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DSMC Simulations of Transient Gas Flows

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DSMC: Fundamentals through Advanced Concepts
Short Course

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

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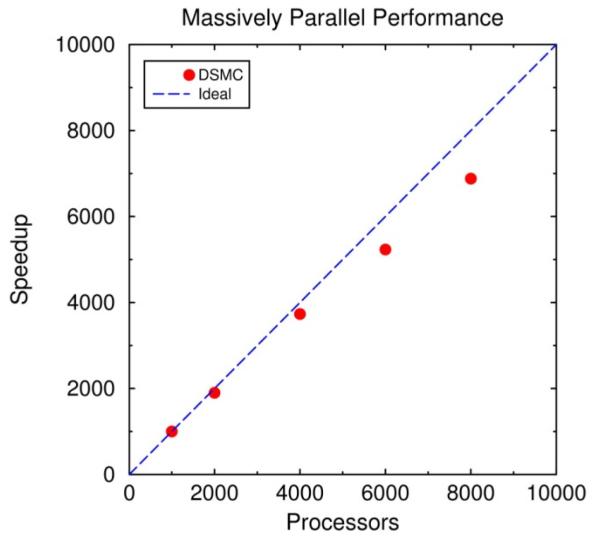
The Limitations of DSMC

- The computational load increases with the density of the flow
- Statistical error decreases as a function of the *square root* of the number of samples
- DSMC can carry more information than actually needed for some applications
- DSMC is an MP empowered technology



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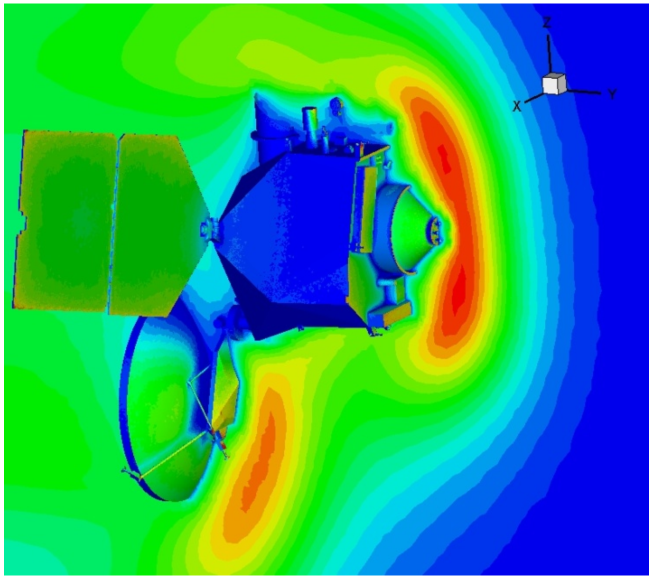
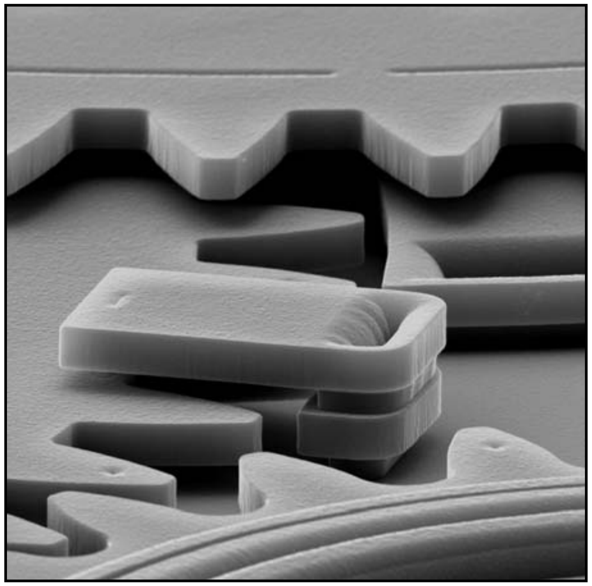
Can DSMC Compute Transient Microscale Gas Flow?



Traditional DSMC application

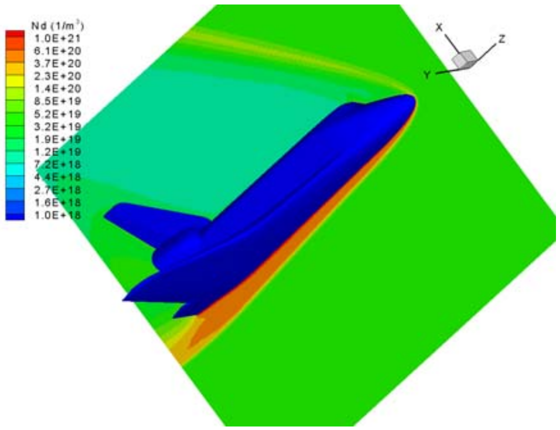


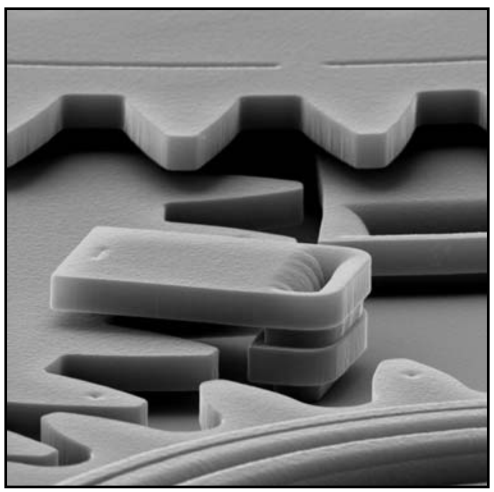
Can DSMC be used?

Perception: DSMC is a "rough and ready" method, sufficiently accurate for hypersonic flows but not adequate (speed, accuracy) for microscale flows (low-speed, nearly-isothermal)

Reality: DSMC can also be used for transient microscale flows if carefully implemented and applied in a massively parallel (MP) environment

Why DSMC for Microscale Gas Flows?





DSMC is accurate for hypersonic <u>and</u> microscale gas flows
- Careful implementation is required – can't "cut corners"
- Pay attention to mesh, time step, number of molecules, statistics

DSMC has been successfully verified against known results
- Low heat fluxes with small molecular mean free path
  - Excellent agreement with Chapman-Enskog theory
- Arbitrary heat fluxes with infinite molecular mean free path
  - Excellent agreement with well-known solutions

DSMC can compute regimes that theory cannot predict
- High heat fluxes with small molecular mean free path
  - Predicts gas state when Chapman-Enskog theory does not apply
- Heat fluxes with molecular mean free path comparable to geometry
  - Predicts gas state when wall interactions are significant

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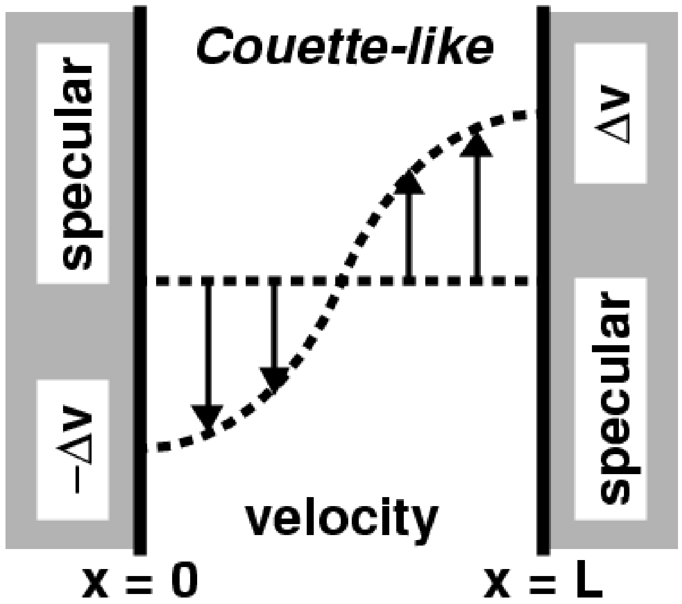
Convergence of Transient DSMC

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

– How does DSMC converge for transient flows?

– Goal: extract maximum accuracy with minimum effort
  - Identify major parameters controlling DSMC accuracy

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 1994)
- Temperature: 273.15 K

Quantities varied in simulations

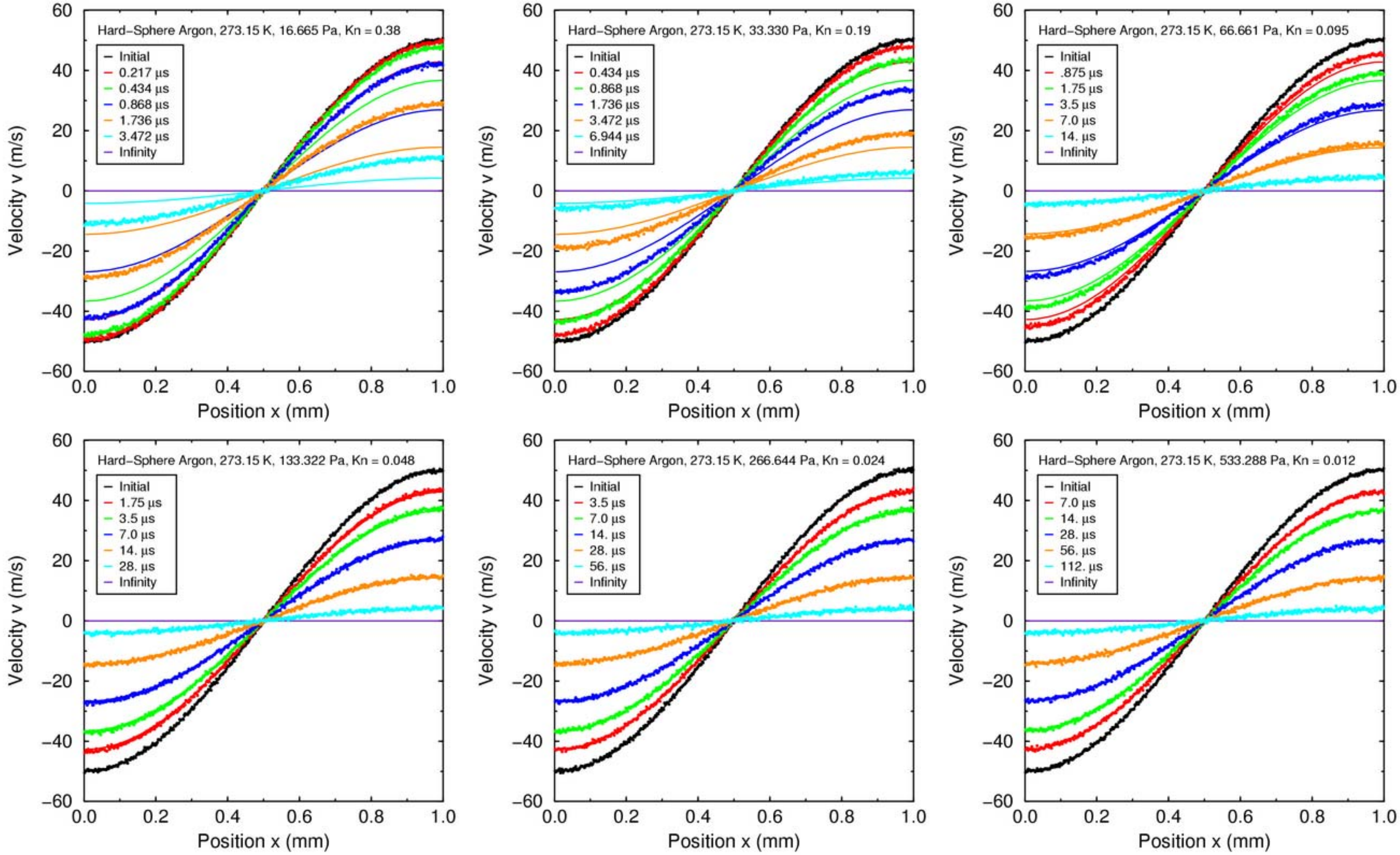
- Velocity: $v = -\Delta v \cdot \cos[\pi x / L]$, Δv = 50-500 m/s, c = 381 m/s
- Pressure: p = 4, 2, 1, 0.5, 0.25, 0.125 torr (focus on 2 torr)

  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

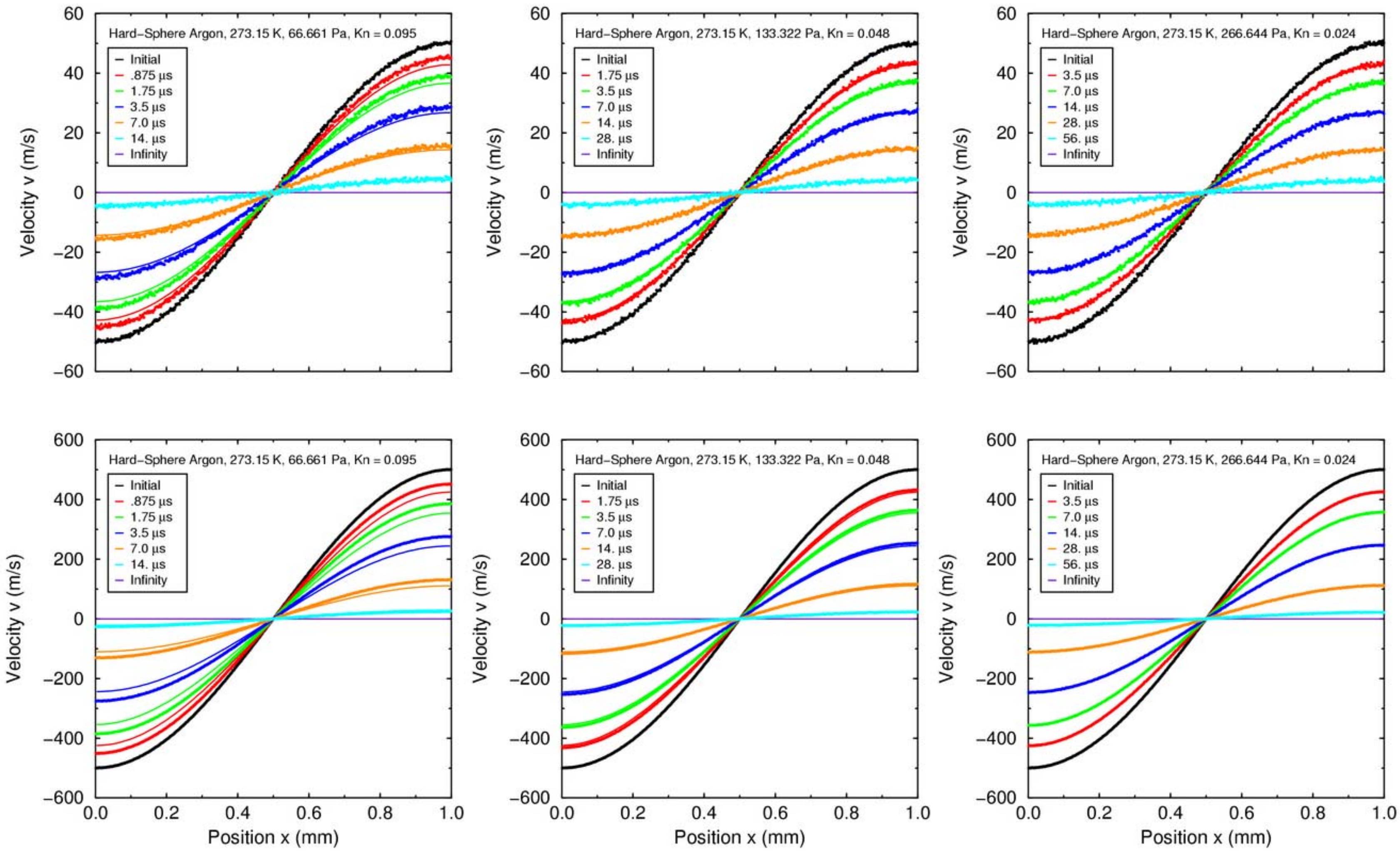
- Algorithm: DSMC94, move-sample-collide-sample
- Molecules: 10,000,000 (25,000-250,000 per cell)

Pressure (Knudsen Number) Dependence



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

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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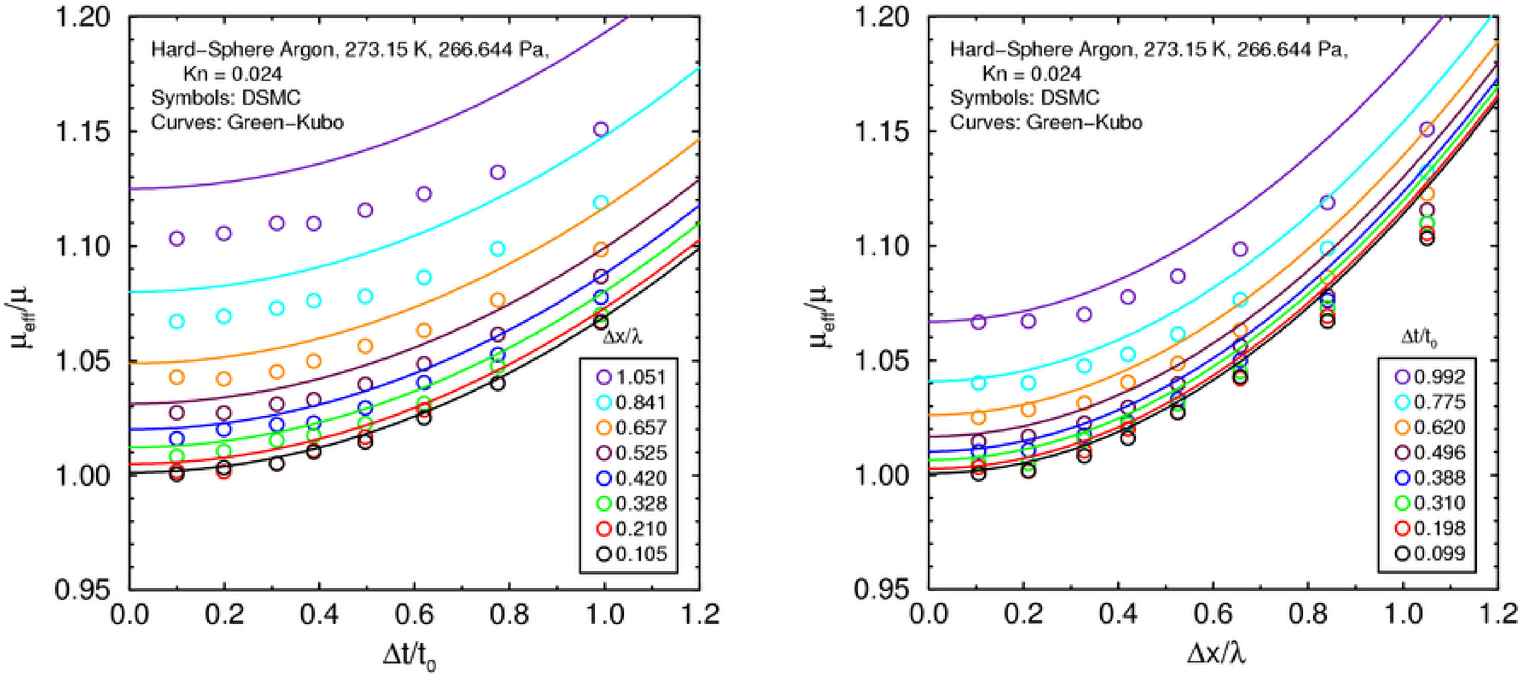
Comparison to Green-Kubo Theory

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

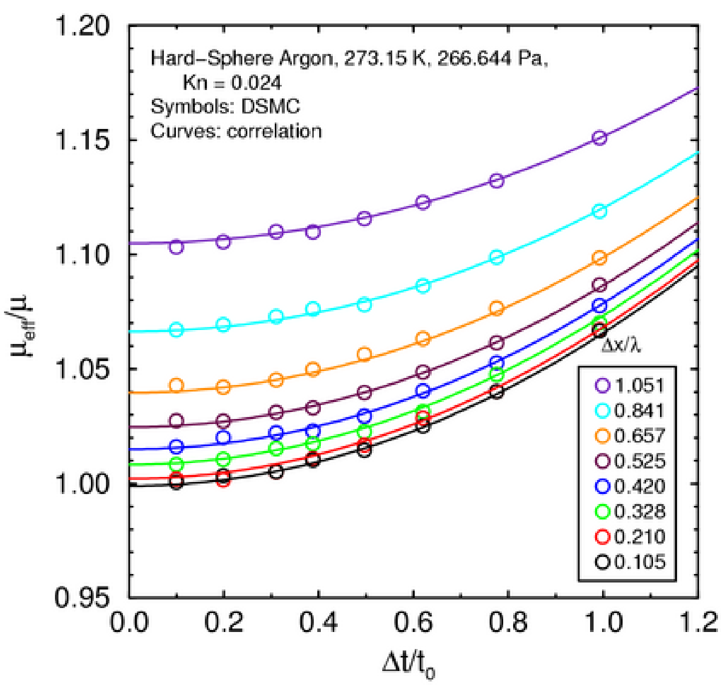


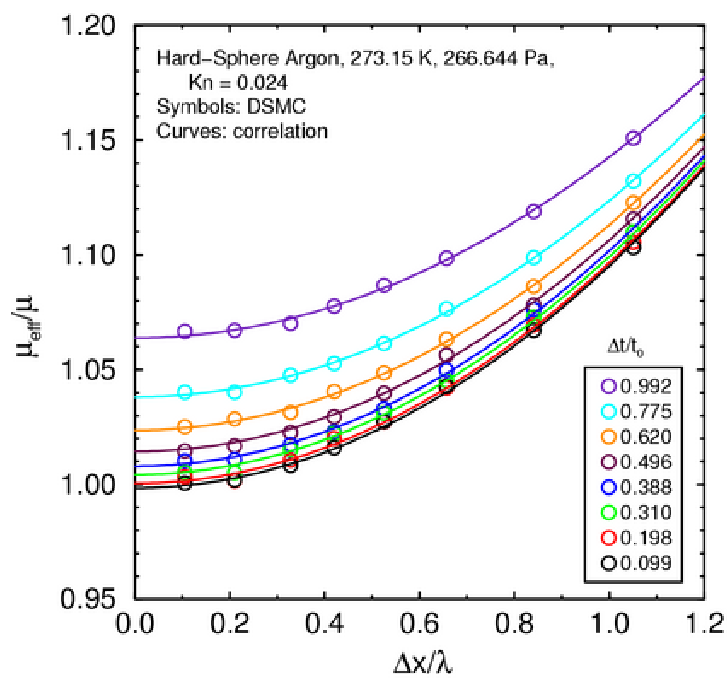
DSMC and Green-Kubo results agree reasonably

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

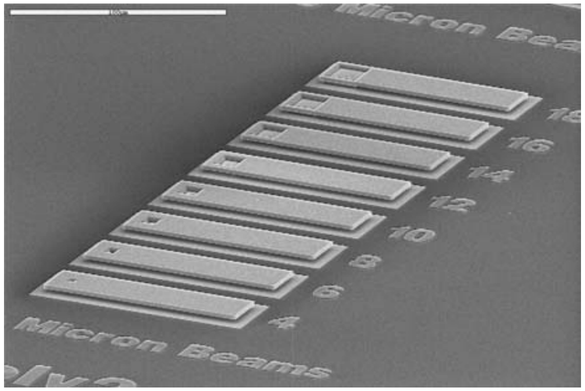
Pure terms agree reasonably with Green-Kubo

Cross terms are required to correlate values

Quasi-Static Assumption

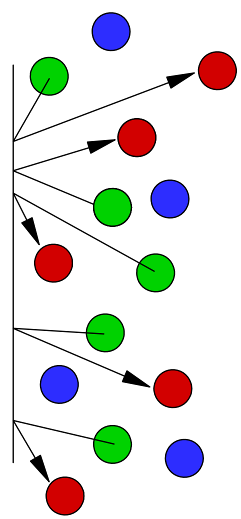
- **The structure movement is quasi-static**
  - *the structure speed is much smaller than the thermal speed of molecules*
  - *the gas is incompressible and isothermal*

- **The moving boundary is replaced by a fixed boundary on which the velocity is applied**



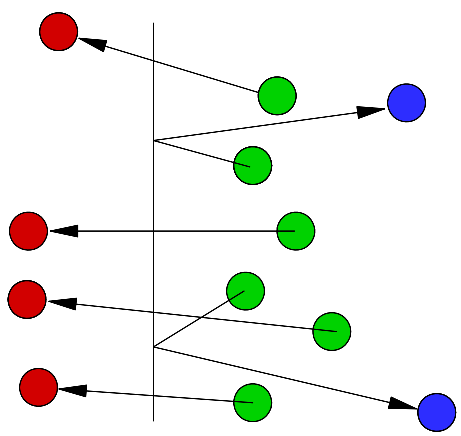
DSMC Inflow BC

- Molecules that “exit” are reintroduced into the domain with new properties.
- Additional molecules are introduced at a rate that corresponds to the net subsonic inflow.
- Properties of entering molecules selected to produce Maxwellian at prescribed velocity and temperature.



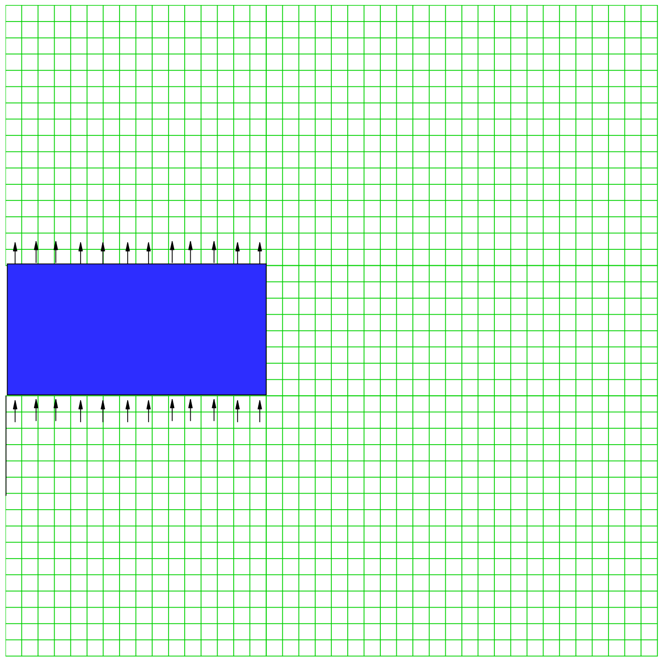
DSMC Outflow BC

- Molecules that “exit” are deleted at a rate that corresponds to the net subsonic outflow.
- The rest of the molecules that “exit” are reintroduced into the domain with new properties.
- Properties of entering molecules selected to produce Maxwellian at prescribed velocity and temperature.



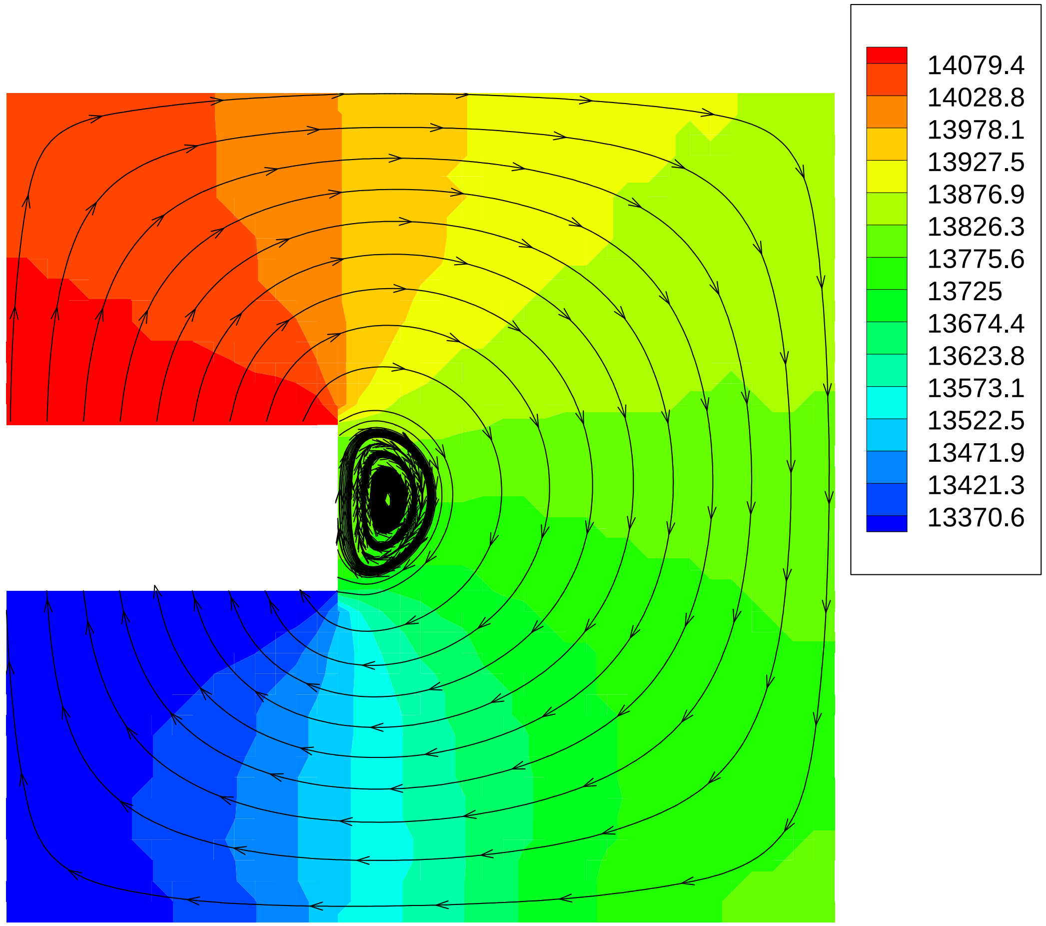
Moving Microbeam

- **Geometry**
  - 2D cross-section
  - Half-width: 4 microns
  - Thickness: 2 microns
  - Gap: 4 microns
- **Gas properties**
  - Gas: rarefied nitrogen
  - Pressure: 100 mTorr
  - Temperature: 295 K
- **Flow condition**
  - Velocity: 10 m/s



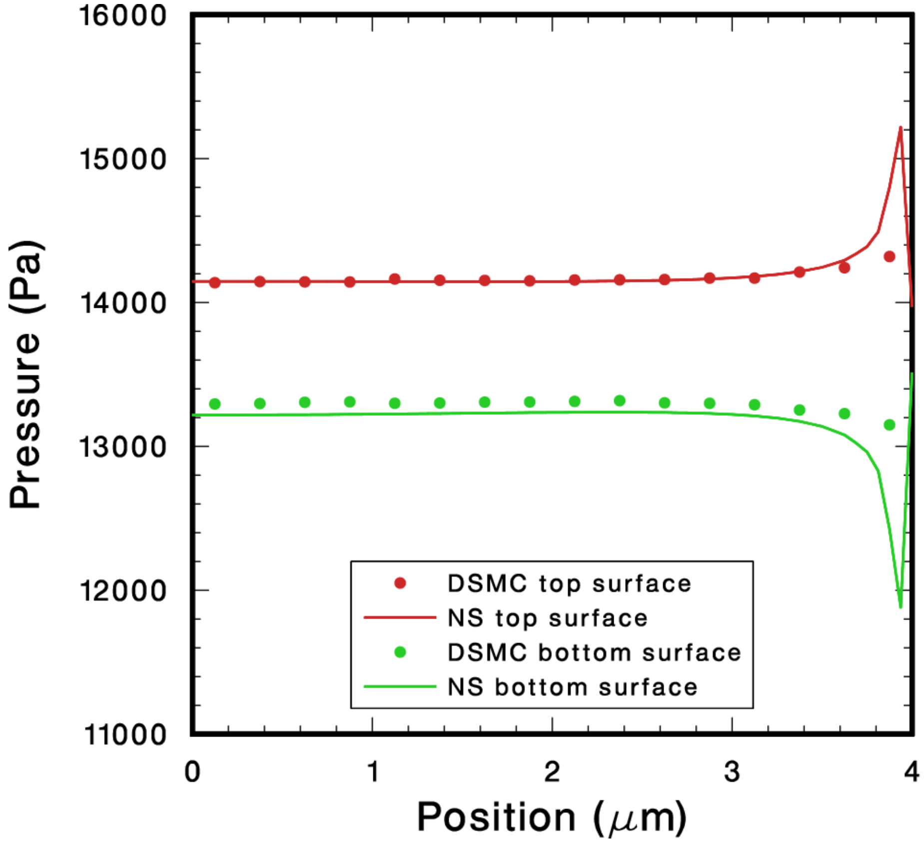
Moving Microbeam

Pressure Contours and Streamlines



Moving Microbeam

DSMC and NS Pressures on the Surfaces

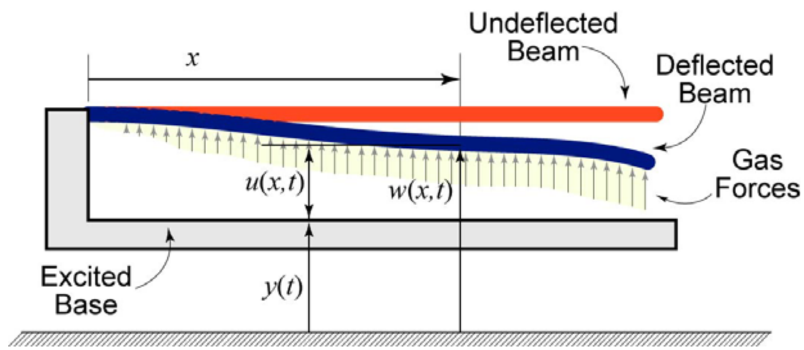


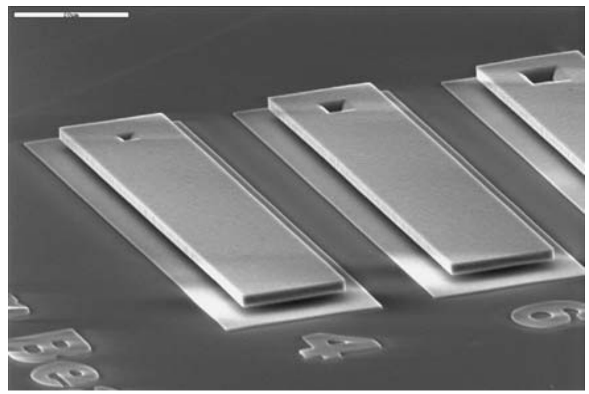
DSMC: Icarus
NS: FIDAP (continuum slip, incompressible, isothermal)

Cantilevered Microbeams

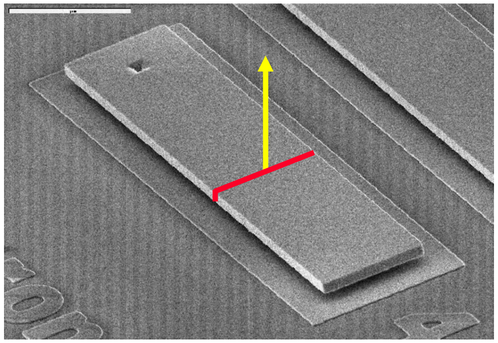
- "Diving boards for bacteria"
  - Polycrystalline silicon
    - Length: 100 microns
    - Width: 20 microns
    - Thickness: 2 microns
    - Gap height: 2-10 microns
    - Frequency: 10-100 kHz
  - Gas: ambient or rarefied air

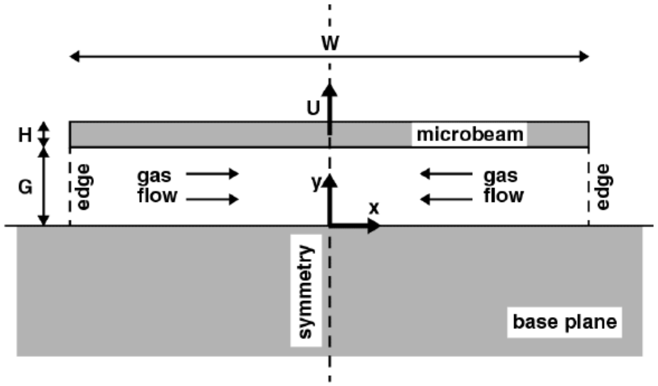
- Good candidate for analysis
  - Geometry, properties known
  - Experimentally accessible





Microbeam Gas Damping

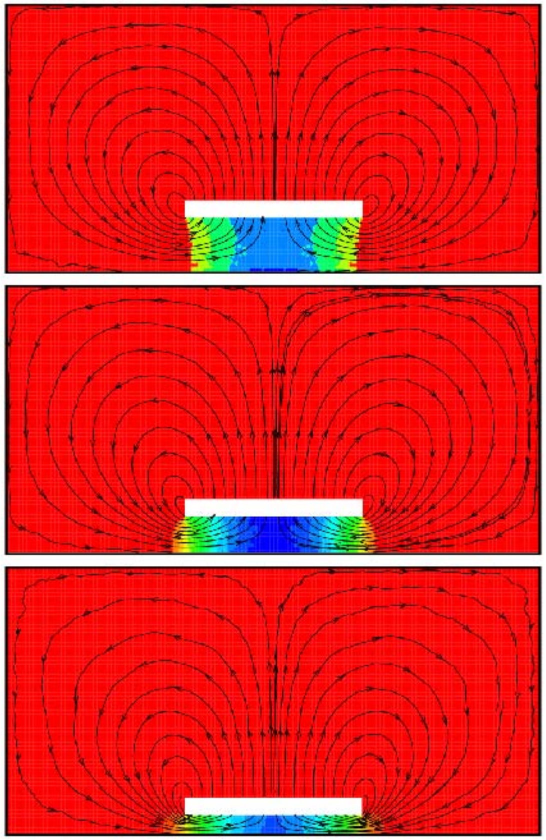




- DSMC simulation of microbeam gas damping

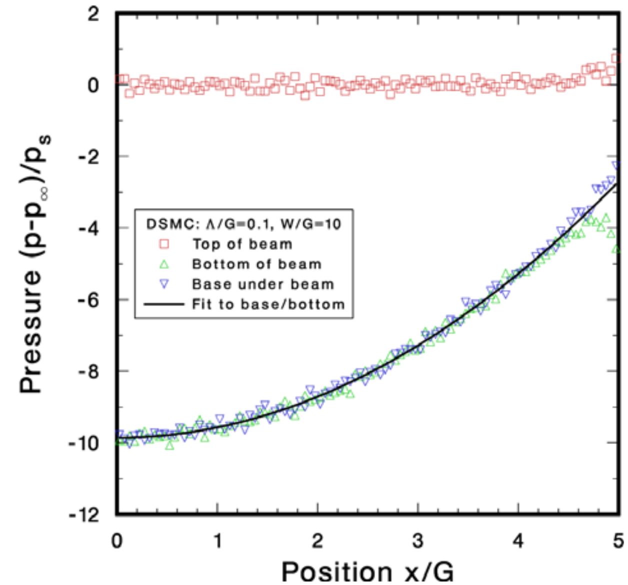
- **Two-dimensional geometry: cross section**
- **Quasi-static flow:**
  - **Moving boundary replaced by fixed boundary**
  - **Velocity applied as boundary condition**
- **Low velocities, small pressure variations**
- **Nearly isothermal, nearly incompressible**

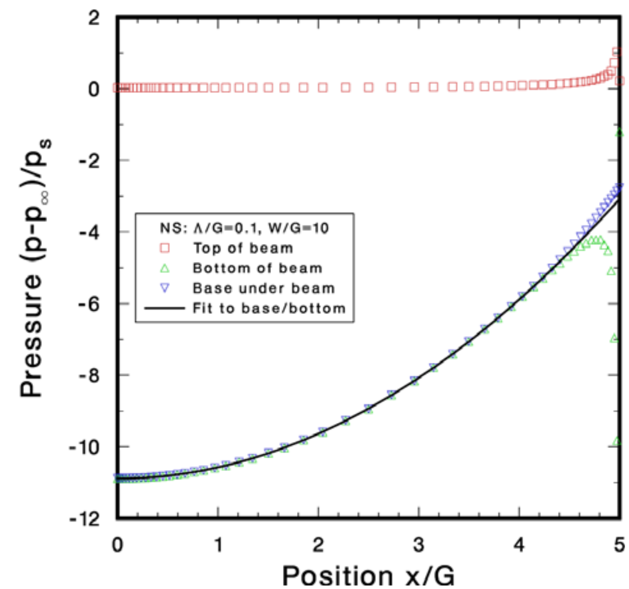
Quasi-Static DSMC



DSMC

NSSJ





DSMC: 24 hours on 3000 processors (ASCI Red)
Sample 10^{10} molecules/cell, ~1 billion time steps
Microbeam: 2x20 μm, 1 m/s
Gas: atmospheric nitrogen

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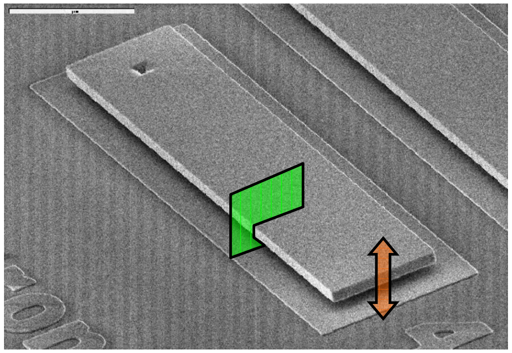
Transient DSMC Simulation

- Goal: Simulate transient gas flow around a moving microbeam
- Microbeam Test Case
  - Geometry (2-D): 2x20-μm cross section, 2-μm gap
  - Gas: atmospheric nitrogen
  - Oscillation: 1 MHz with peak speed of 1 m/s
- DSMC Simulation
  - Sandia MP implementation (Icarus)
  - Simulation: 24 hours on 8000 processors (ASCI Red, 3 Tflop)
  - Total time simulated: 3 μs (3 cycles)
  - Computational molecules: 13,000 per cell, ~1 billion total
    - 3 million sampled per cell per frame (uncertainty 50 Pa, 0.2 m/s)



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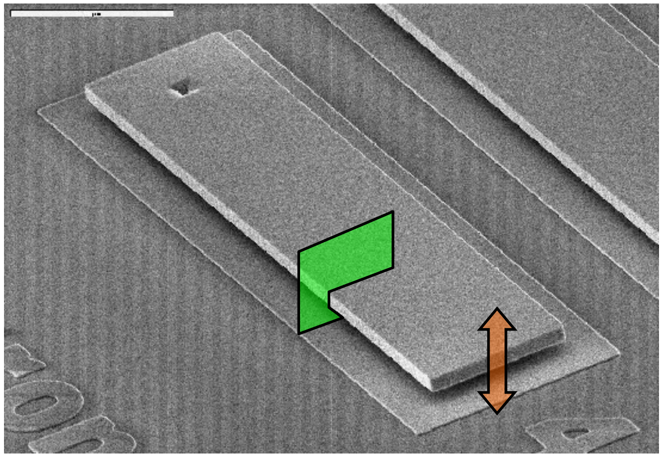
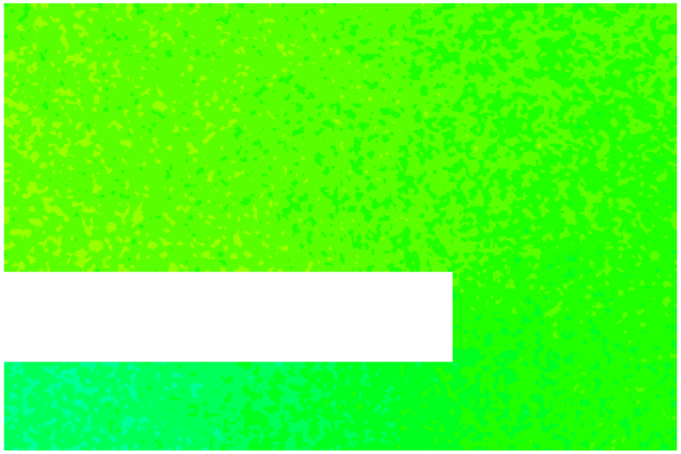
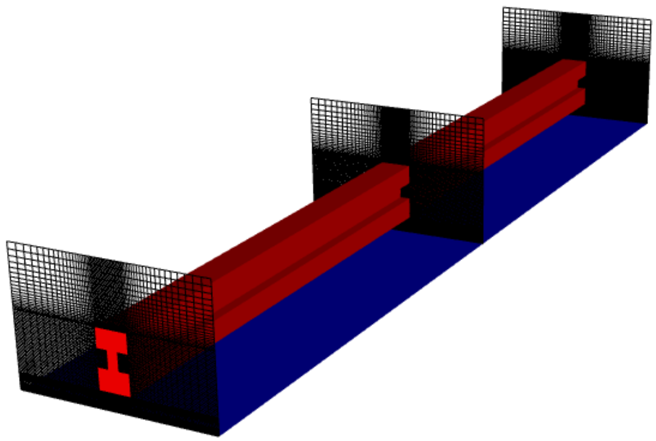
Oscillating Microbeam Flow Field from DSMC

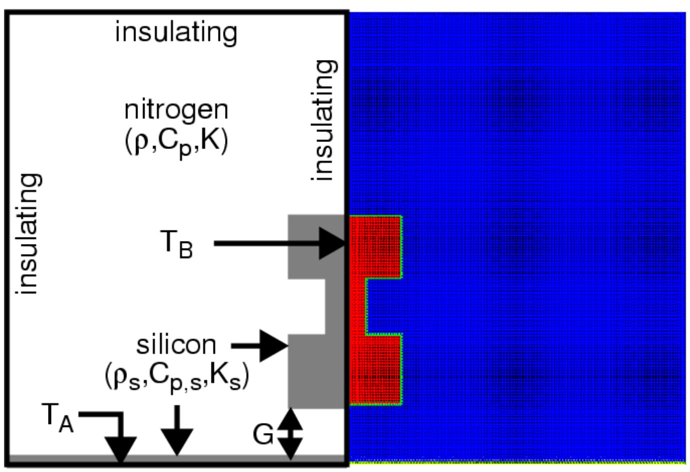




- Microbeam motion creates pressure variations in gap beneath it
- Pressure on top remains practically unchanged

Heated Microbeam Near Substrate





Solid regions: silicon

- **Geometry: 2-micron gap**
- **Beam temperature: ~900 K**
- **Substrate temperature: ~300 K**

Gas region: nitrogen

- **Pressure: atmospheric**
- **Initial temperature: ~300 K**

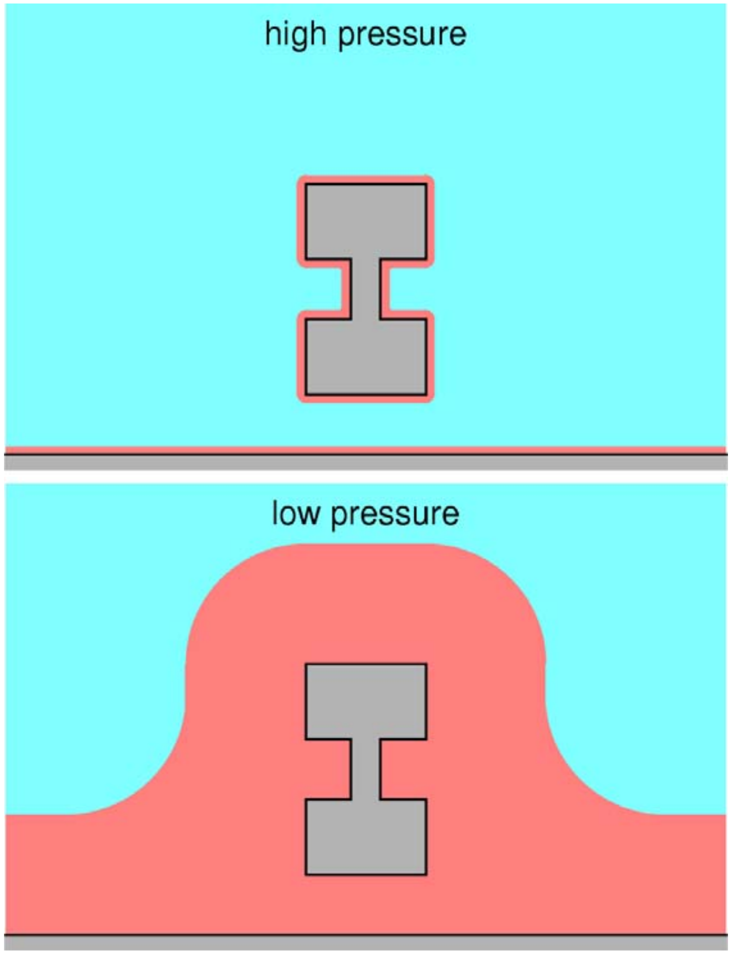
NSSJ simulations

- **Finite-element (Calore, FIDAP)**

DSMC simulations

- **Two-dimensional, transient**
- **100 computational molecules/cell**
- **24 hours, 3000 processors, 3 Tflop (ASCI Red)**

Microbeam Noncontinuum Regions



High pressure

- **Thin, isolated, planar Knudsen layers**
- **Heat transfer = continuum + jumps**

Low pressure

- **Thick, merged, convex Knudsen layers**
- **Heat transfer = free-molecular finite body**

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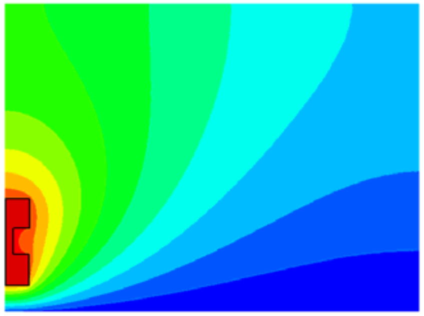
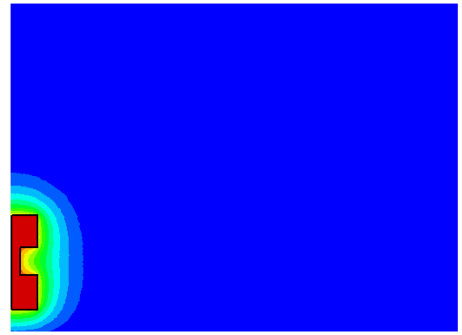
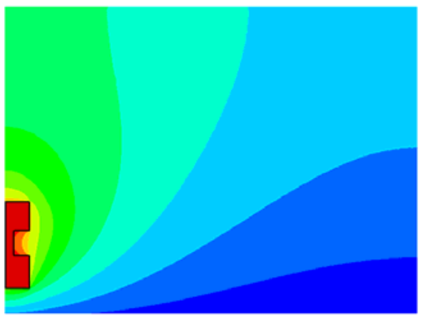
Steady State

Transient Motion

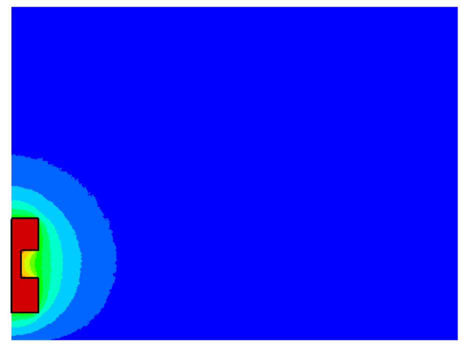


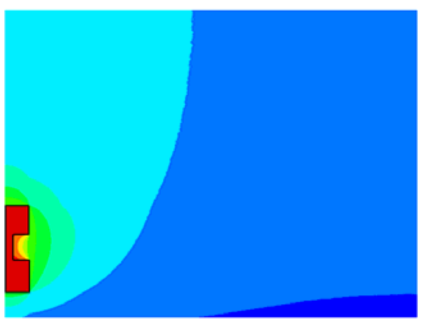
1 atm





0.1 atm





0.01 atm

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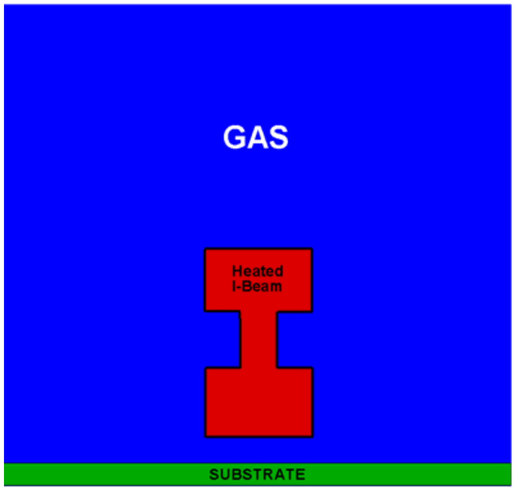
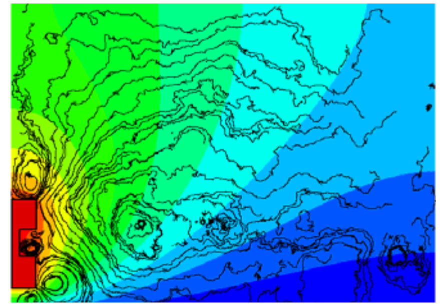
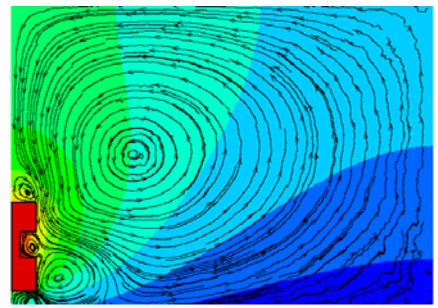
Heated Microbeam Makes Gas Move



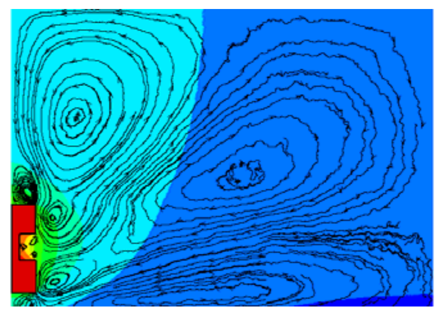
1 atm
~0.1 m/s



0.1 atm
~2 m/s



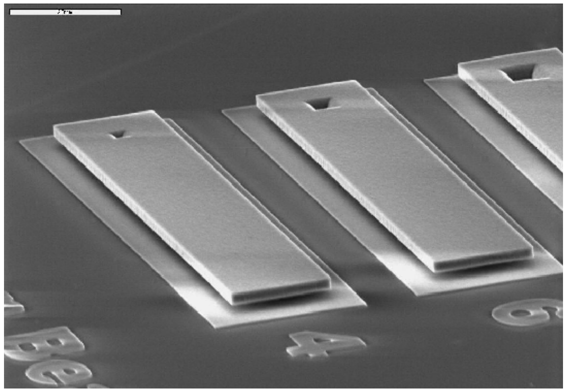
0.01 atm
~1 m/s

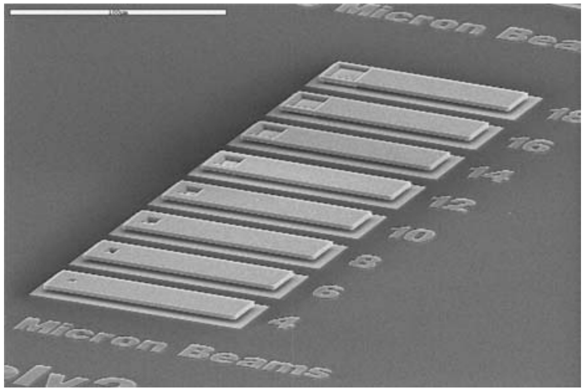


- DSMC microbeam simulations
- Steady gas motion is induced by temperature differences
  - *Not* buoyancy, *not* transient
- Noncontinuum effects cause motion
  - *Not* seen in NSSJ simulations

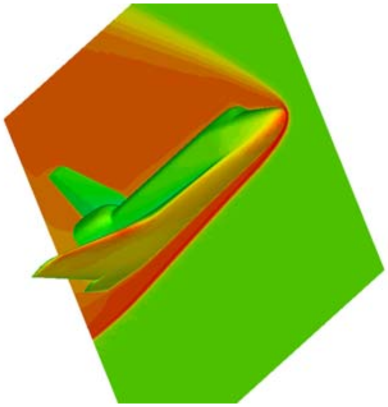
DSMC for Subsonic Flows

- Massively parallel (MP) implementation is the enabling technology for transient DSMC simulations
- 8000 processors (3 Tflop) for 24 hours is marginally adequate to simulate a few cycles of a 2-D microbeam oscillation
- Simulation of 3-D transient flow is projected to require about 10^3 times greater computational power (0.1-10 Pflop)

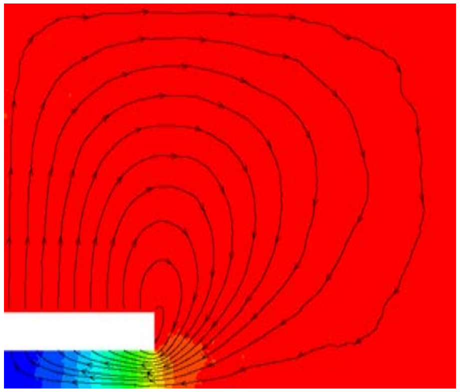




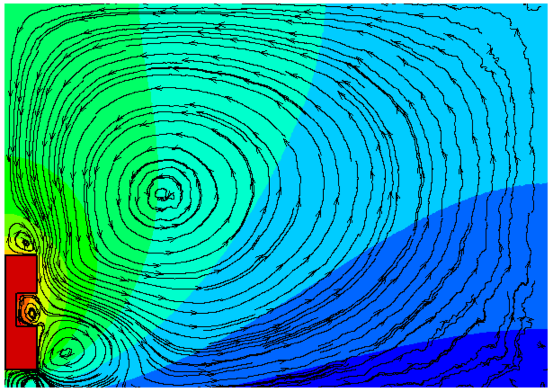
Summary



Hypersonic Vehicles



Moving microbeam



Heated microbeam

DSMC for Gas Dynamics

- **DSMC can be applied to almost any regime of gas dynamics, including low-pressure, microscale, or hypersonic gas flows.**
- **DSMC can offer physical insight to processes where physical, chemical, thermal non-equilibrium plays a role.**

DSMC for transient MEMS-type flows

- **Possible even with today's computational resources**
- **Computational effort remains high compared to continuum CFD**

Microscale devices cannot be designed using only macroscale tools

- **DSMC reveals true characteristics of microscale flow fields**
- **DSMC can be used to derive engineering models for designers**

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