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# DSMC Algorithms for Moving-Boundary Problems


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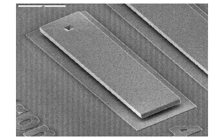
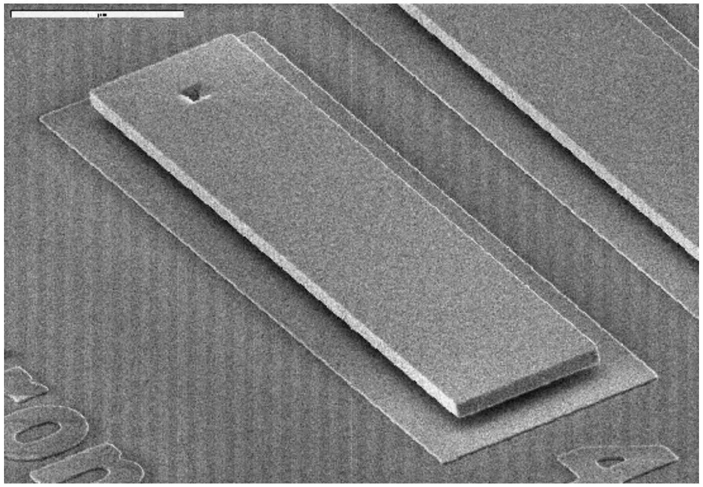
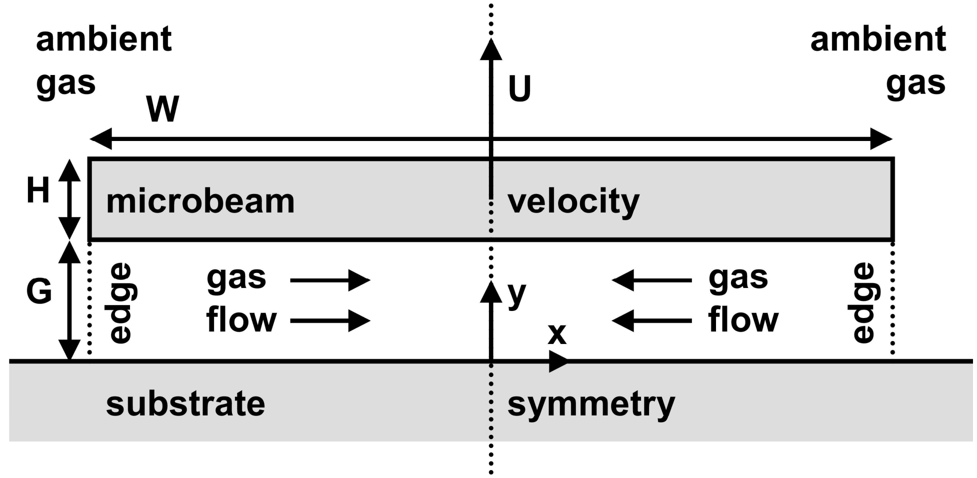
# Motivation








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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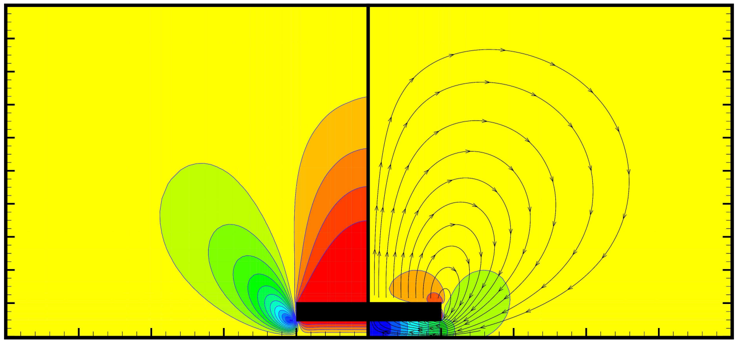
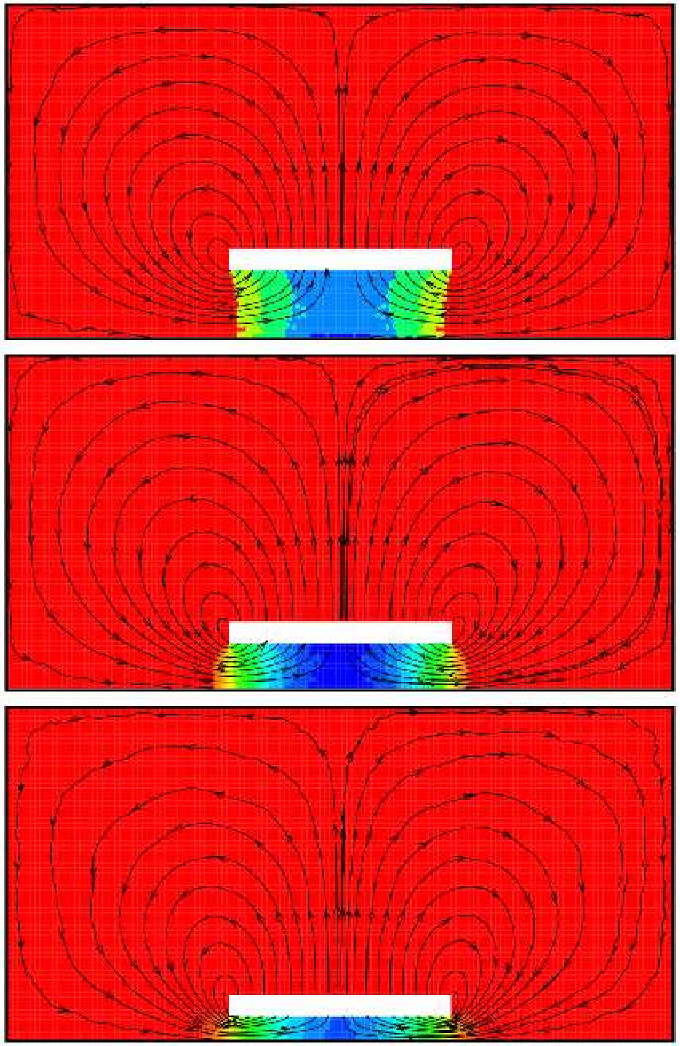
# Previous Work



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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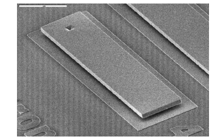
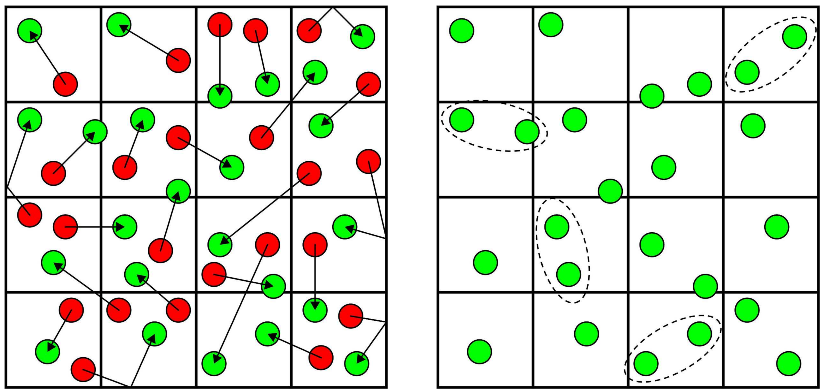
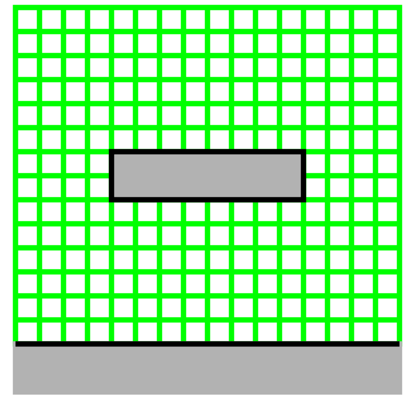


# Current Approach



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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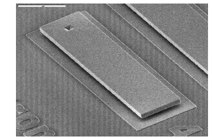
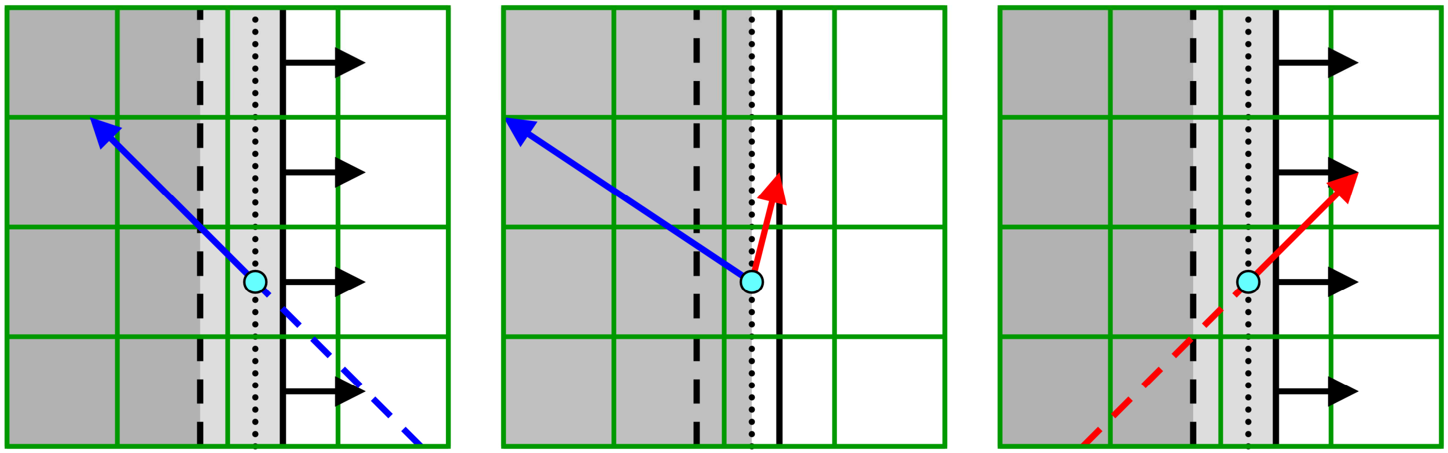
# Rigorous Algorithm





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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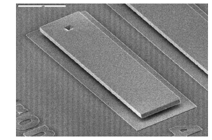
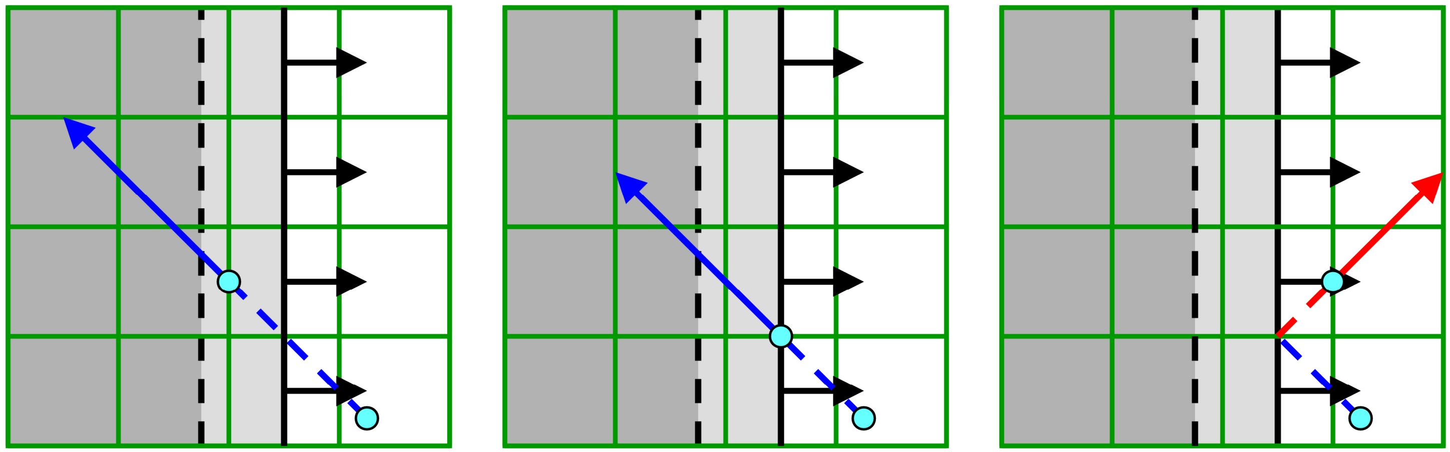


# Approximate Algorithm



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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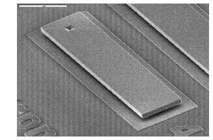
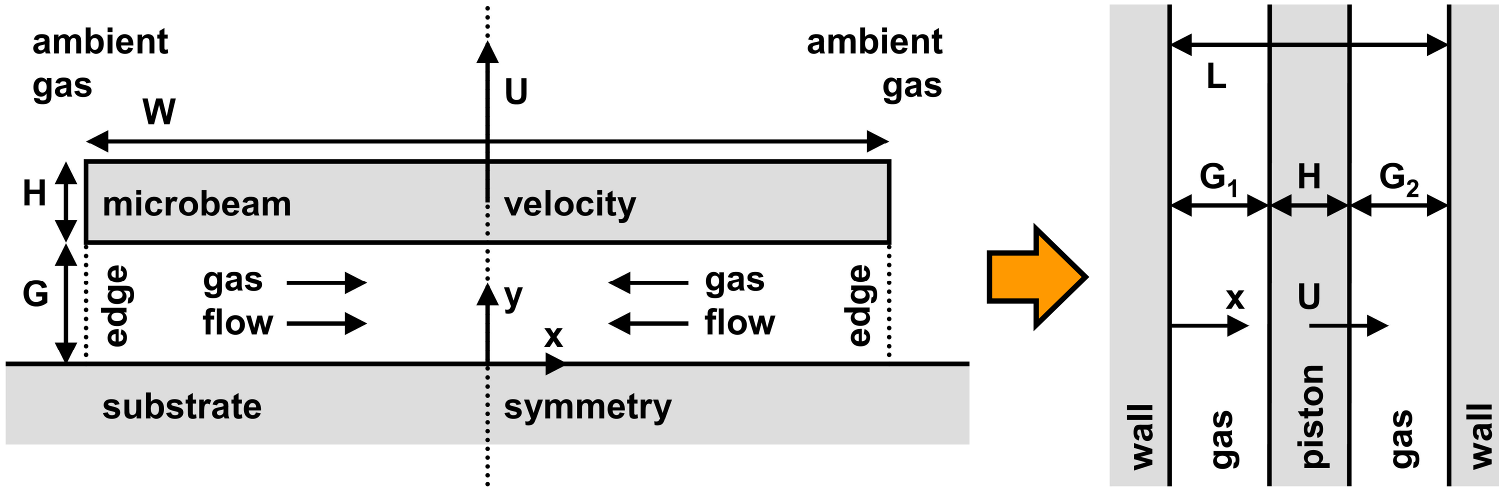


# Simplified Geometry




**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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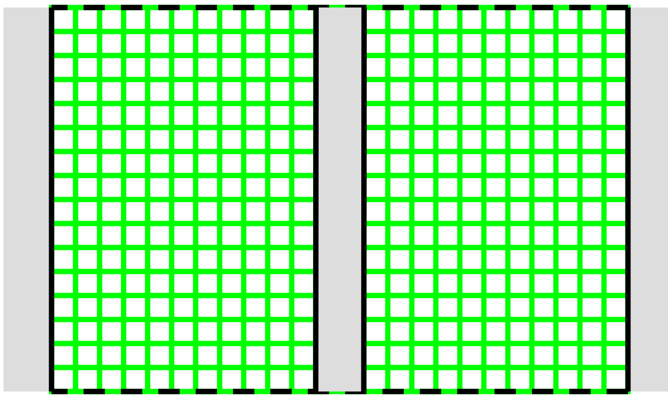
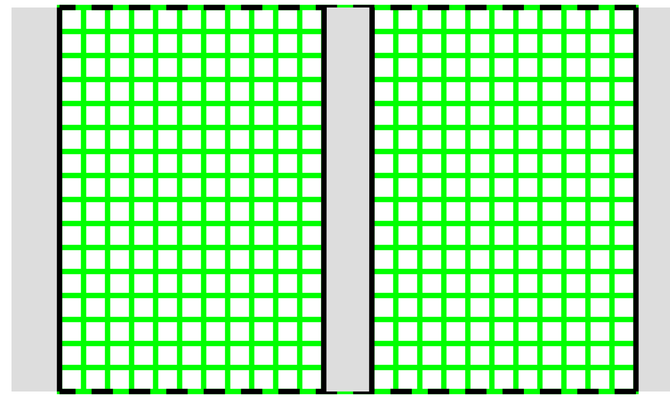
# Piston Motion



Impulsively starts and stops



Sinusoidally oscillates continually

## Simulation conditions

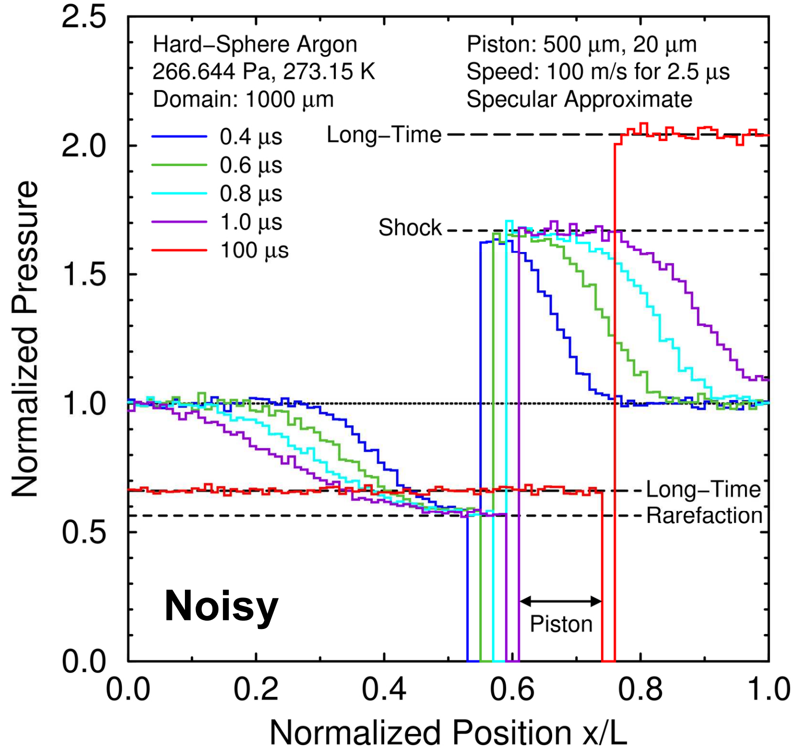
- Gas is hard-sphere argon at 266.644 Pa and 273.15 K
- Domain is 1000 μm, cells are 10 μm (100 cells)
- End walls are motionless, diffuse at 273.15 K
- Piston is 20 μm (2 cells), specular or diffuse at 273.15 K
- Time step is 1 ns, no averaging over multiple time steps
- Molecules per cell: $10^4$ (“noisy”)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

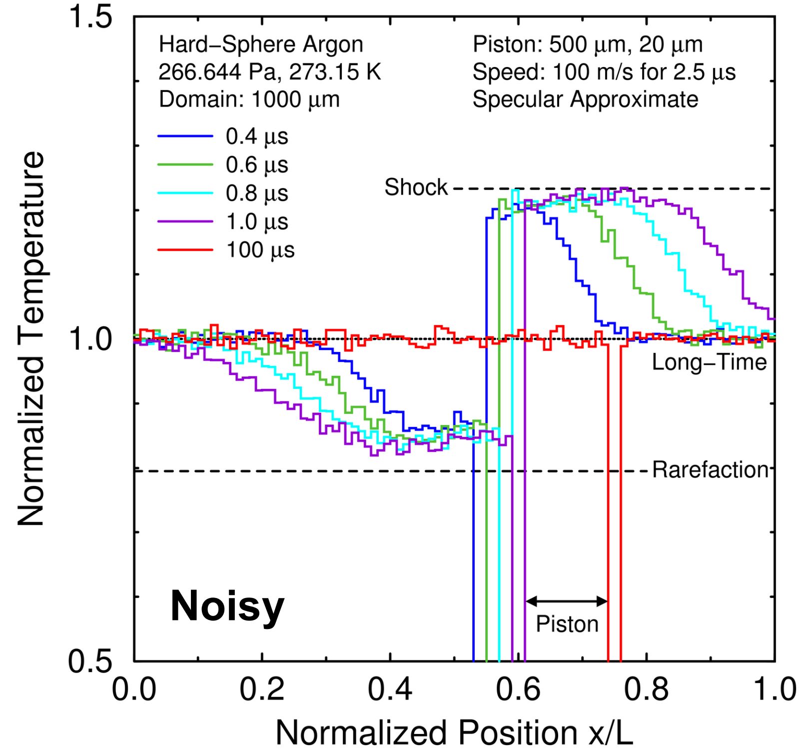
**Case 1:** starts at 50%, moves at 100 or 10 m/s, stops at 75%

**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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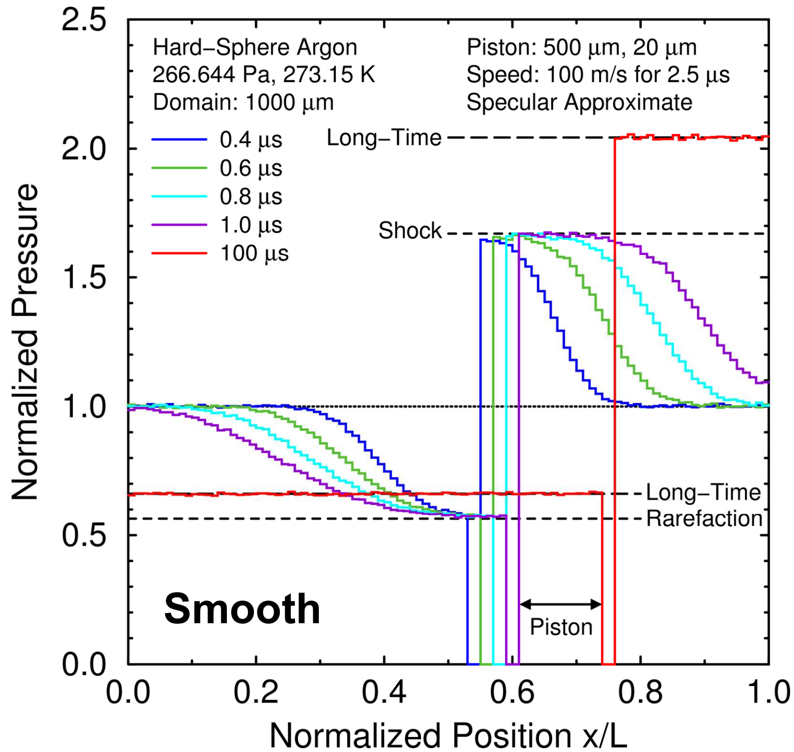
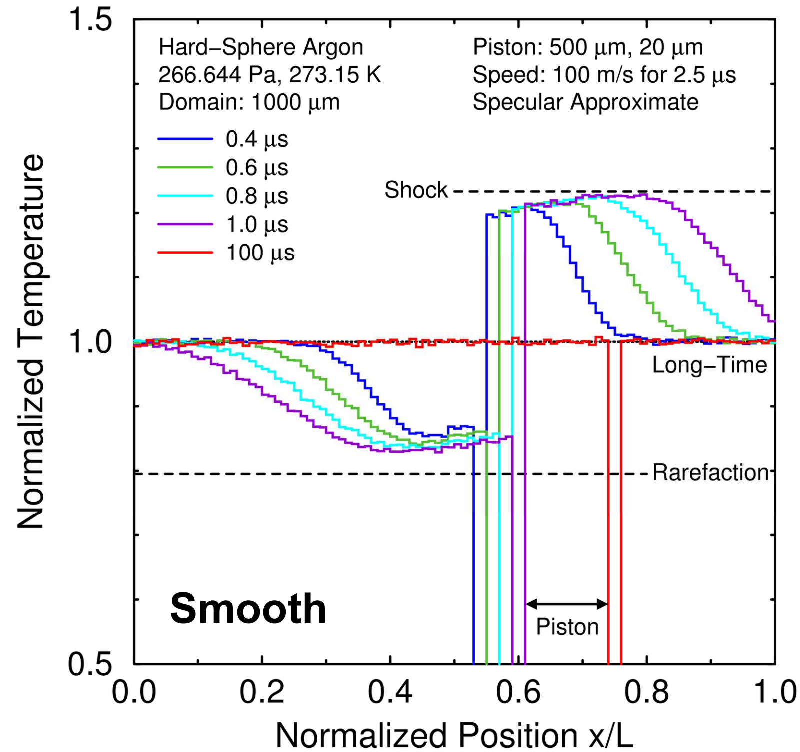
# Impulsive Fast Specular Approximate




**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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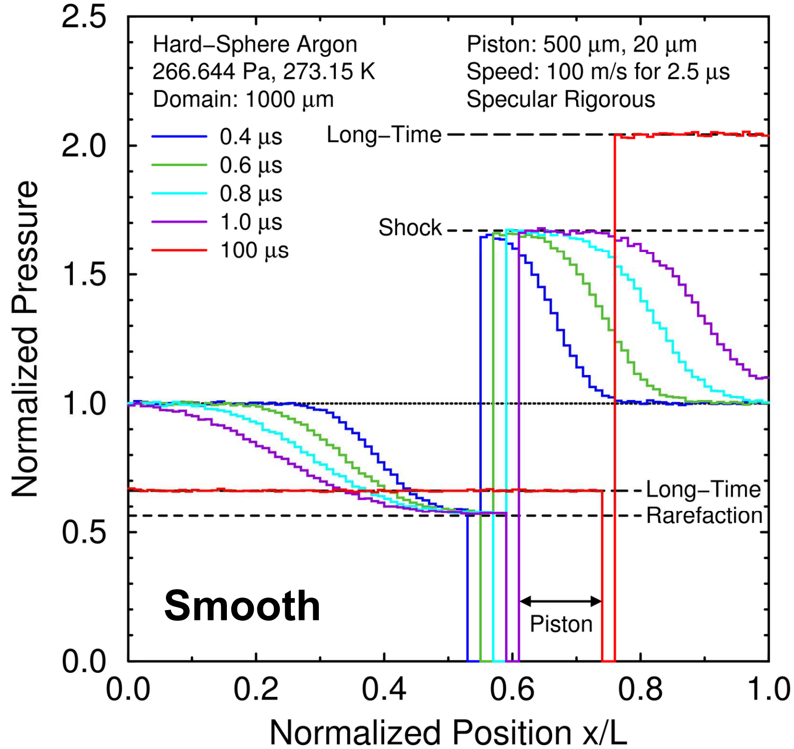
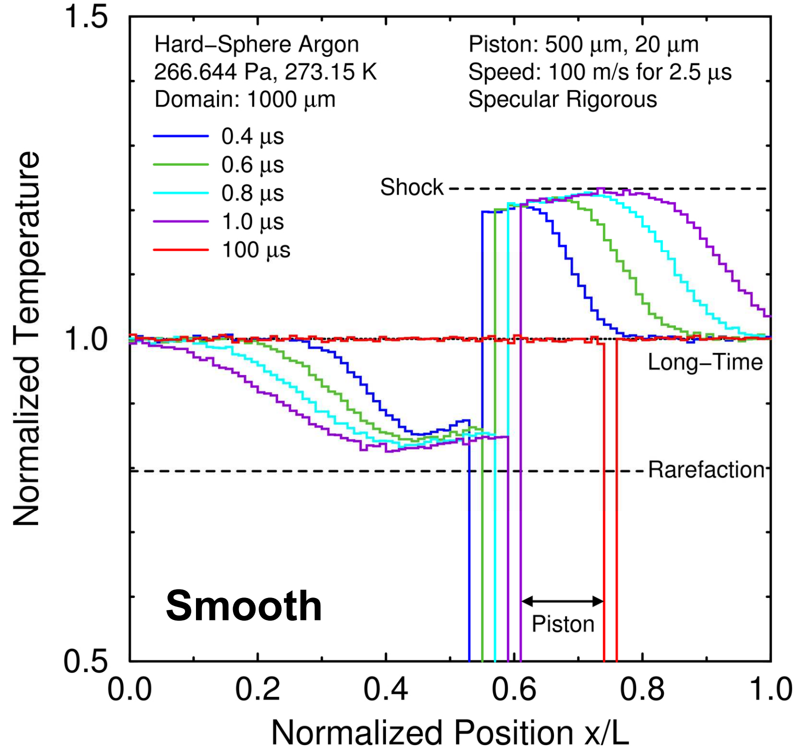
# Impulsive Fast Specular Rigorous




**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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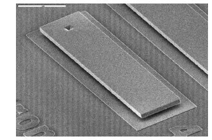
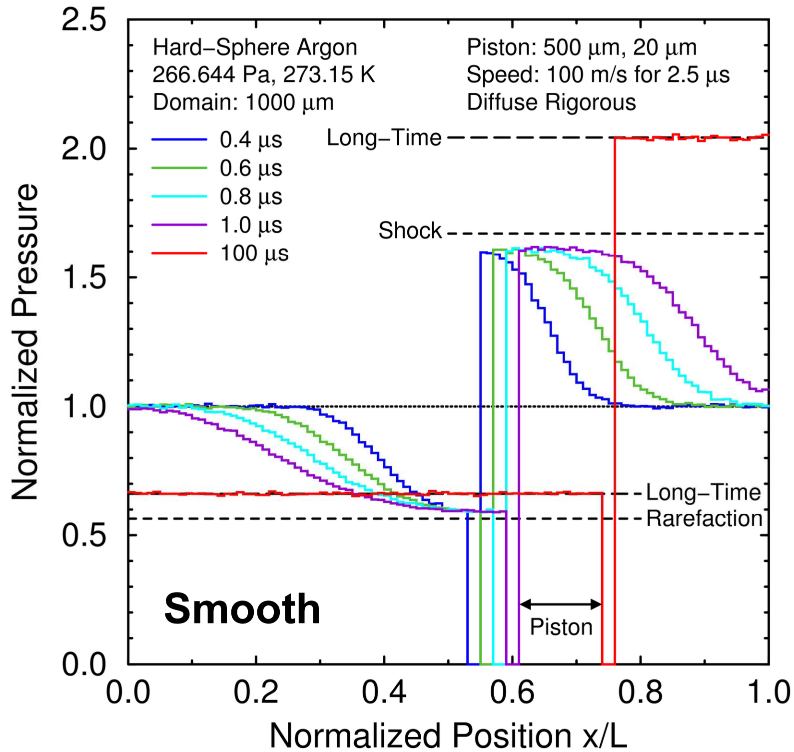
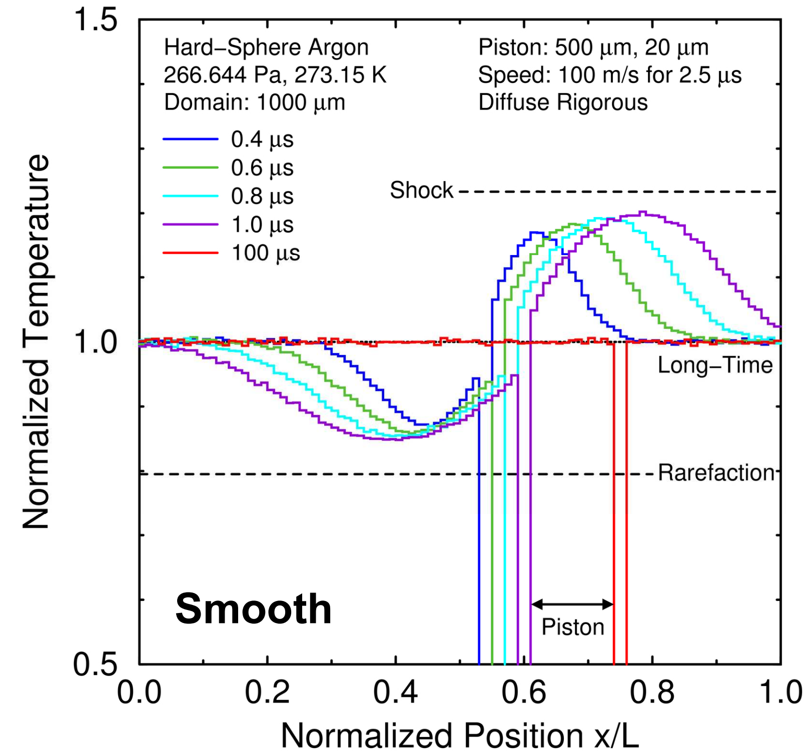


# Impulsive Fast Diffuse Rigorous




**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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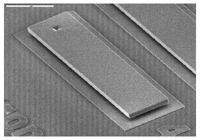
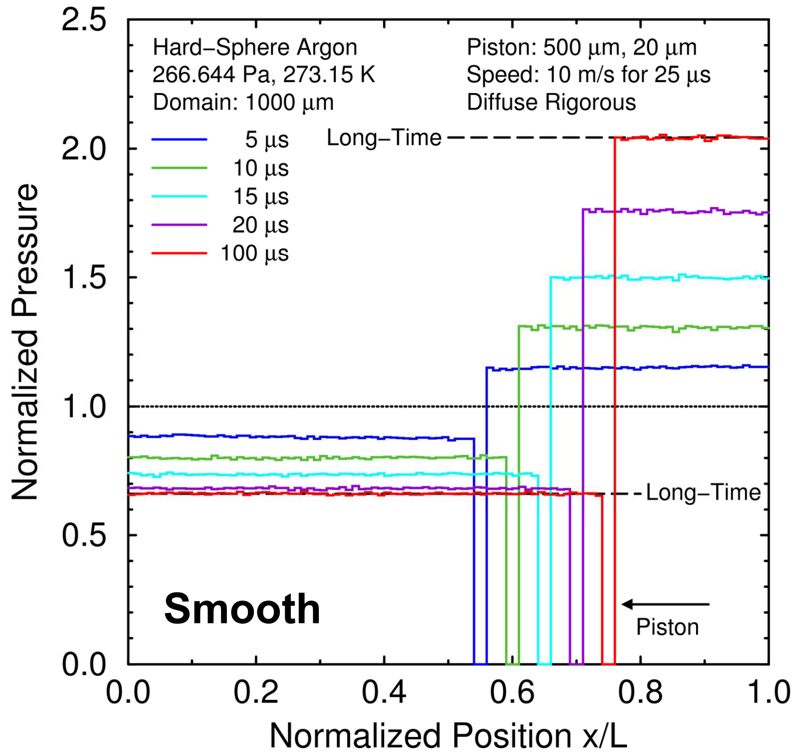
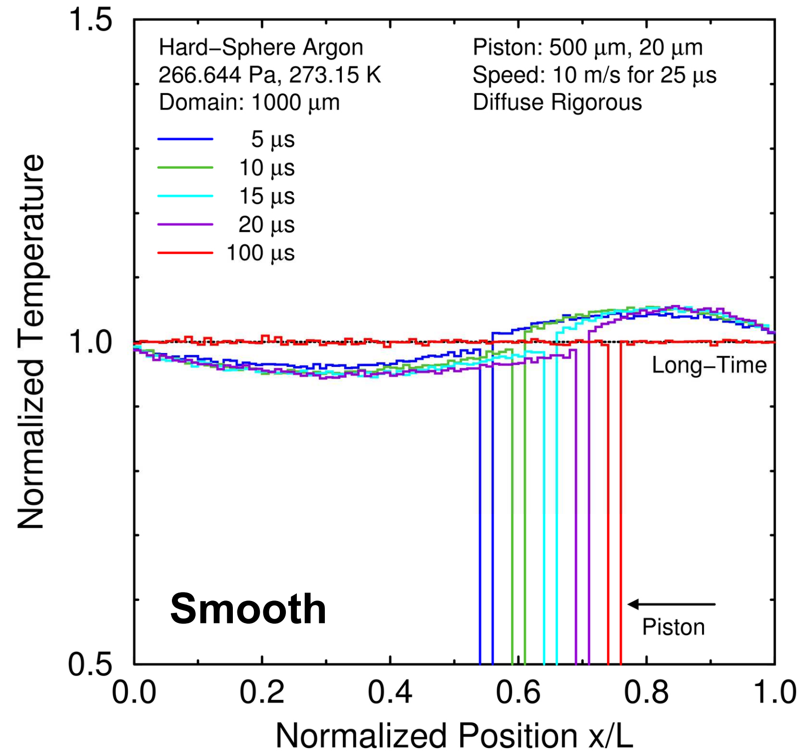
# Impulsive Slow Diffuse Rigorous






**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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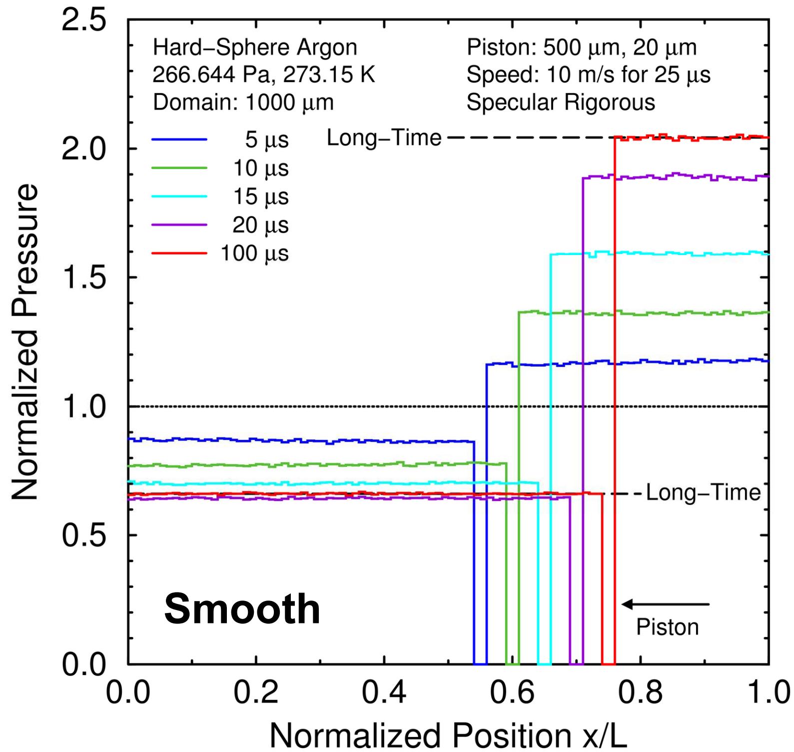
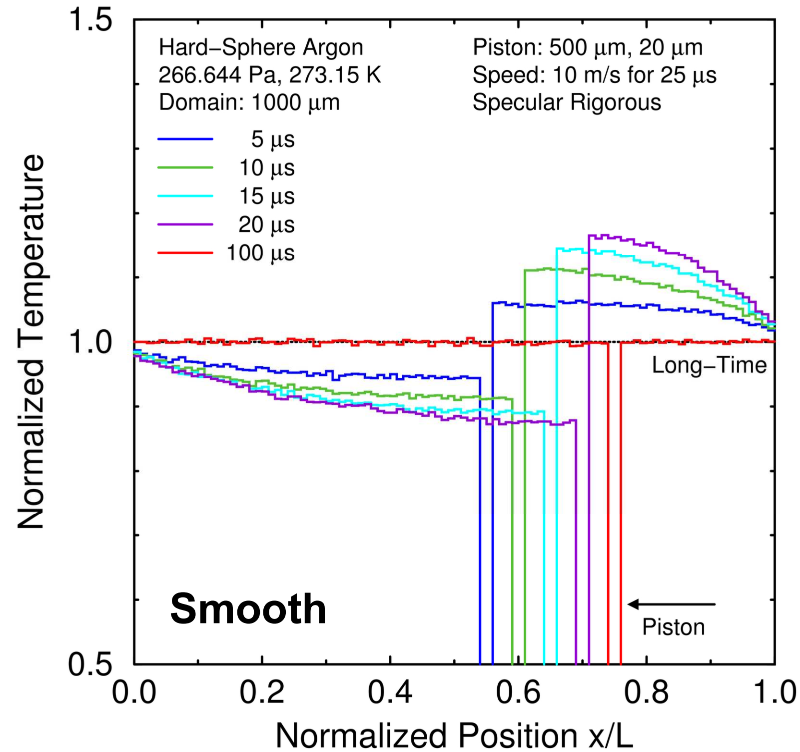
# Impulsive Slow Specular Rigorous




**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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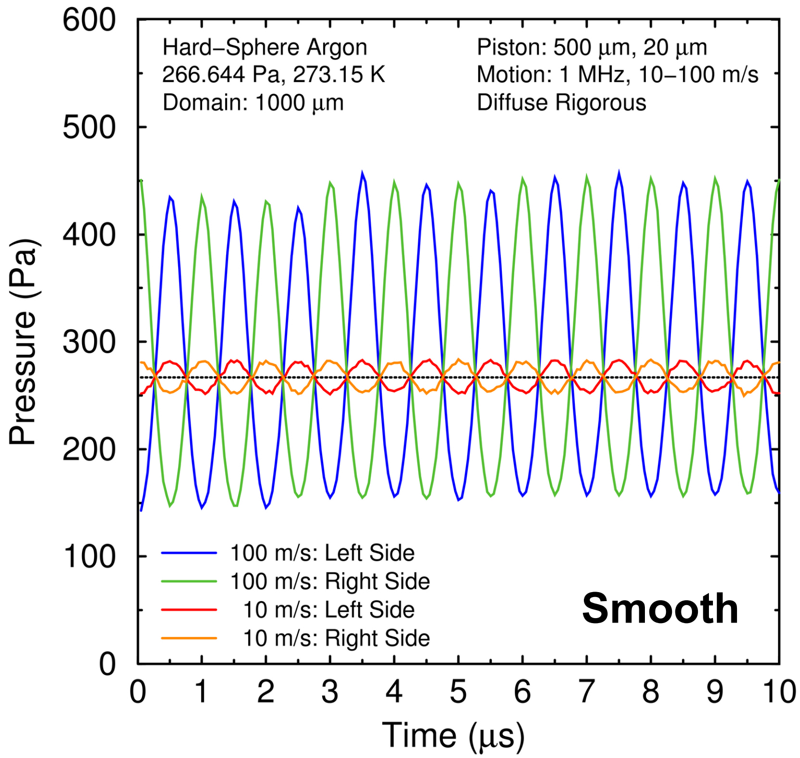
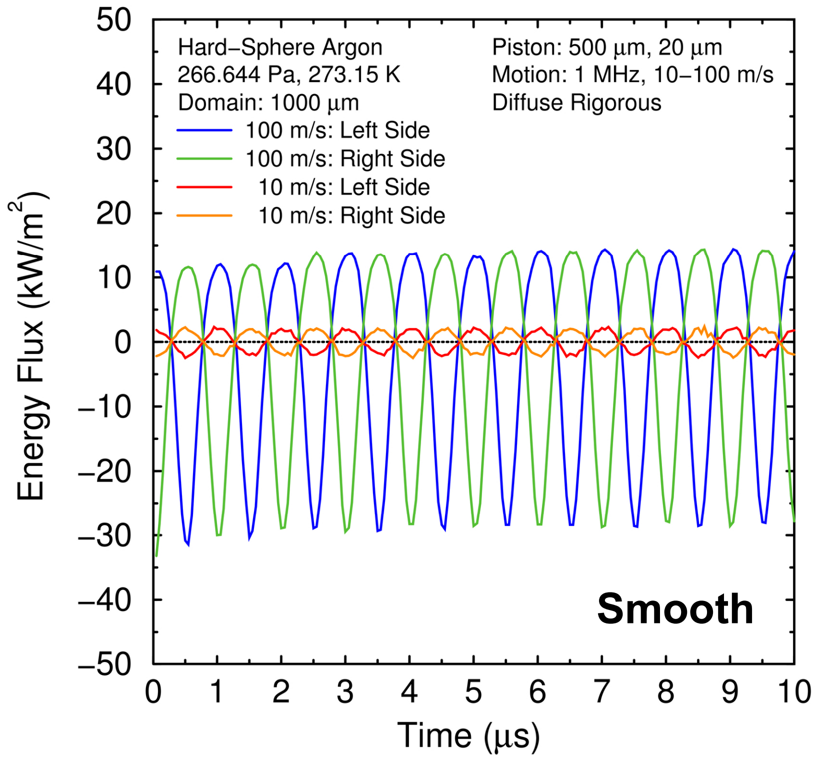
# Oscillating Fast and Slow Diffuse




**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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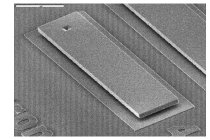
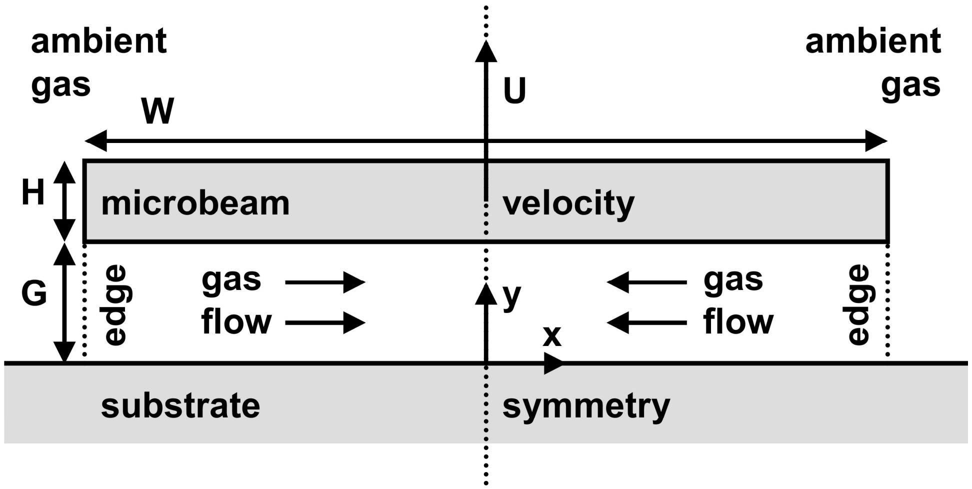
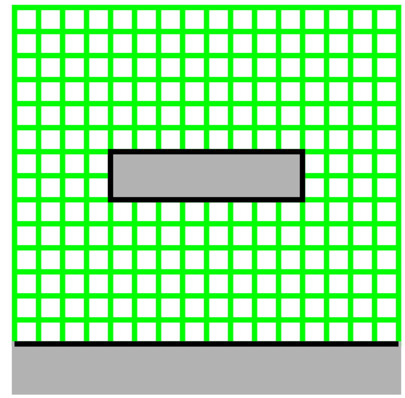


# Conclusions and Future Efforts



**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