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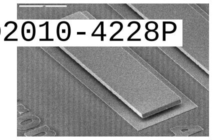

DSMC Moving-Boundary Algorithms for Simulating MEMS Geometries with Opening and Closing Gaps

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Sandia National Laboratories

Albuquerque, New Mexico

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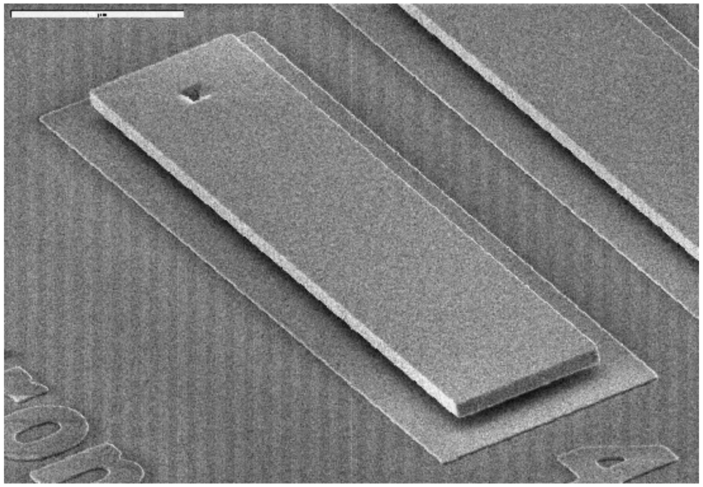
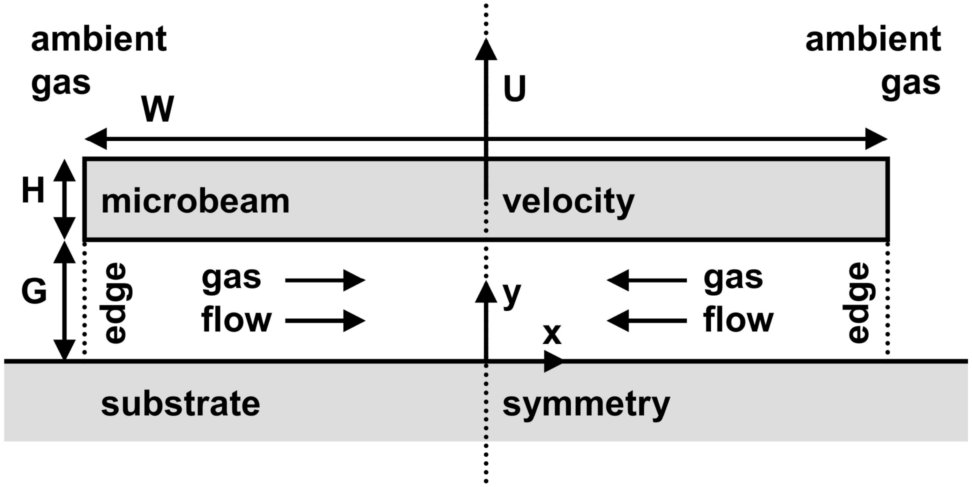
Motivation





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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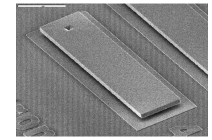
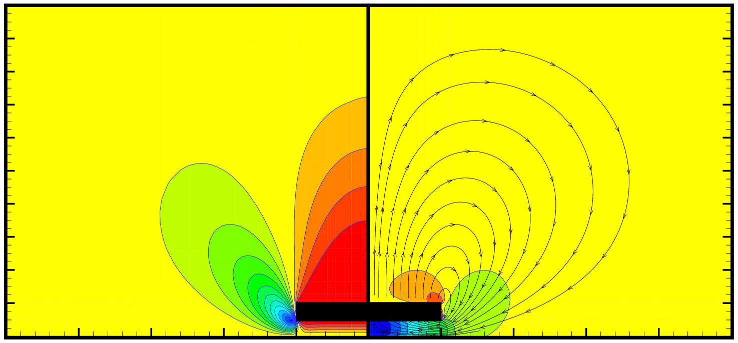
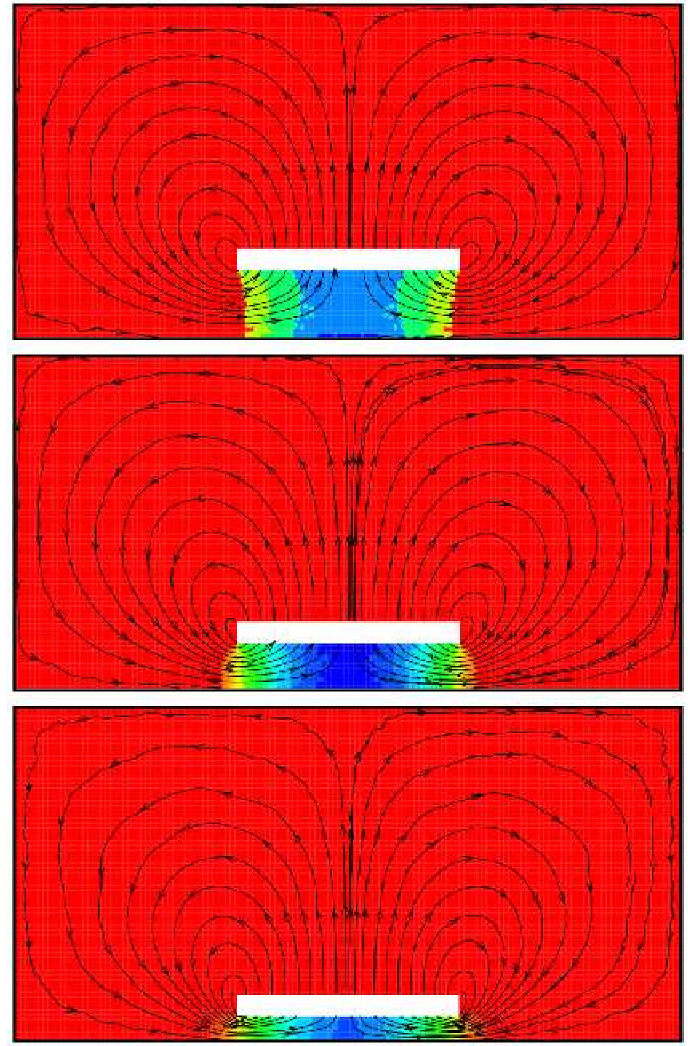


Previous Work



Alexeenko et al. (2006): Ellipsoidal Statistical



Gallis et al. (2003): Quasi-Static 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)
- **Kinetic model:** Ellipsoidal statistical, Alexeenko et al. (2006)

DSMC for noncontinuum gas with moving object

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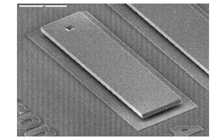
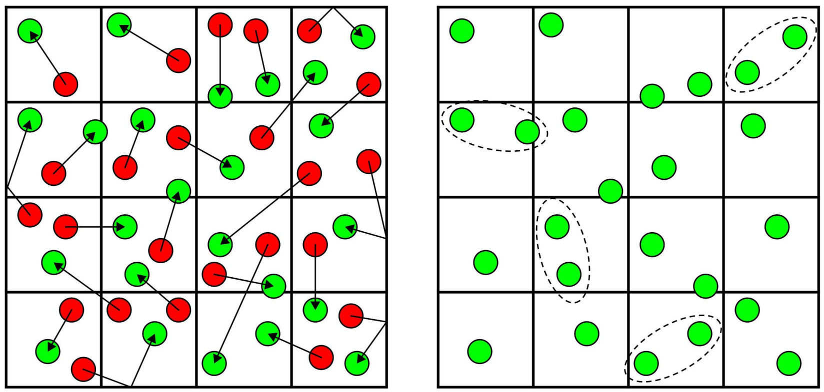
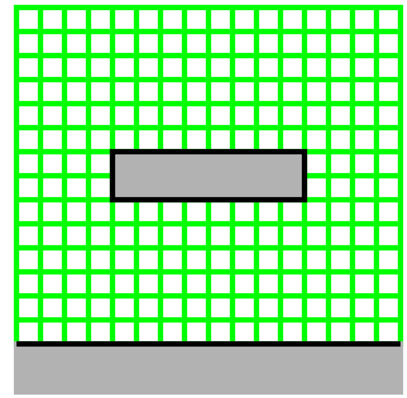


Current Approach



DSMC molecules move over mesh, collide within cells



Object moves over mesh

Direct Simulation Monte Carlo (DSMC) with moving object

- Object moves over mesh just like molecules do
- Molecules reflect from moving object (diffuse, specular)

Advantages and disadvantages

- Gas motion is inherently transient and noncontinuum
- Requires significant computational resources

Surface fluxes to object are most important quantities

- Gas force on object, gas energy transfer to object
- Can tolerate stochastic noise out in bulk gas

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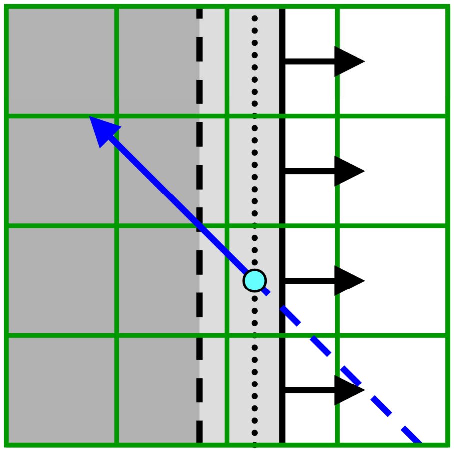
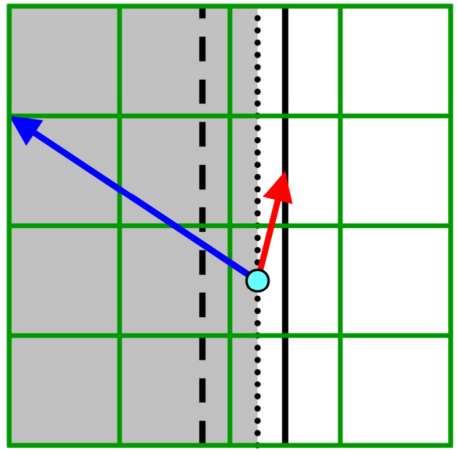
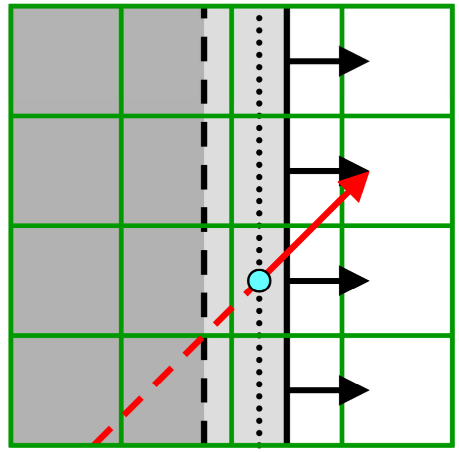
Rigorous Algorithm



mesh frame
incident molecule



object frame
ordinary reflection



mesh frame
reflected molecule

Reflection occurs where molecule and object paths intersect

- Molecule & object move with fixed velocities over time step
- Intersection point and remaining time are determined

Molecule reflection is performed in object reference frame

- Object velocity is subtracted from molecule velocity
- Reflected molecule velocity is selected (diffuse, specular)
- Object velocity is added to reflected molecule velocity

Molecule travels for remainder of time step

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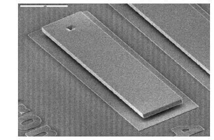
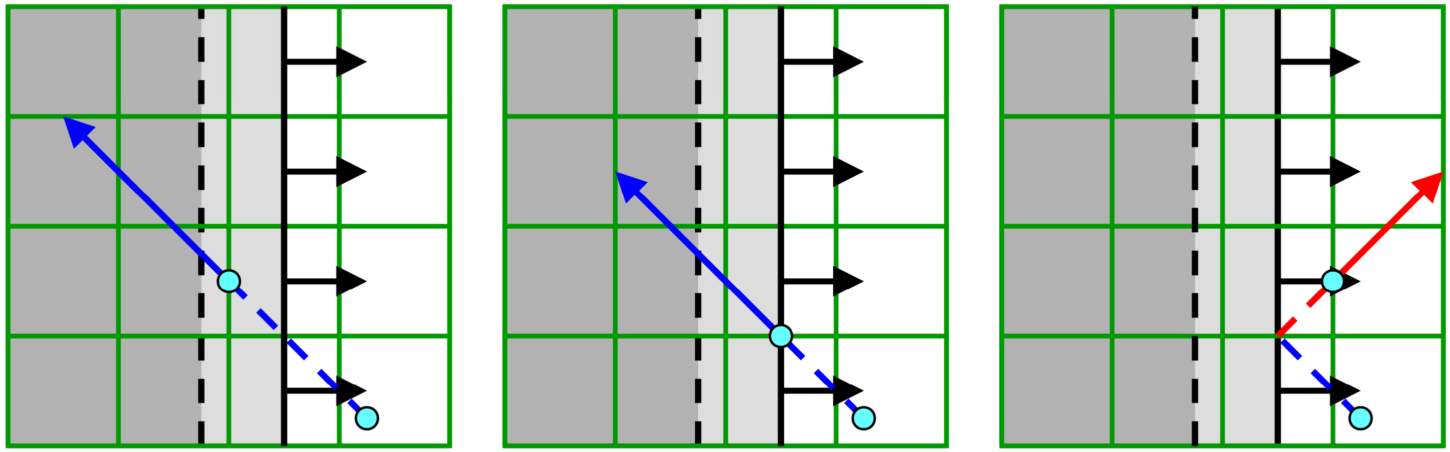


Approximate Algorithm



object & molecule move, overlap | intersect path with new object position | molecule reflects from new object

Reflection occurs from envelope of object over time step

- Advancing/receding: reflect from new/old object position
- Ensures that reflected molecule remains outside object

If object is slow w.r.t. molecules, approximate → rigorous

- Molecule's reflected velocity is same as rigorous algorithm

Advantages and disadvantages

- Faster than rigorous since reflection point is not calculated
- Positions of molecules near surface approximated

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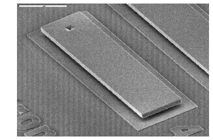
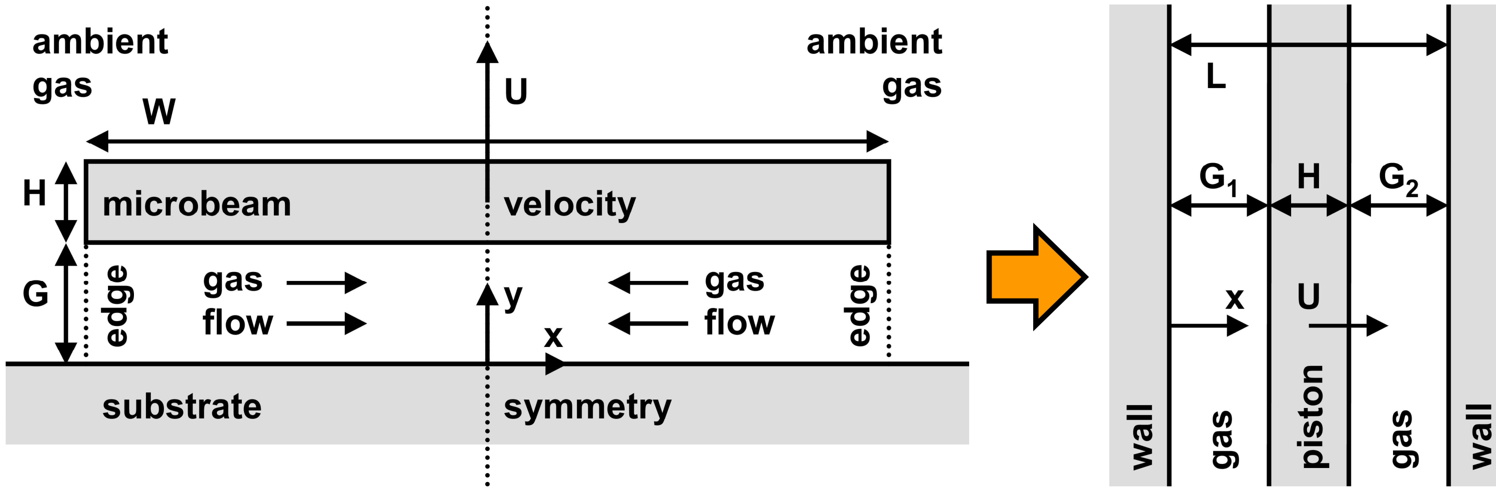


Simplified Geometry



Initially, implement/assess algorithms for simple geometry
- Need less computational resources, verification is easier

Replace 2D microbeam cross section with 1D piston
- Piston has opening and closing gaps like microbeam
- Molecule-surface intersection point is easy to determine
- Know early (wave) & long-time behavior for some cases

Prescribe piston position analytically for all time
- Piston velocity is constant over each time step: average
- Could couple piston motion to gas force

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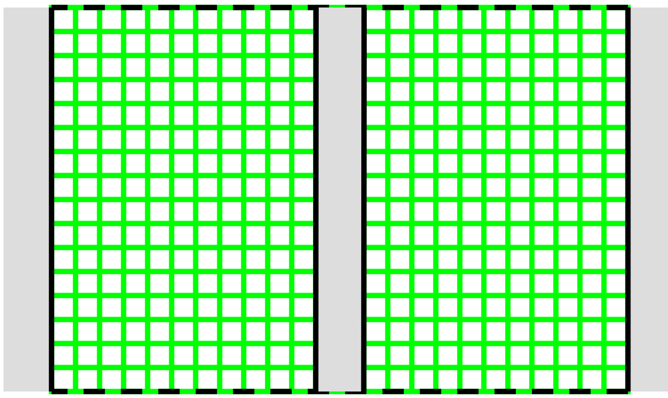
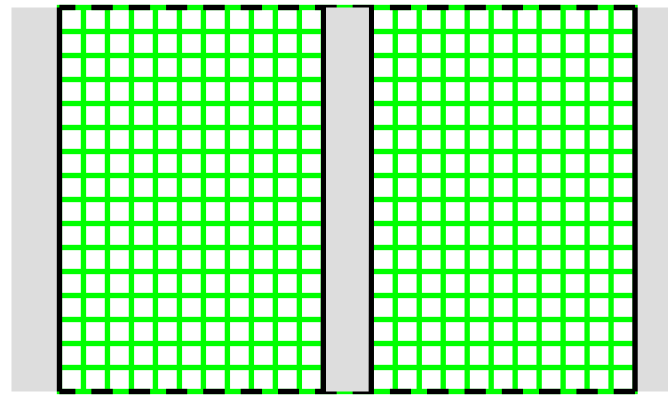
Piston Motion



Impulsively starts and stops



Sinusoidally oscillates continually

Simulation conditions

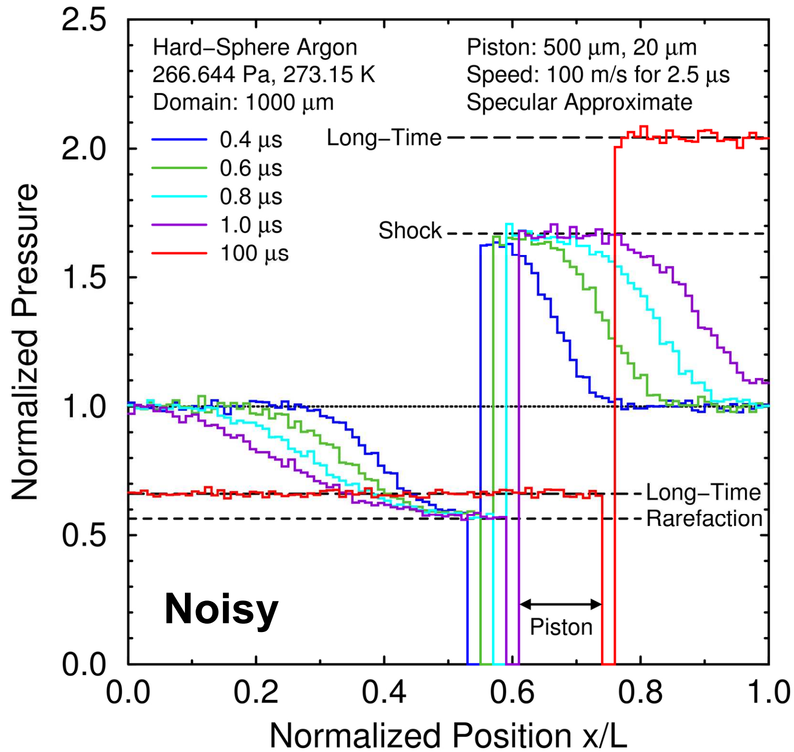
- Gas is hard-sphere argon at 266.644 Pa and 273.15 K
- Domain is 1000 μm, cells are 10 μm (100 cells)
- End walls are motionless, diffuse at 273.15 K
- Piston is 20 μm (2 cells), specular or diffuse at 273.15 K
- Time step is 1 ns, no averaging over multiple time steps
- Molecules per cell: 10^4 (“noisy”) or 10^5 (“smooth”, most)

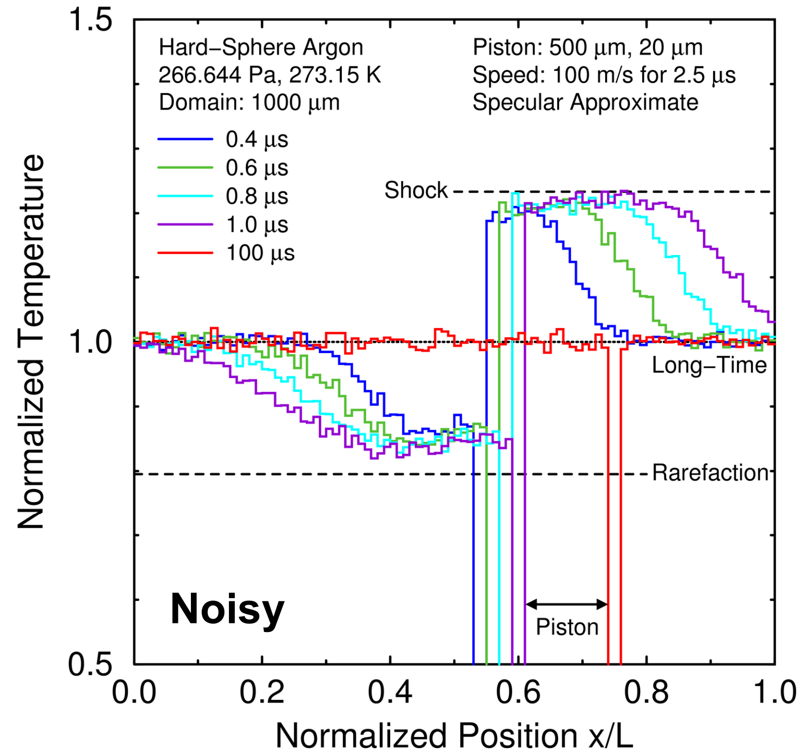
Case 1: starts at 50%, moves at 100 or 10 m/s, stops at 75%

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 Fast Specular Approximate





Excellent agreement with theoretical predictions

- **Shock pressure and temperature on compression side**
- **Rarefaction pressure and temperature on expansion side**
- **Long-time temperatures are the wall temperature**
- **Long-time pressures correspond to new volumes**

Noise is significant with 10^4 molecules per cell

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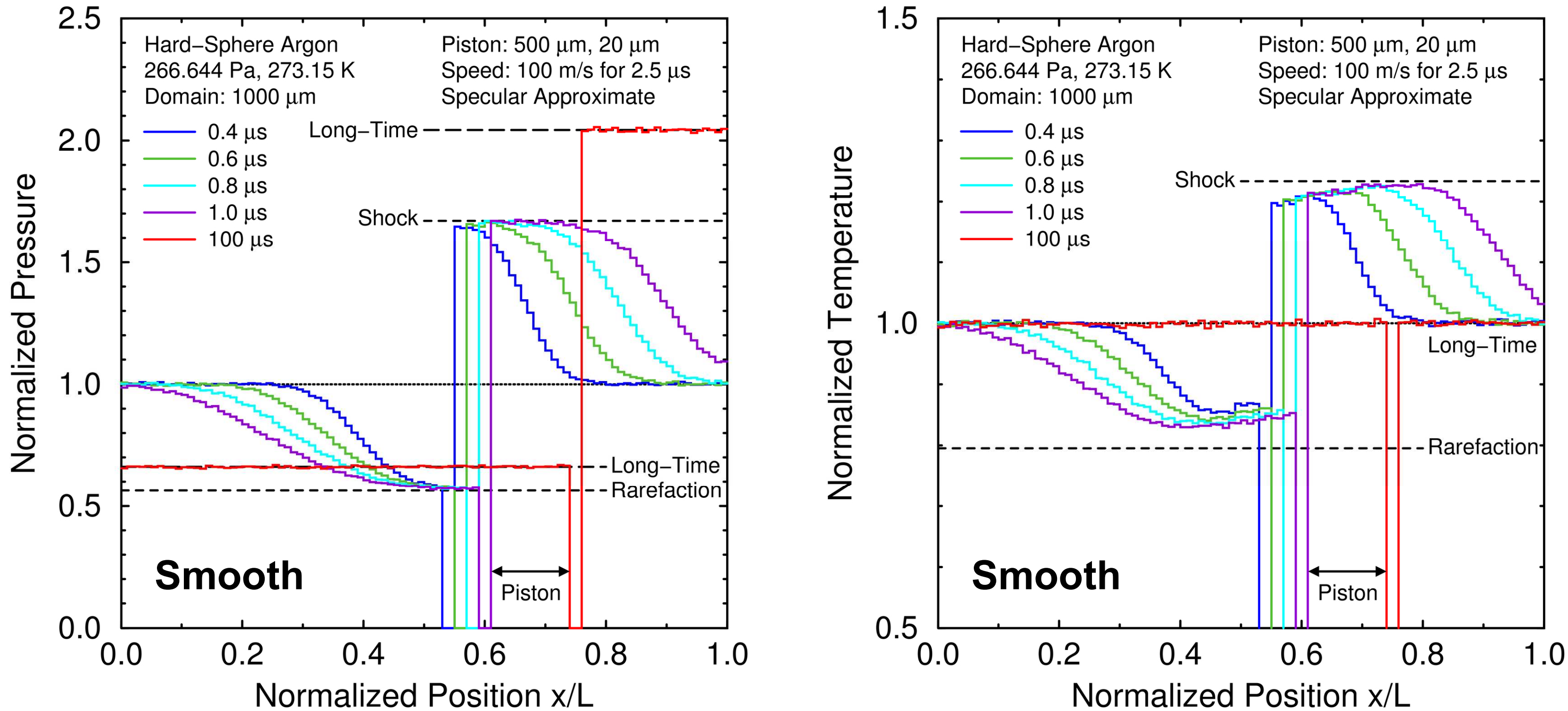
Impulsive Fast Specular Approximate



Excellent agreement with theoretical predictions

- **Shock pressure and temperature on compression side**
- **Rarefaction pressure and temperature on expansion side**
- **Long-time temperatures are the wall temperature**
- **Long-time pressures correspond to new volumes**

Noise is insignificant with 10^5 molecules per cell

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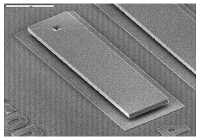
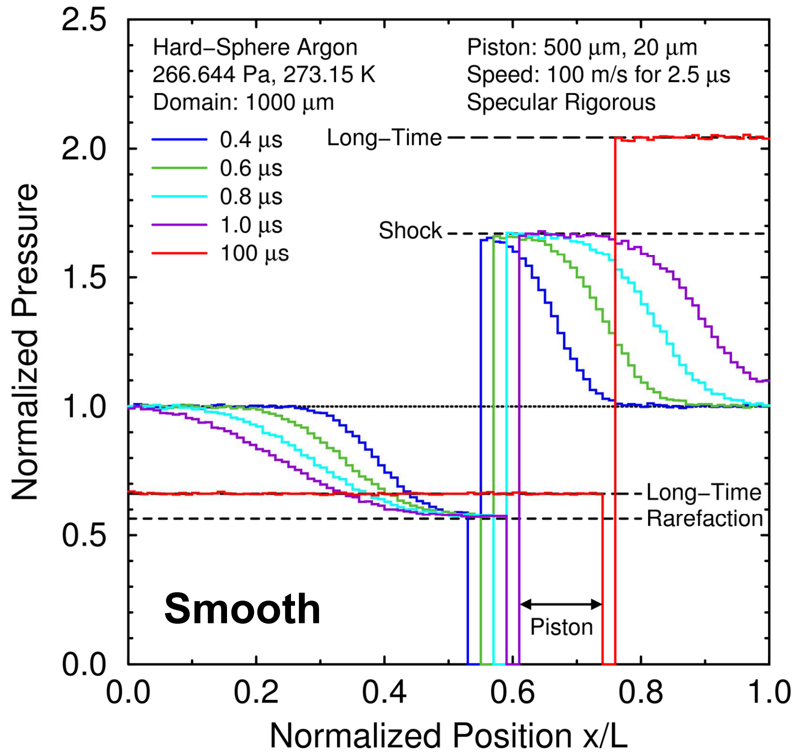
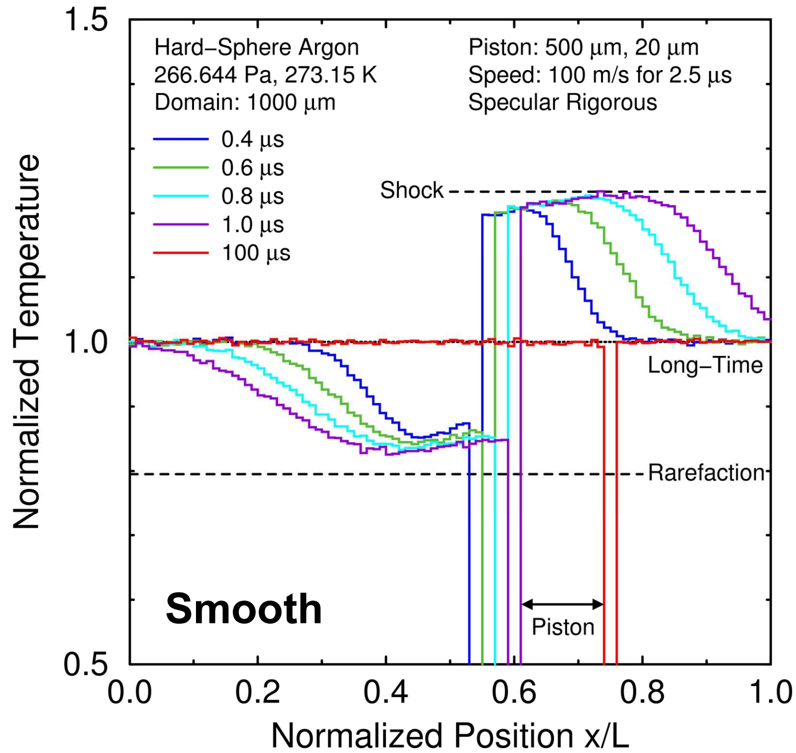
Impulsive Fast Specular Rigorous







Excellent agreement with theoretical predictions

- **Shock pressure and temperature on compression side**
- **Rarefaction pressure and temperature on expansion side**
- **Long-time temperatures are the wall temperature**
- **Long-time pressures correspond to new volumes**

Virtually same as approximate except for noise

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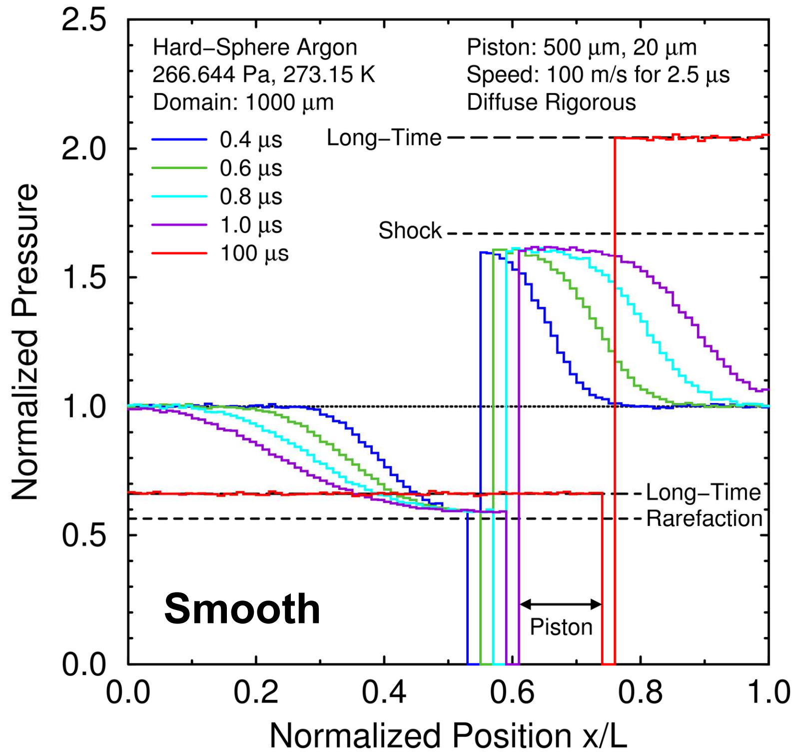
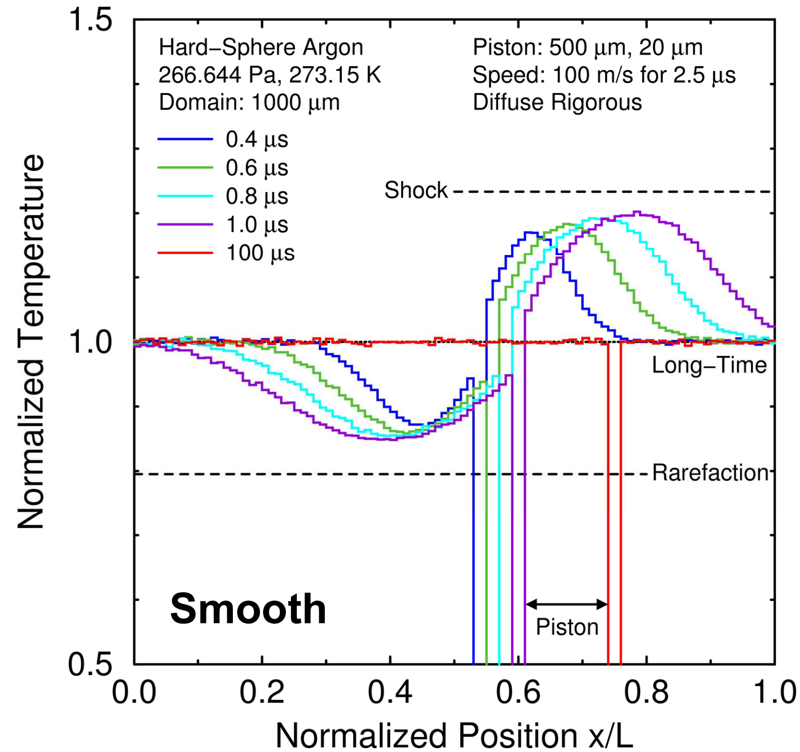
Impulsive Fast Diffuse Rigorous





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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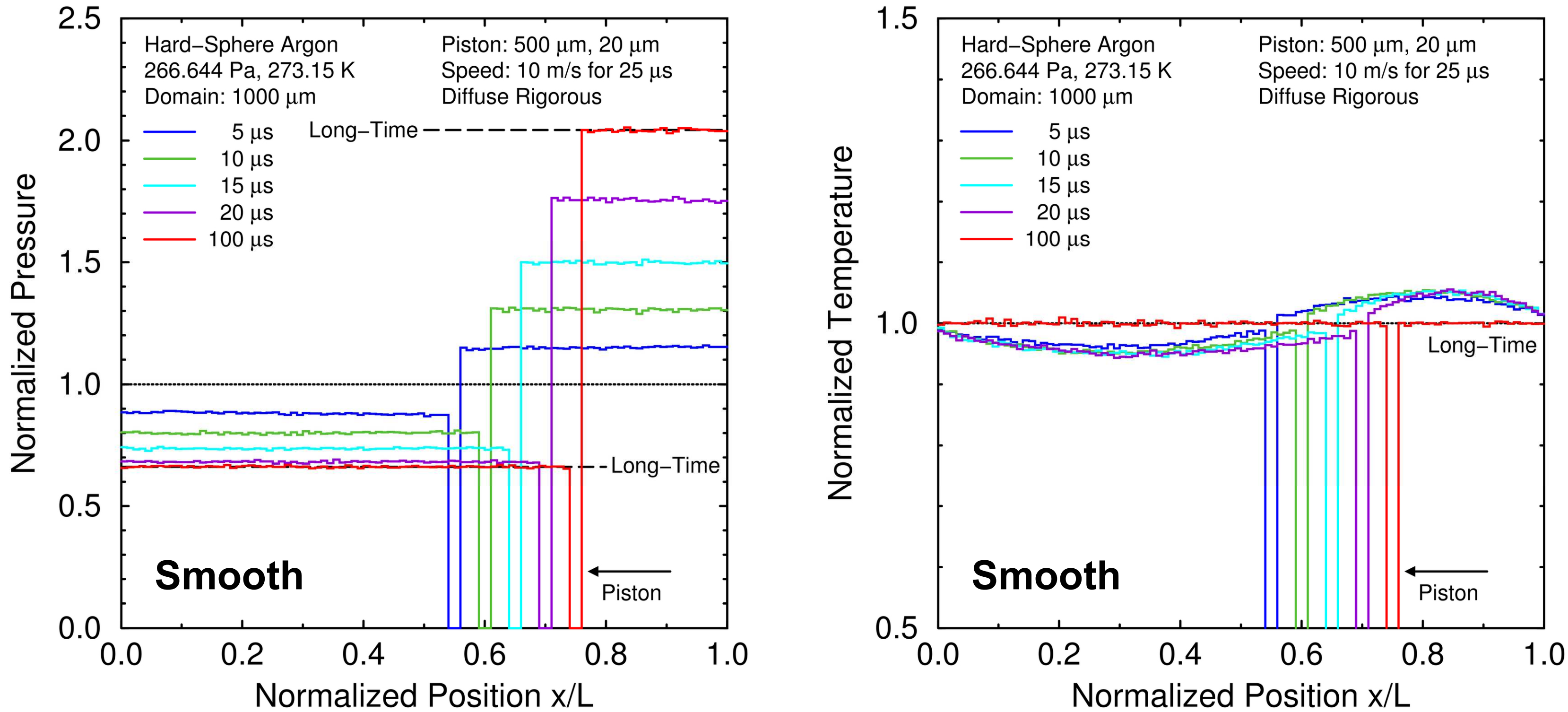
Impulsive Slow Diffuse Rigorous



Good agreement with theoretical expectations

- **Gas temperatures near piston are close to piston value**
- **Temperature jumps at piston and walls are small**
- **Pressures are spatially uniform, waves are negligible**
- **Long-time pressures and temperatures are as expected**

Qualitatively different from fast piston

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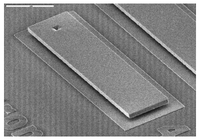
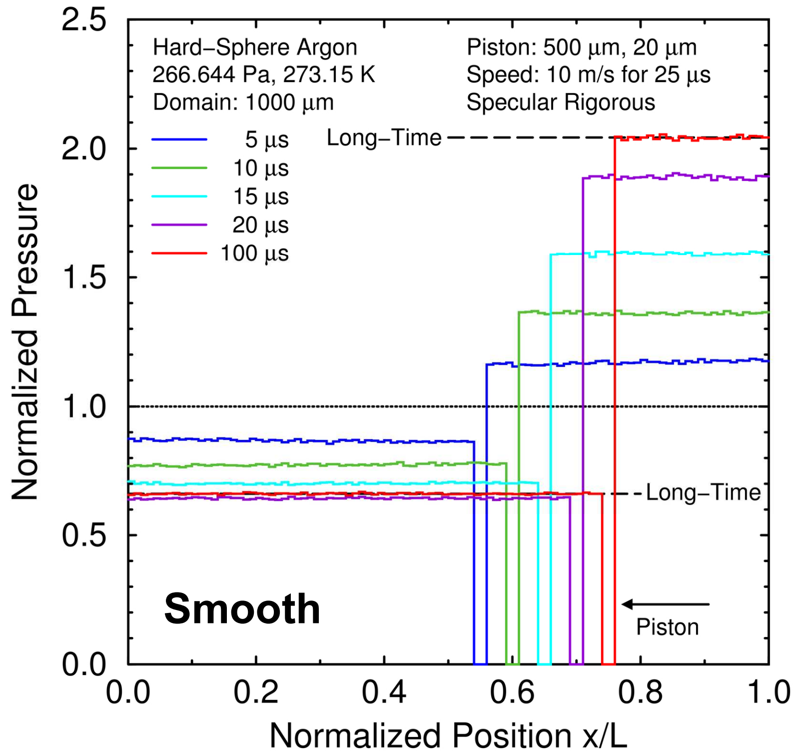
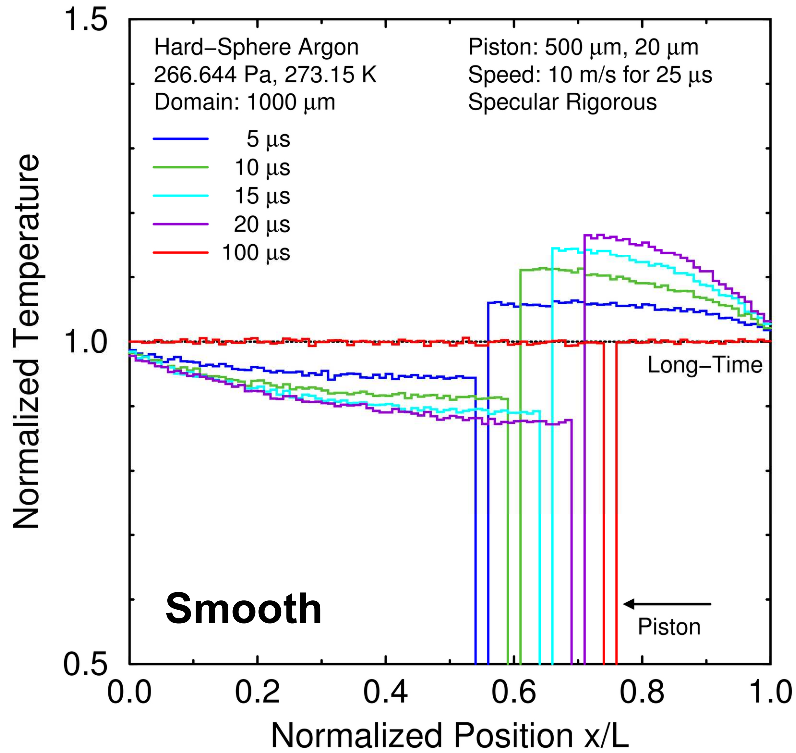
Impulsive Slow Specular Rigorous







Good agreement with theoretical expectations

- **Temperature gradients (heat fluxes) near piston are small**
- **Temperature jumps at walls are small**
- **Pressures are spatially uniform, waves are negligible**
- **Long-time pressures and temperatures are as expected**

Qualitatively similar to diffuse piston

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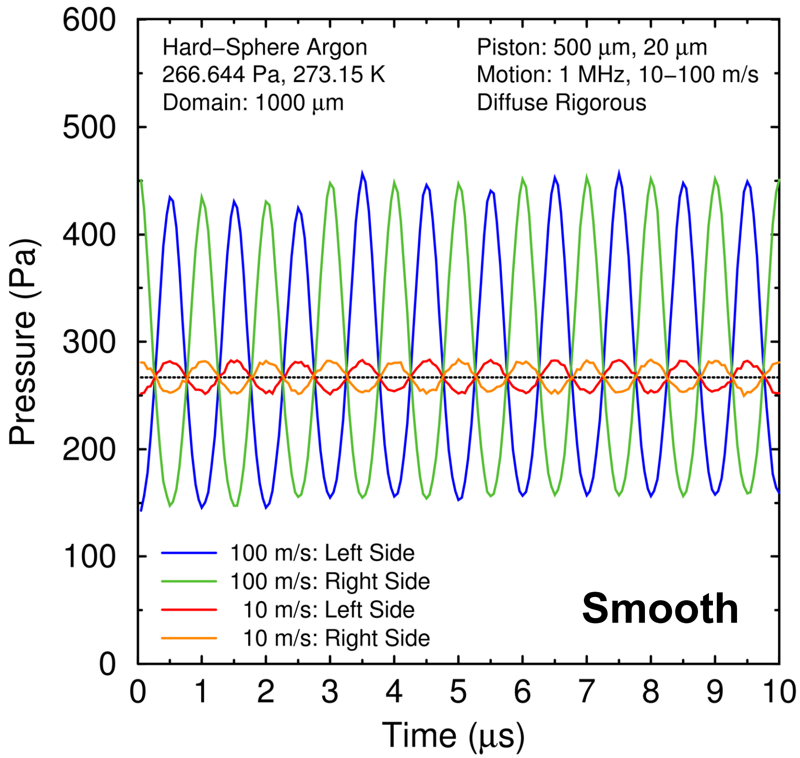
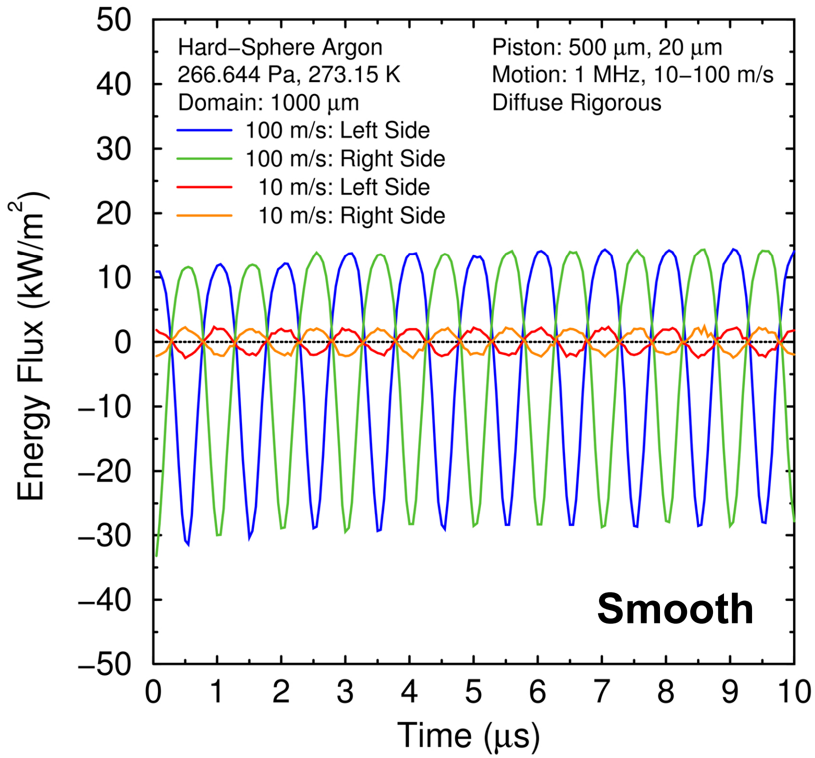
Oscillating Fast and Slow Diffuse





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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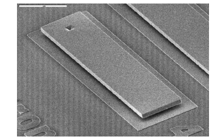
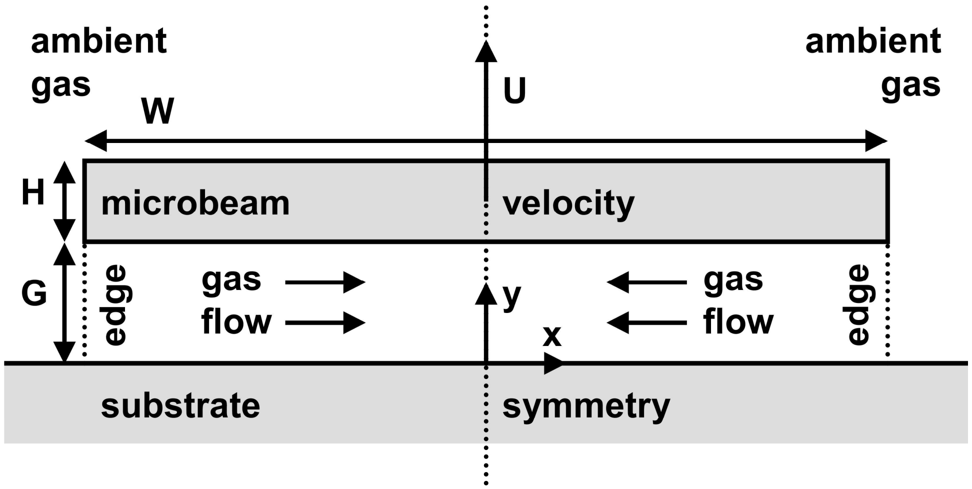
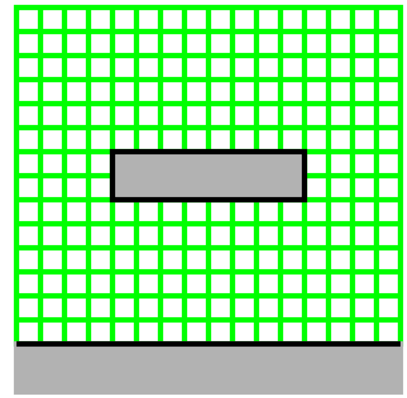


Conclusions and Future Efforts





Moving-boundary DSMC algorithms have been developed

- Implemented for 1D piston moving between end walls
- Rigorous and approximate results agree with theory

Future work will focus on 2D implementation

- Harder to find where object and molecule paths intersect
- Must maintain good scaling for massively parallel cases