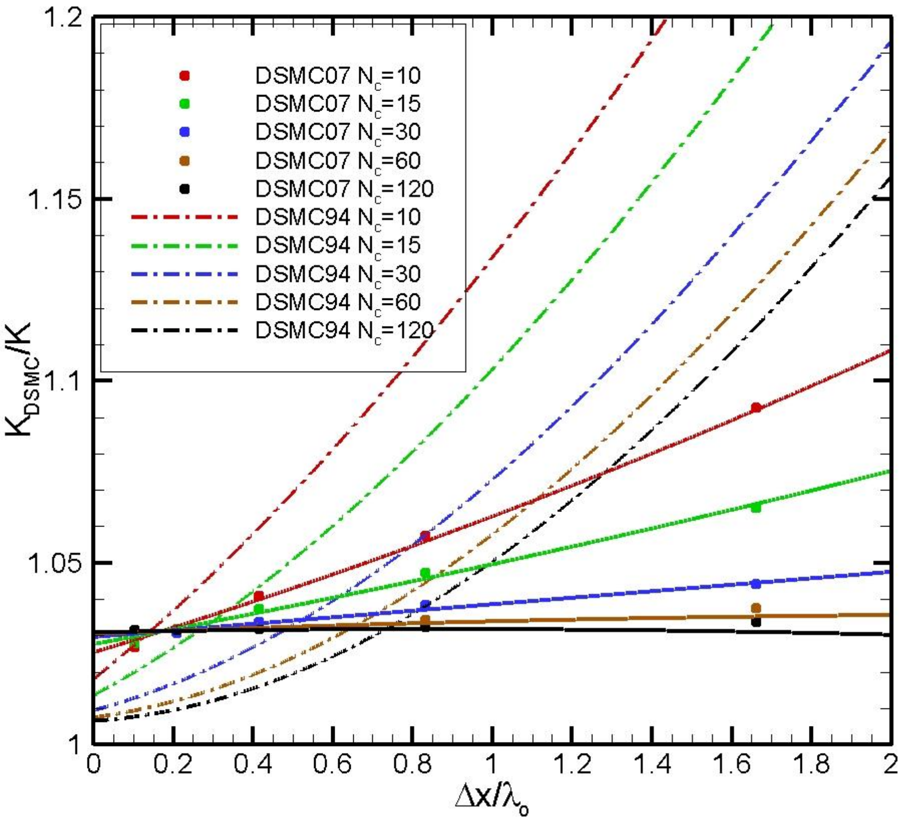
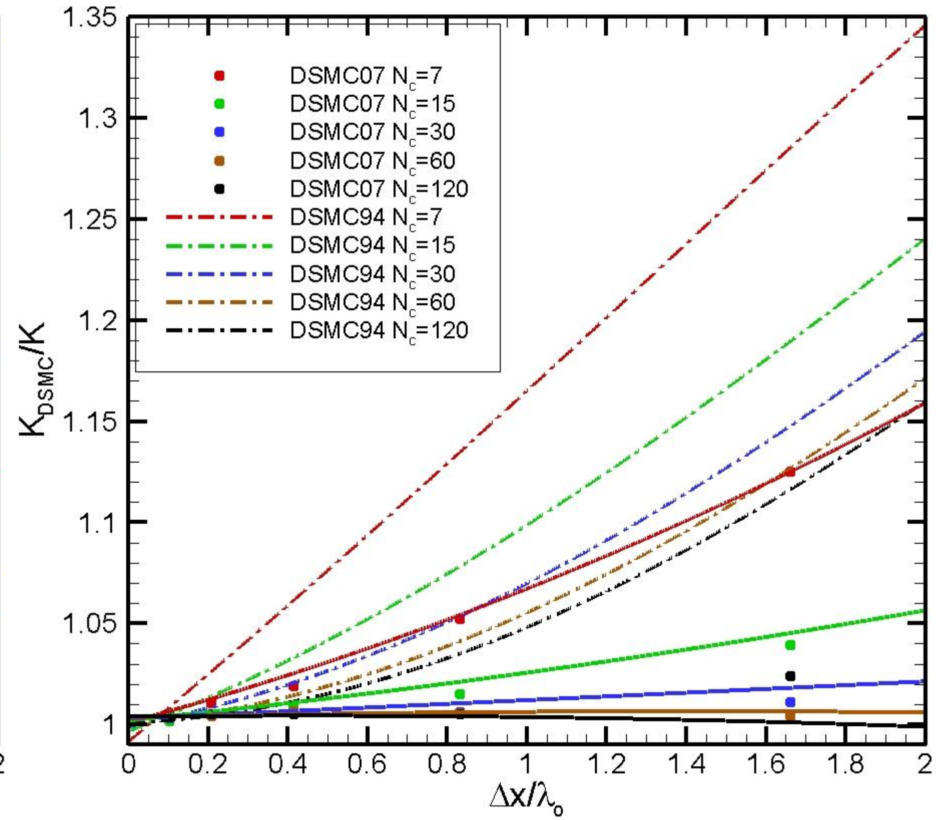
Effect of Time-Step Selection

$\Delta t/t_o=5$



$\Delta t/t_o=10$



- Time-step selection must be based on both
  - Local collision time
  - Local transit time

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.

Allowing nearest-neighbor collisions when MCS~MFP introduces an error that is linear in time step.

Similar to DSMC94 sub-cells, time step should conform to sub-cell structure.

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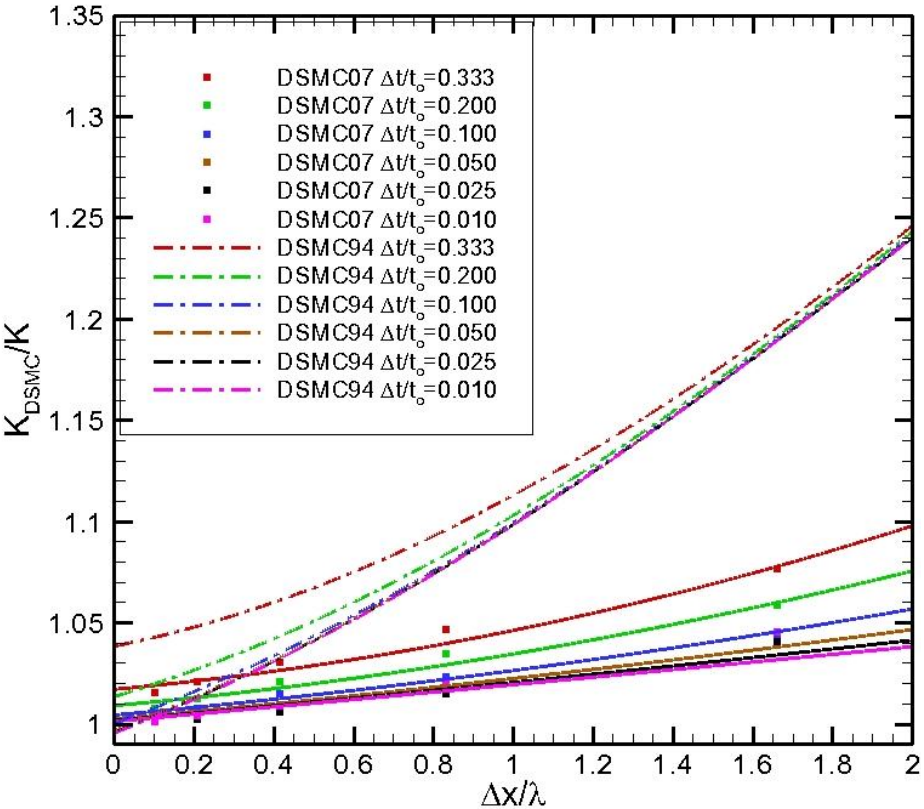
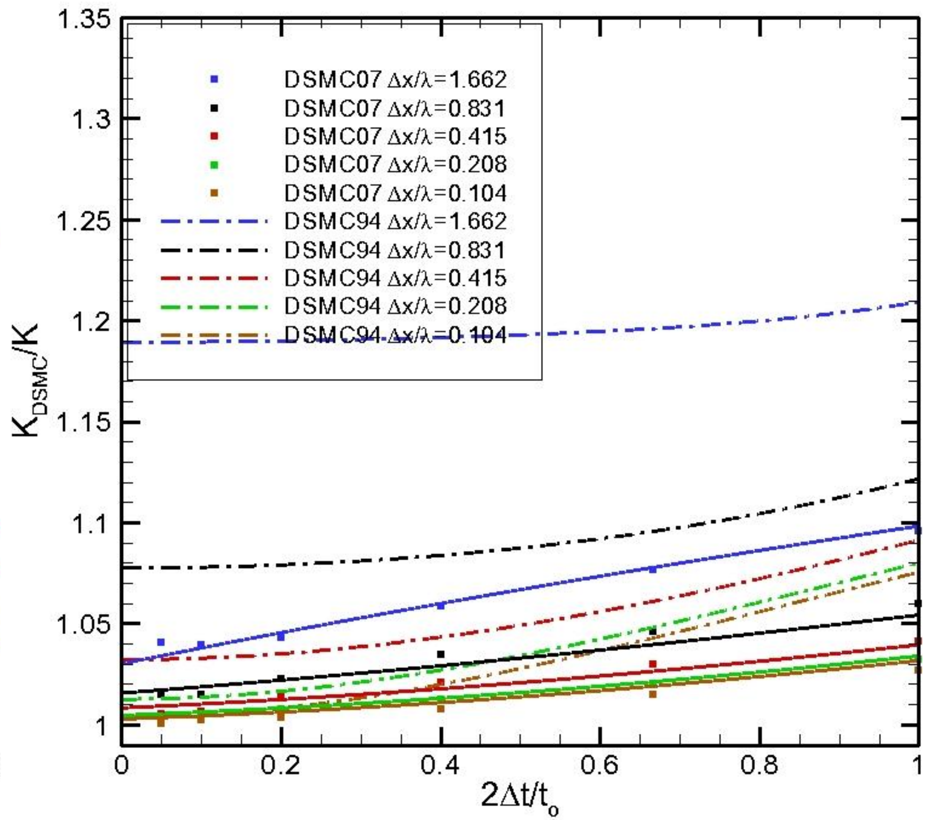
Convergence Behavior for $N_c = 15$
Trajectory dependent selection (D)



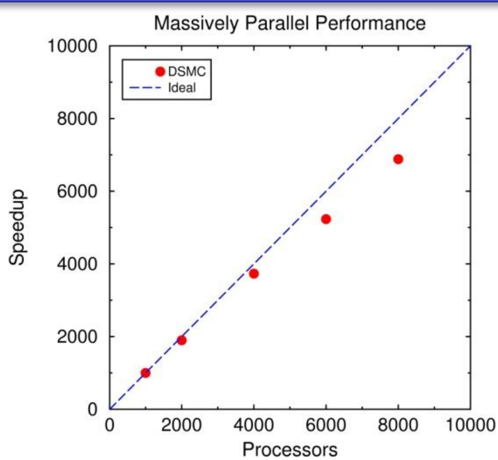


- Significant improvement of convergence rate due to decrease in linear term of temporal discretization error.

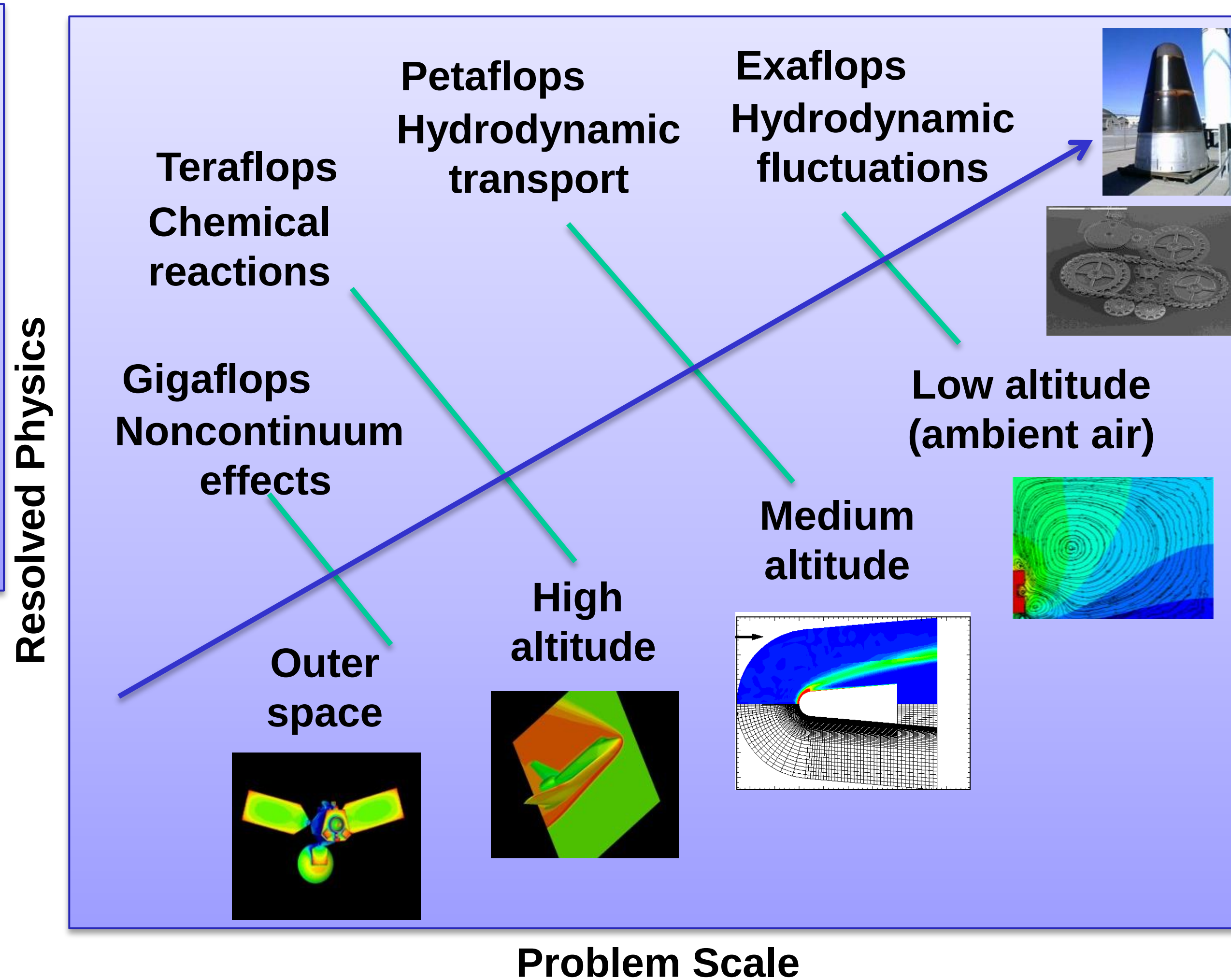
DSMC & Exascale Computing

Develop a validated, predictive, first-principles, massively-parallel computational simulation tool to predict aerodynamic heating and loading to optimize the design and operation of reentry vehicles.

A single numerical technique of higher accuracy than standard CFD that is limited only by computer power and fully parallelizable can provide fundamental insights into gas behavior at molecular scales.



Molecular Gas Dynamics can fully utilize exascale massively parallel technologies.



The road to exascale will enable simulations in this important area and will directly impact the design of US reentry vehicles.

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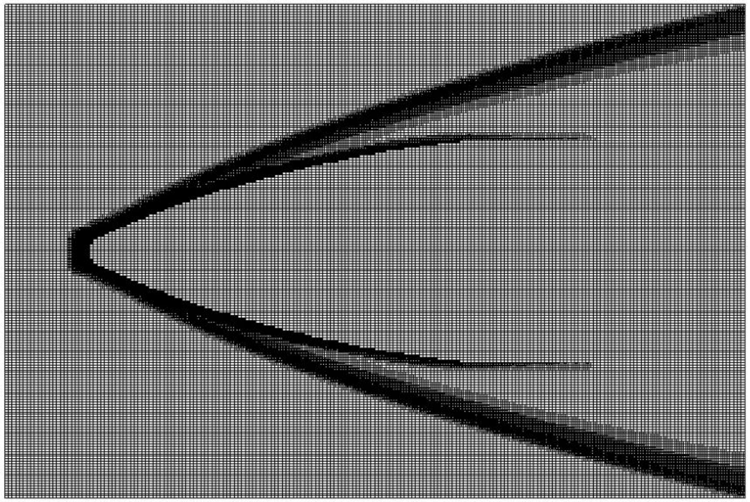
Computational Efficiency

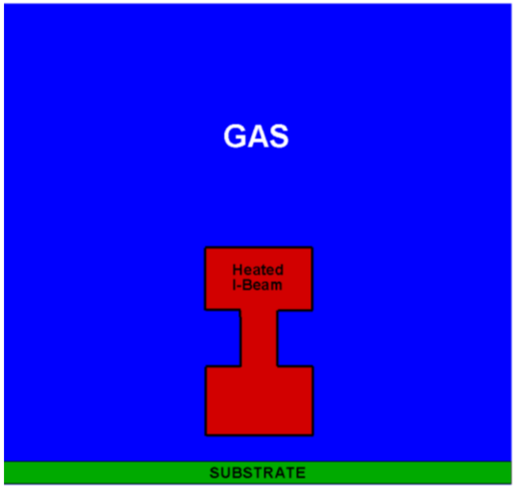
Exploit the inherent MP efficiency of DSMC

- Extend to millions of processors.
- The key to efficient DSMC simulation is inter-cell operations: move phase.
- The most promising option of achieving MP DSMC efficiency is through using Cartesian grids.

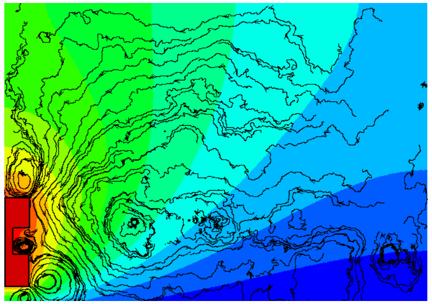


Simulations of MEMS in Air Reveal New Physics

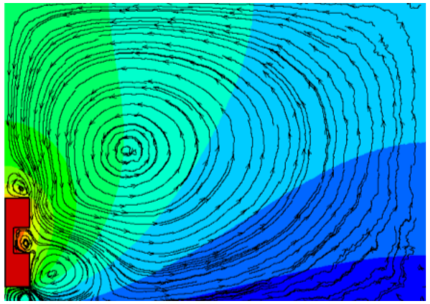
Heated Microbeam Makes Gas Move



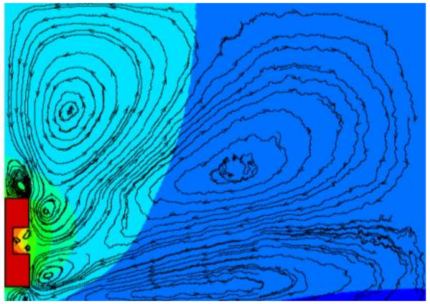
1 atm
~0.1 m/s



0.1 atm
~2 m/s



0.01 atm
~1 m/s



DSMC microbeam simulations

- **Steady gas motion is induced by nonuniform heat flux**

  ***Not* buoyancy, *not* transient**
- **Noncontinuum effects cause motion**

  ***Not* in Navier-Stokes simulations**

Gallis M. A., Torczynski J. R., and Rader D. J., "A Computational Investigation of Noncontinuum Gas-Phase Heat Transfer between a Heated Microbeam and the Adjacent Ambient Substrate", *Sensors and Actuators: A*, 134, 57-68, 2007.

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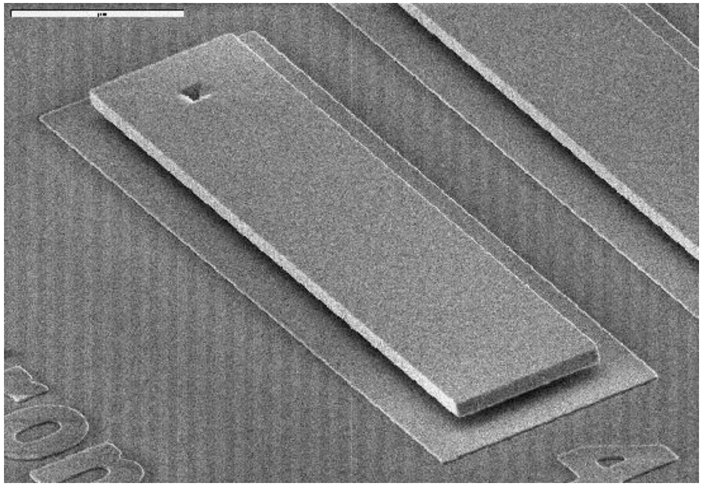
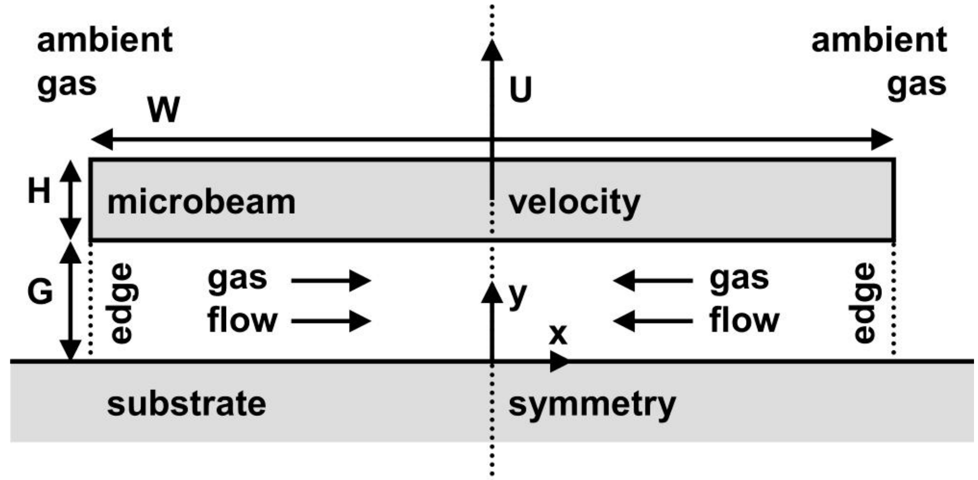
Moving Microbeams





- **MicroElectroMechanical Systems (MEMS) devices in air**
  - Beams often oscillate out-of-plane at high frequencies
  - Gas in gap between beam and substrate damps motion
- **Gas motion producing damping force is noncontinuum**
  - Gaps are small: ~2 μm nominal, smaller while closing
  - Mean free path: ~0.07 μm, larger in low-pressure package
- **Gas motion is driven by time-varying geometry**
  - Closing and opening gaps, gas motion to/from ambient
- **Simulate noncontinuum gas with moving object**

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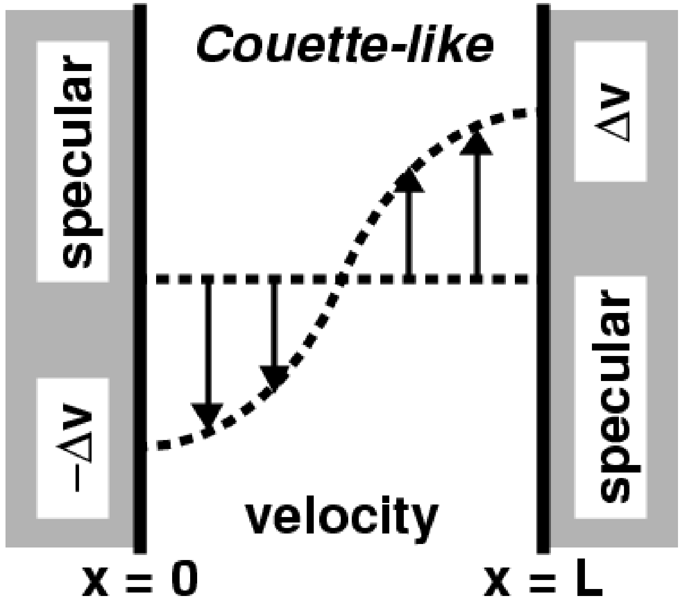
Couette-like Transient Flow

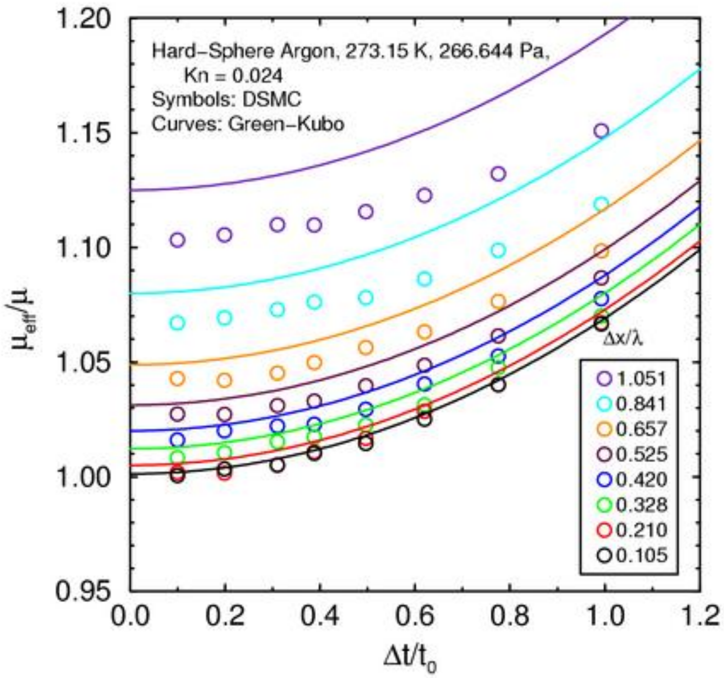


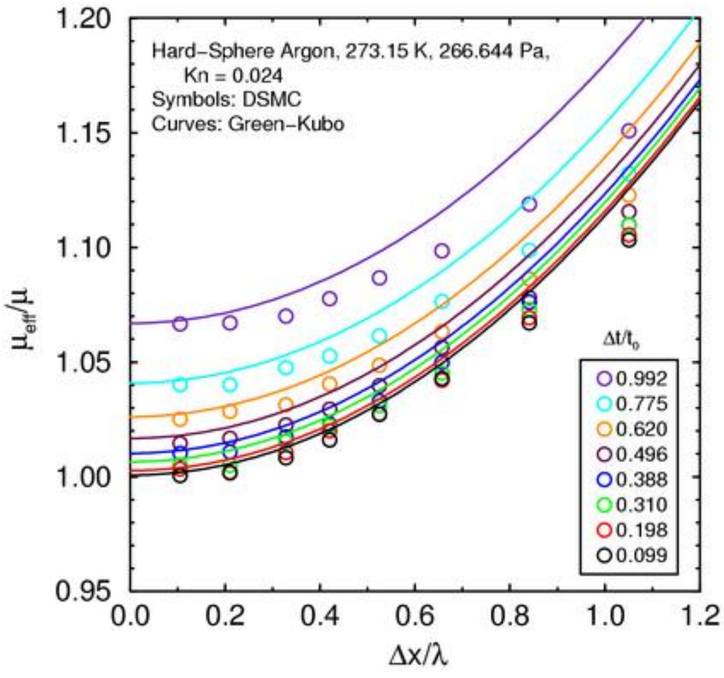
Decaying shear flow with slippery walls

- 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

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

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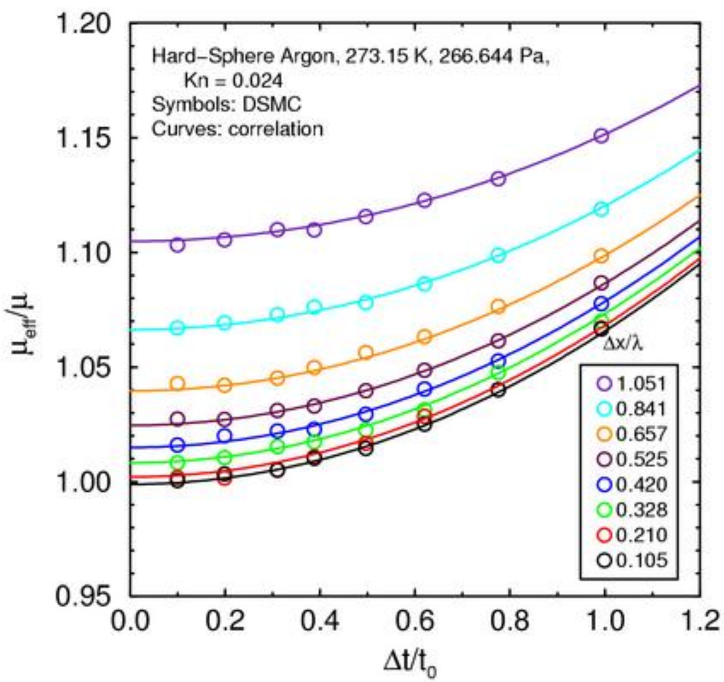
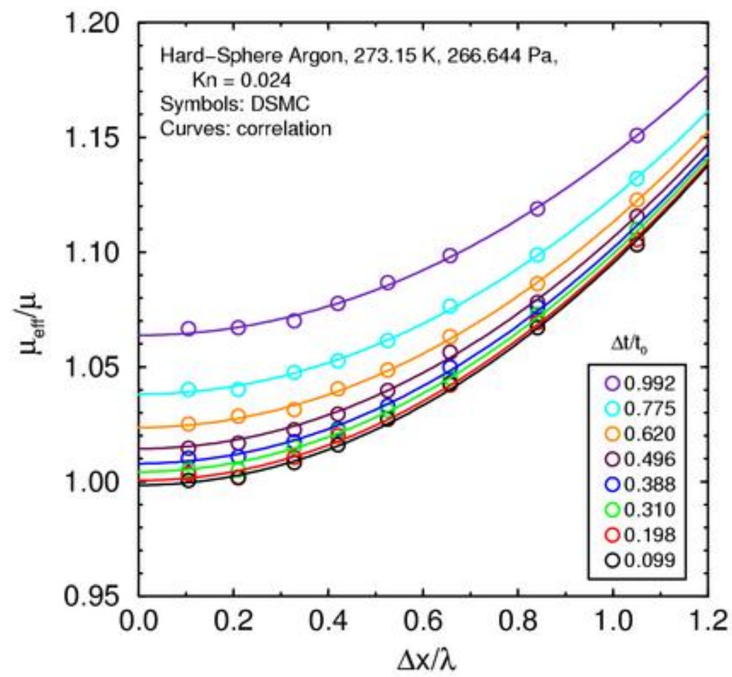
Polynomial Correlation

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





Viscosity differs by 0.3%, close to thermal variation

Pure terms agree reasonably with Green-Kubo

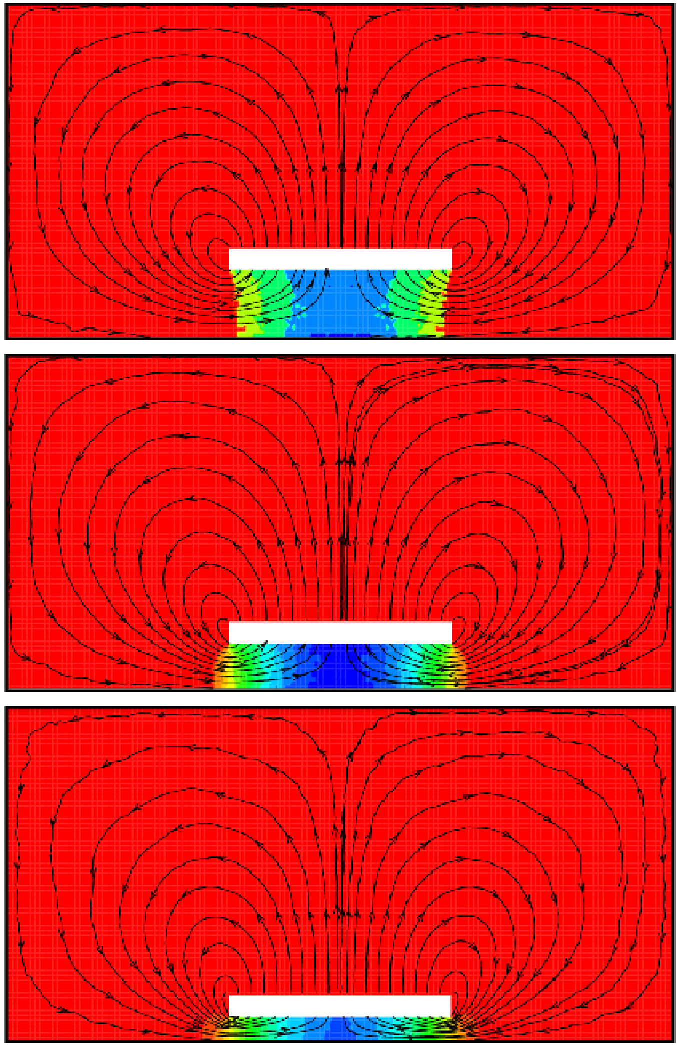
Cross terms are required to correlate values

Modeling Moving Objects with DSMC

Several approaches have been used

- Continuum: Navier-Stokes slip-jump,
  Torczynski et al. (2002)
- Quasi-static DSMC: fixed geometries,
  Gallis et al. (2003)
- Simpler physics: Reynolds equation,
  Gallis and Torczynski (2004)

DSMC for noncontinuum gas with moving object



Gallis et al. (2003): Quasi-Static DSMC

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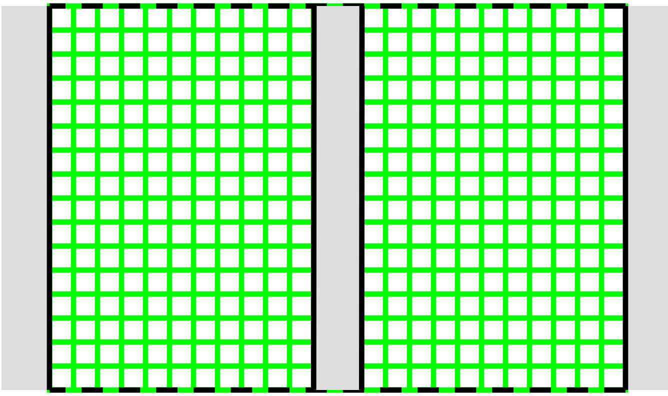
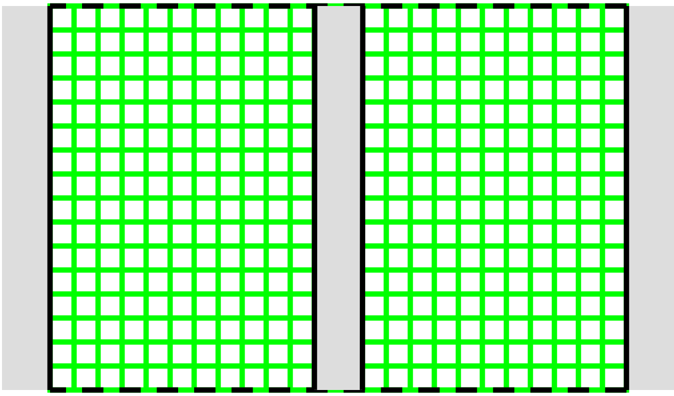
Piston Motion



Impulsively starts and stops



Sinusoidally oscillates continually

Simulation conditions

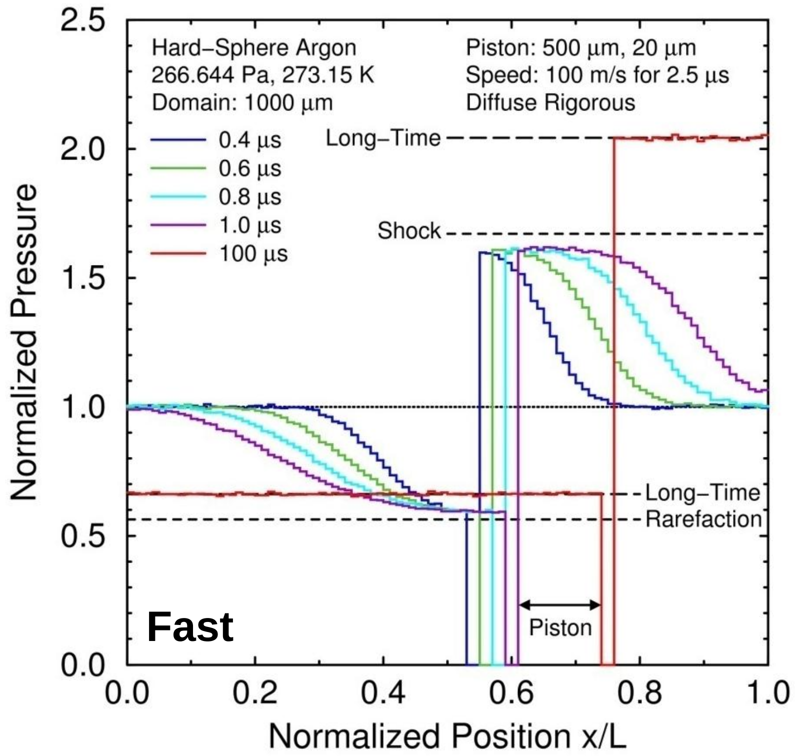
- Gas is hard-sphere argon at 266.644 Pa and 273.15 K
- Domain is 1000 μm, cells are 10 μm (100 cells)
- End walls are motionless, diffuse at 273.15 K
- Piston is 20 μm (2 cells), specular or diffuse at 273.15 K
- Time step is 1 ns, no averaging over multiple time steps
- Molecules per cell: 10^5

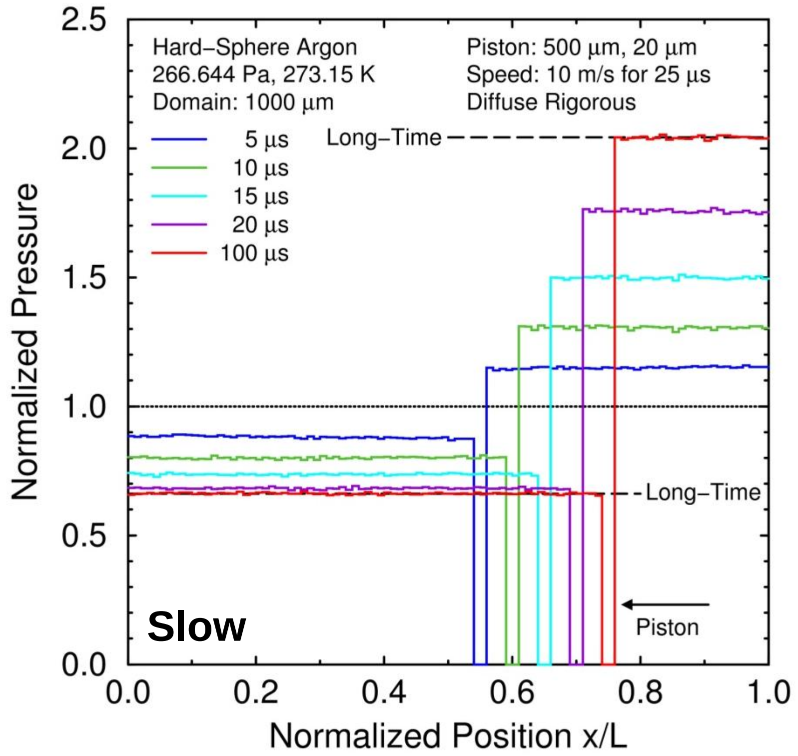
Case 1: starts at 50%, moves at 100 or 10 m/s, stops at 75%

Case 2: centered, 1 MHz, velocity amplitude 100 or 10 m/s

- Denote 100 m/s as “fast” and 10 m/s as “slow”

Impulsive Moving Piston





Good agreement with theoretical expectations

- **Gas temperatures near piston are close to piston value**
- **Temperature jumps at piston and walls are evident**
- **Thermal boundary layers from piston weaken both waves**
- **Long-time pressures and temperatures are as expected**

Qualitatively similar to specular piston

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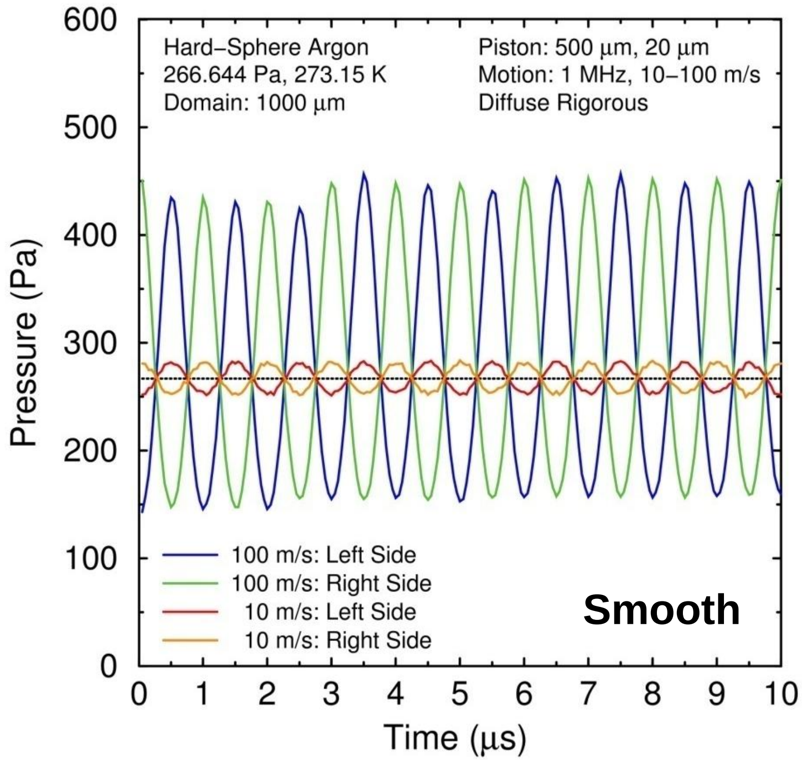
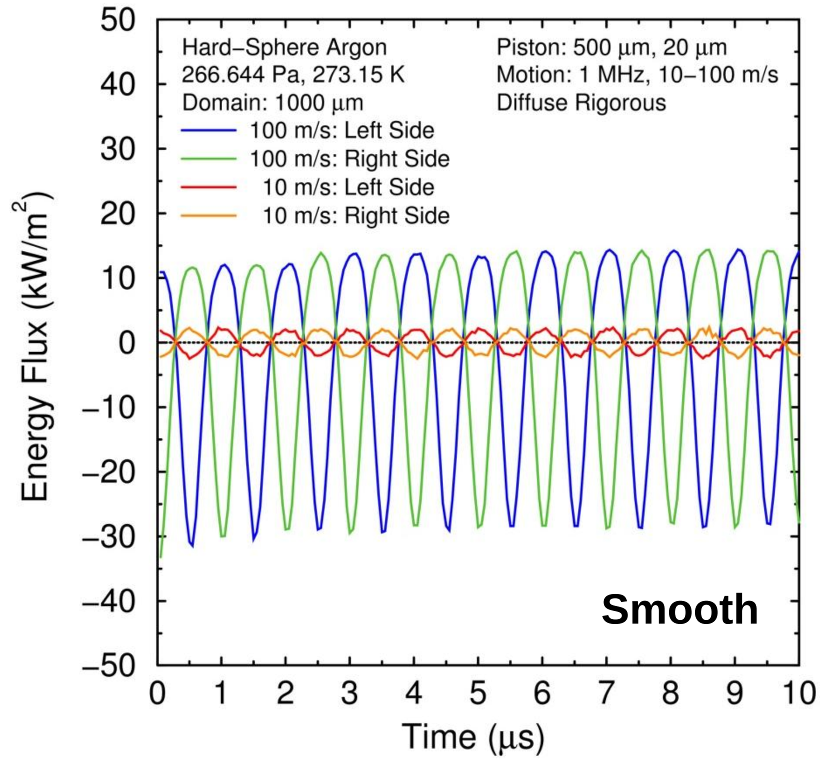
Oscillating Fast and Slow Diffuse





Force on and energy transfer to object are most important

- **Slow has linear waves, advancing and receding are same**
- **Fast has nonlinear waves, advancing and receding differ**
- **Increasing velocity 10x does not increase response 10x**
- **Slight rise over time is attributed to net heating of gas**

Energy flux is mainly work, not heat transfer

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Non-equilibrium Gas Modeling
Future Directions for Research

To address problems of national importance, research must focus on major technical issues

- **Analysis**
  - Simulation *accuracy* for noncontinuum gas
  - Noncontinuum-gas *models* for engineering codes
  - Improved *understanding* of physical processes
  - Address *multi-discipline* problems
- **Codes**
  - Much faster *algorithms*
  - Efficient *massively parallel implementations*
  - New *computer technologies*
- **Data**
  - Accurate *physical properties* for gases and solids
  - Reliable, complete *validation* experimental results

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