

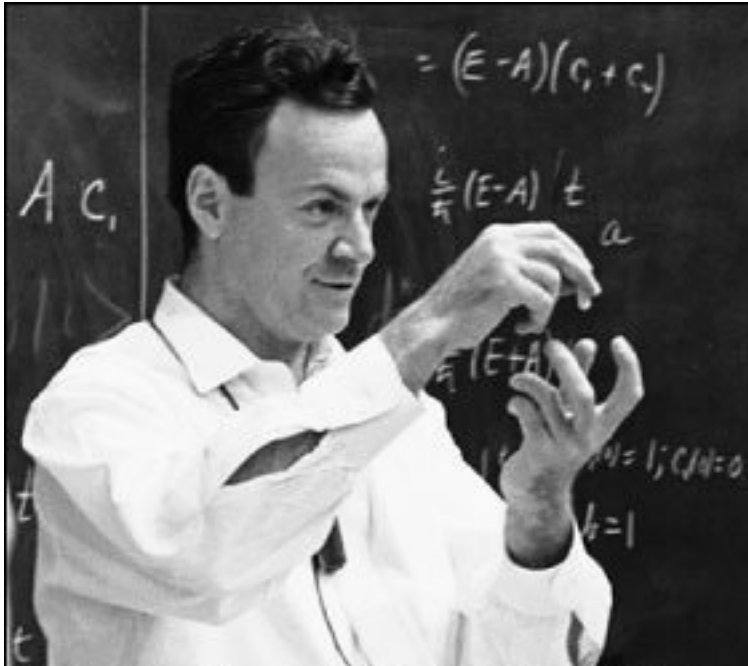


# **Rarefied Micro/Nanoflows: a brief tour**

**Alina Alexeenko**

*AAE, Purdue*

# All Science in 1 Sentence



Richard Feynman,  
*Six Easy Pieces*, Ch. 1

*I believe it is the **atomic hypothesis** that **All things are made of atoms—little particles that that move around in perpetual motion, attracting each other when they are a little distance apart, but repelling upon being squeezed into one another.***”

# Boltzmann Kinetic Equation

Kinetic Theory of Gases

Molecular Hypothesis

Classical Conservation Laws

Statistics

$$f = f(t, \vec{x}, \vec{u})$$



Ludwig Boltzmann, 1844-1906

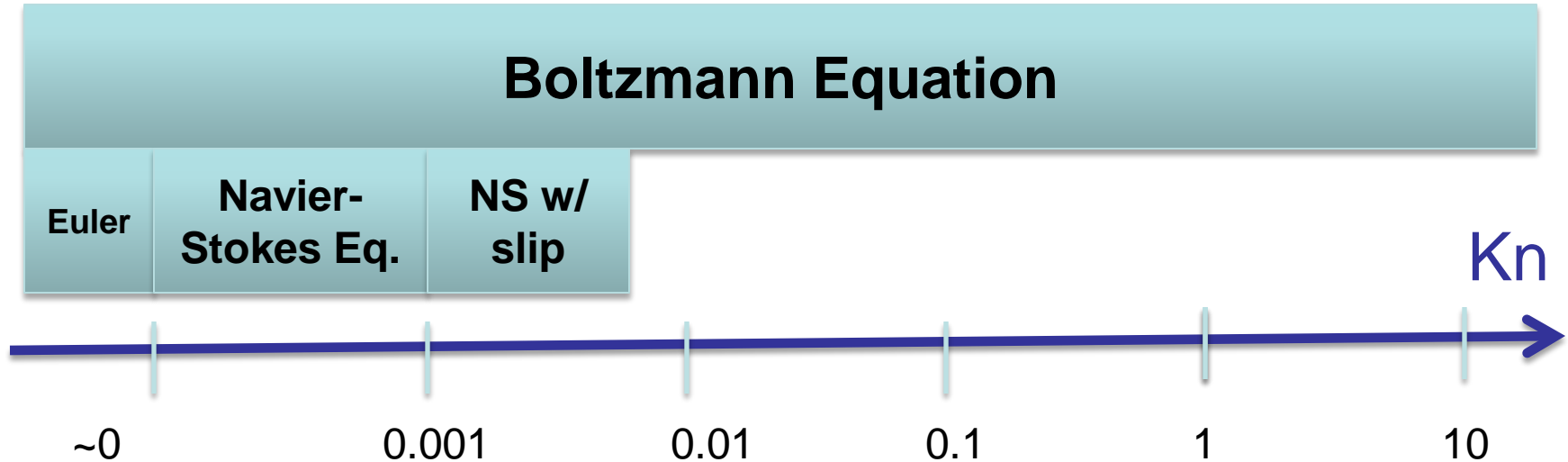
$$\frac{\partial(nf)}{\partial t} + \vec{u} \cdot \nabla_x(nf) + \frac{\vec{F}}{m} \cdot \nabla_v(nf) = n^2 \int_0^{4\pi} \int (f^* f_1^* - ff_1) |\vec{u}_r| \frac{d\sigma_T}{d\Omega} d\Omega d\vec{u}_1$$

Molecular Interaction Law

Purdue course **AAE590 Molecular Gas Dynamics** (Fall 2014; offered online)

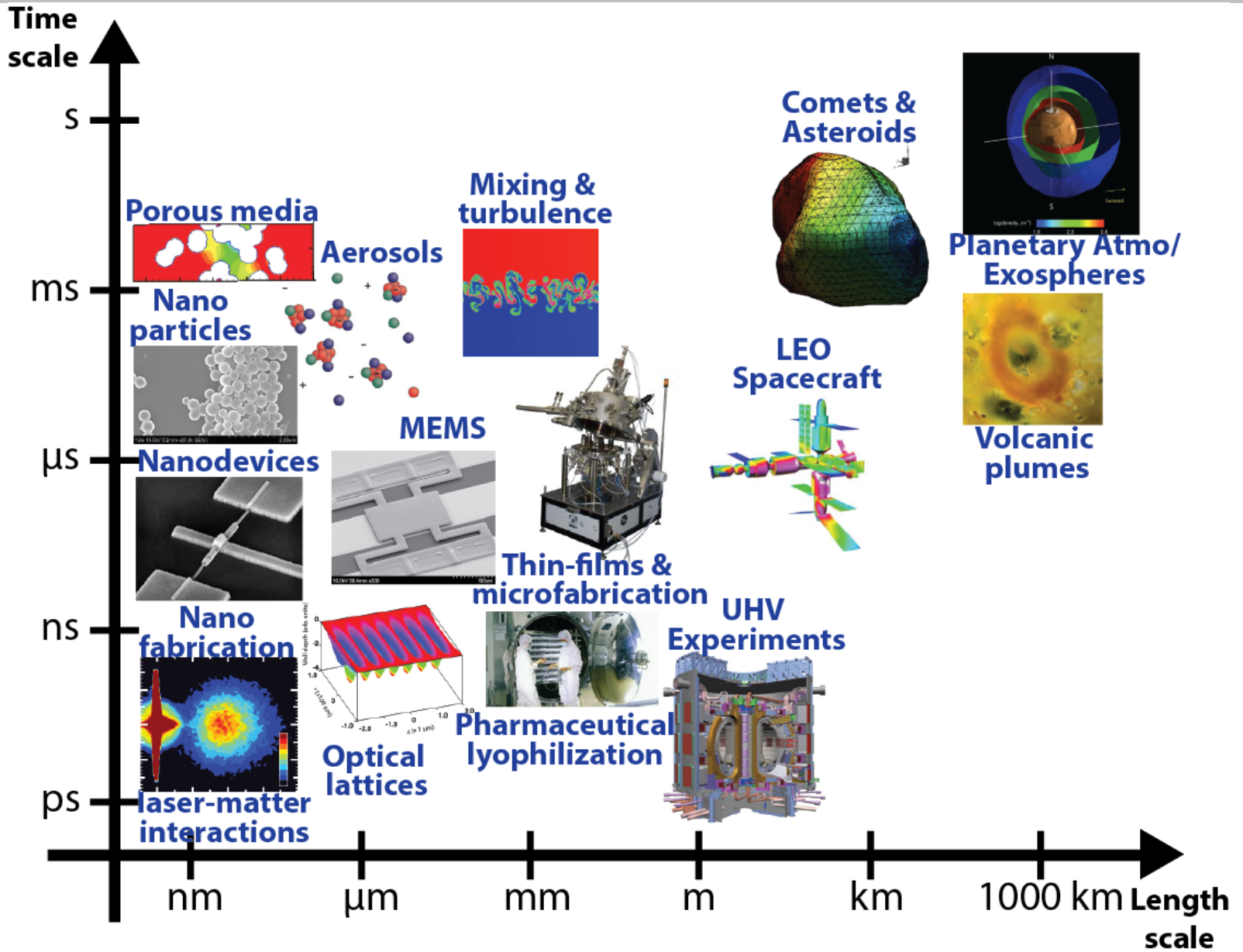
# Flow Rarefaction Regimes

Knudsen number:  $Kn = \frac{\lambda}{L}$



Mean free path calculator **Gas Dynamics Toolbox:**  
<http://web.ics.purdue.edu/~alexeenk/GDT/>

# Applications of Rarefied Gas Dynamics

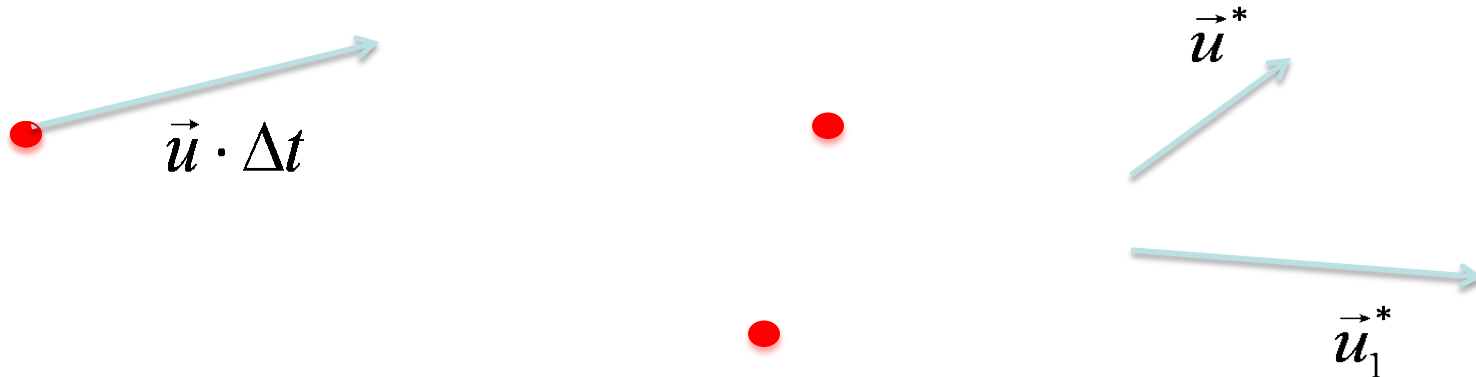


# Stochastic Simulation Method: DSMC

**Direct Simulation Monte Carlo (DSMC)** is a stochastic method to obtain solution of the Boltzmann equation governing the dilute gas flows in molecular regime:

$$\frac{\partial(nf)}{\partial t} + \vec{u} \cdot \nabla_x(nf) = n^2 \int_0^{4\pi} \int (f^* f_1^* - ff_1) |\vec{u}_r| \frac{d\sigma_T}{d\Omega} d\Omega d\vec{u}_1$$

*Free flight* *Binary molecular collisions*



Input: geometry; boundary conditions (thermal, evaporation/condensation);  
molecular interaction model !!

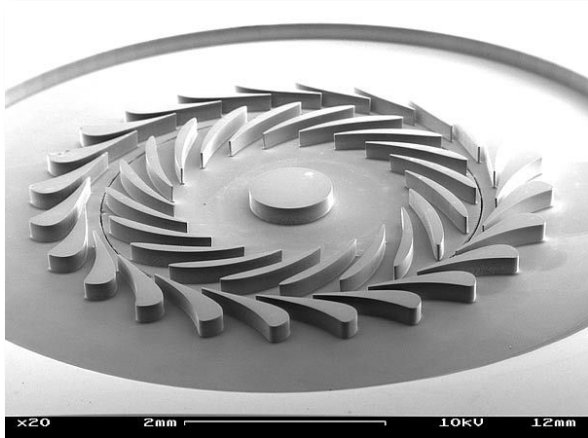
# Deterministic Approach: ES-BGK

Unsteady Boltzmann model kinetic equation for velocity distribution function:

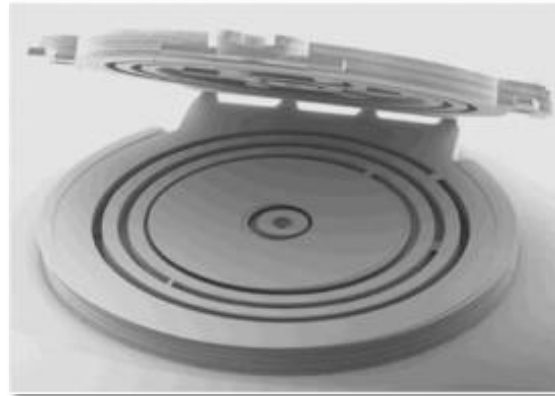
$$\frac{\partial f}{\partial t} + \vec{u} \cdot \nabla_x f = \frac{1}{\tau} (f_0 - f)$$

- ESBGK collision operator
  - H-theorem proved by Andries et al, 2000.
- discrete-ordinate method in velocity space with high-order quadratures
- FVM in physical space with 3<sup>rd</sup>-order WENO fluxes.
- 2<sup>nd</sup> and 3<sup>rd</sup> -order time integration with Runge-Kutta TVD schemes
- domain decomposition in physical space

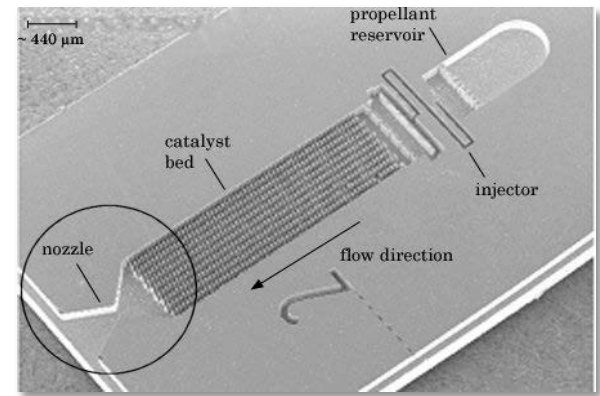
# Gas-Based Microdevices



MIT micro-turbine



USC micro-burner



NASA GSFC/UVM H<sub>2</sub>O<sub>2</sub>  
Monopropellant Micro-Thruster

## Microscale Challenges:

- Gas-phase extinction limit, min  $Re \sim 40$ . Catalyst needed
- Amplified heat transfer losses
- Increased viscous losses:  $I_{sp}$  drops for  $Re < 200$ .

**Rarefied flow analysis provides methods for design to overcome these challenges**

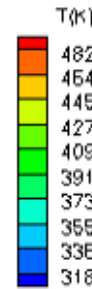
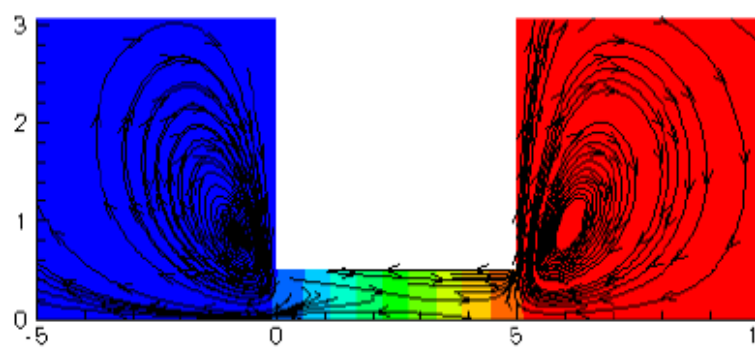


# Exploiting Rarefied Microflows

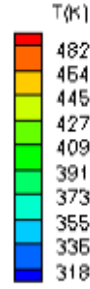
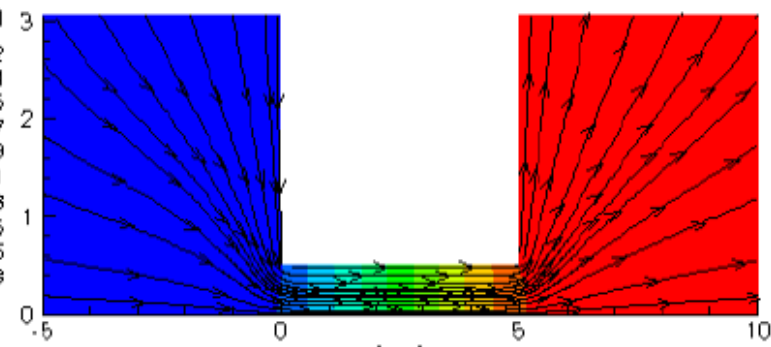
1

$L/H = 5$ ,  $Kn = 0.2$ ,  $T_1 = 300K$ ,  $T_2 = 500K$ , linear wall temperature profile.

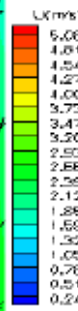
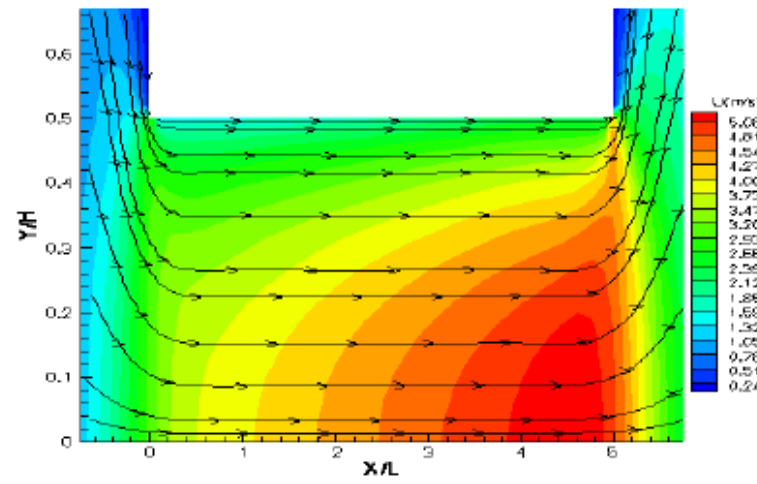
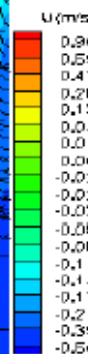
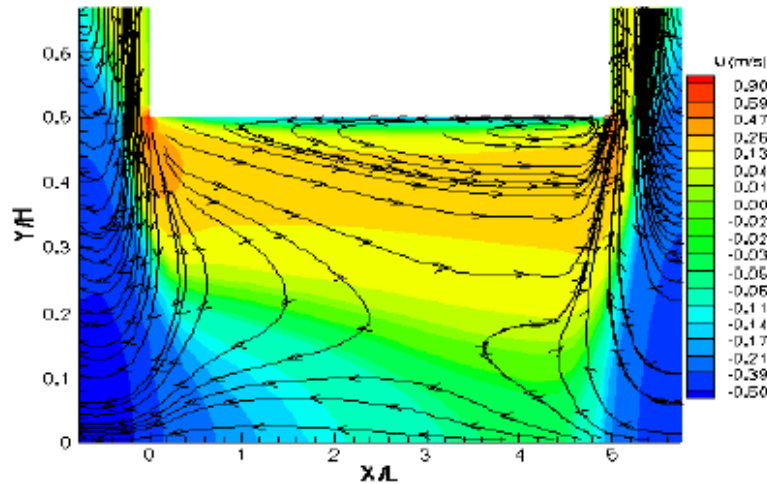
Closed Flow:



Open Flow:



•Temperature contours and streamlines for thermal creep flow in a 2D channel



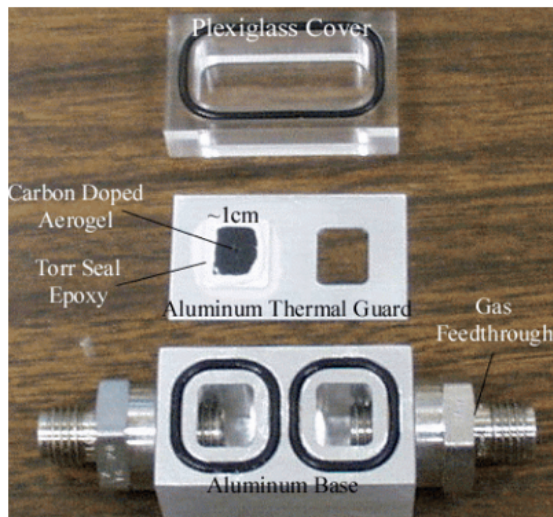
•X-component of velocity contours and streamlines (zoom) in a 2D channel

# Exploiting Rarefied Microflows

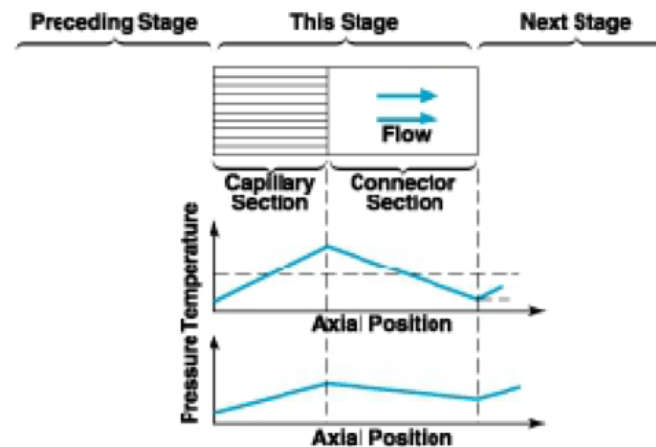
## Knudsen Compressor

A Knudsen compressor is a cascade of multiple, individually heated compressor stages that exploit the pumping effect of thermal transpiration.

Phil Muntz et al, USC



- **Aerogel pore diameter 20-50 nm**
- **Multistage**
- **Resistant and radiant heating.**



Schematic diagram of gas flow

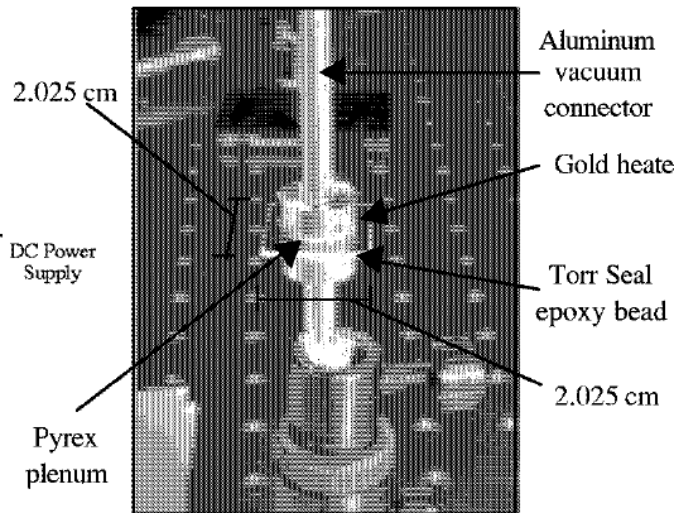
15-stage: radiant  
20 MW/cm<sup>2</sup>, 30cm<sup>2</sup>x2cm  
760 → 640 torr

# Exploiting Rarefied Microflows

Vargo, Muntz, Shiflett, Tang, “Knudsen Compressor as a Micro/Meso-scale Vacuum Pump”, *JVST A*, 1999:

*a cascade of multiple, individually heated compressor stages that exploit the pumping effect of rarefied thermal transpiration.*

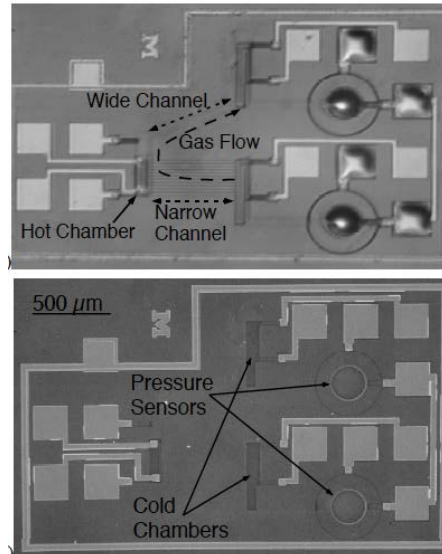
Vargo and Muntz  
(USC), 2001



1-stage:

1.5 W, 2 cmx2cm  
760 → 750 torr

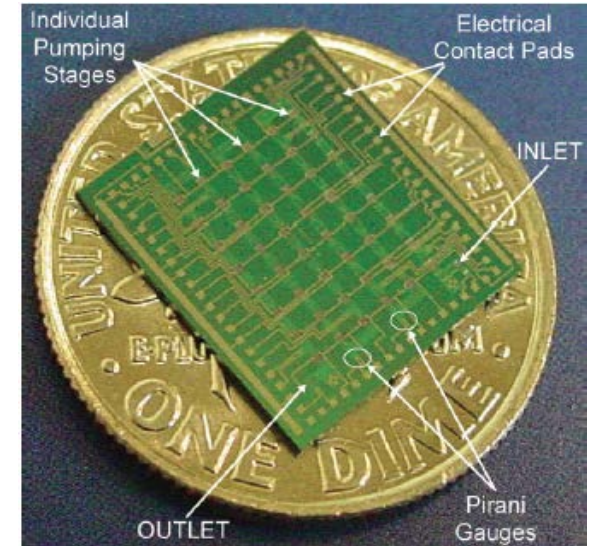
McNamara&Gianchandani  
(UMich), 2003



1-stage:

80 mW, 2 x 2 mm<sup>2</sup>  
760 → 350 torr

Gupta, Ann, Gianchandani  
(UMich), 2012



48-stage:

1350 mW, 1cm<sup>2</sup>  
760 → 50 or 250 → 5 torr

# Emerging Applications of RGD

- Knudsen force actuation/sensing
  - Rarefied thermally-driven flow + thermoelectrics
- Microplasmas
  - Rarefied flows + Field-emission cold plasmas



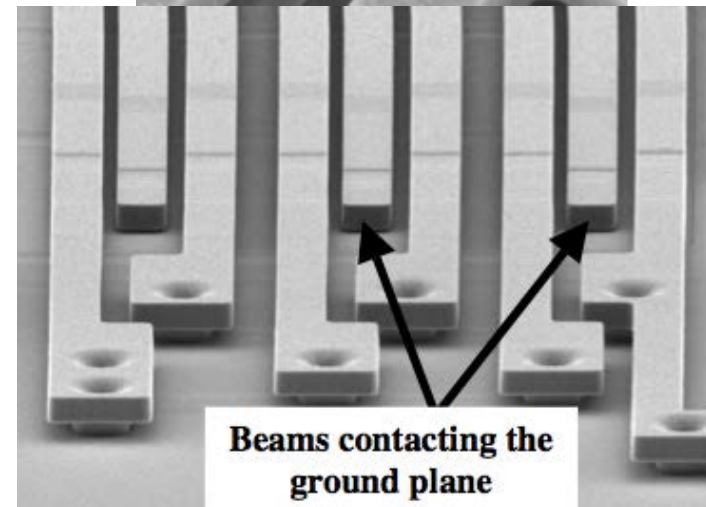
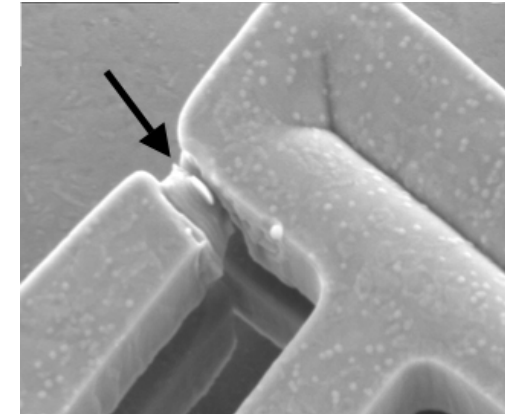
# Actuation Mechanisms in MEMS

- Electrostatic Force:

$$F_e = \frac{1}{2} \epsilon_0 A \frac{V^2}{g^2}$$

$\epsilon_0$ : permittivity  
A: normal area  
V: voltage  
g: gap size

- + Large force output at small geometry scales.
  - Electrostatic discharge at high E-fields (MV/cm)
  - Stiction due to the non-linear force that increases quadratically with distance.
- Piezoelectric Materials
  - Pneumatic Actuation
  - Fluidic Thermal Actuation = Knudse force



J. A. Walraven, *Failure Mechanisms in MEMS*,  
International Test Conference, 2003

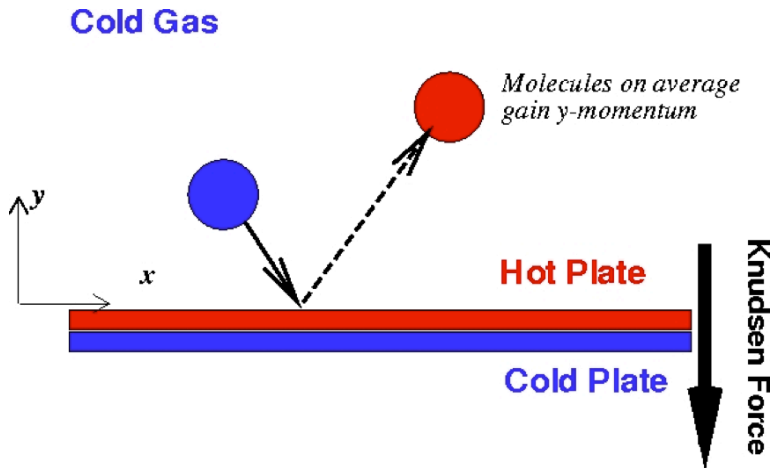
# Thermal Knudsen Forces



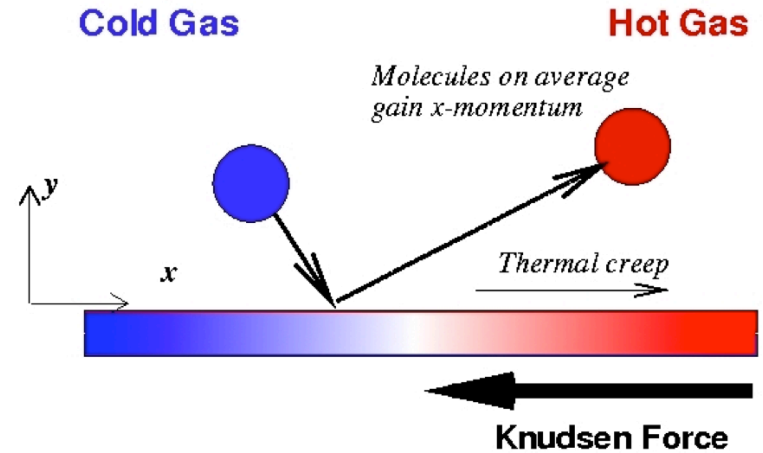
Crookes' Radiometer  
(Sir William Crookes, 1874)

- Initially misattributed to light pressure
- Reynolds (1876) explained that gas reflecting from dark vanes is hotter and thus faster
- Maxwell (1879) introduced the notion of thermal creep around the edges
- Einstein (1925) suggested that thermal force was localized near edge of the vane and the force proportional to perimeter of vane.
- Observed also in
  - Vacuum microbalance gauges
  - Thermal transpiration and creep through porous media
  - Thermophoresis on small unequally heated particles
- Direct measurements at **microscale** using laser heating by Passian *et al* (2003, 2004).

# Knudsen Forces



*Crookes Radiometer: Transverse*

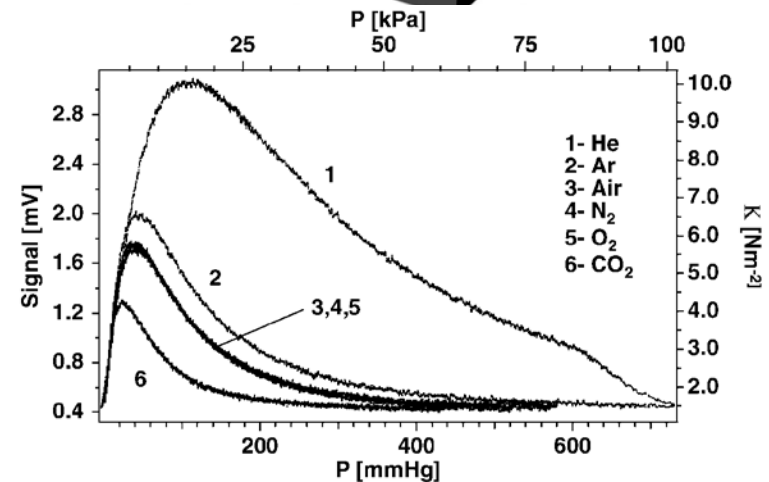
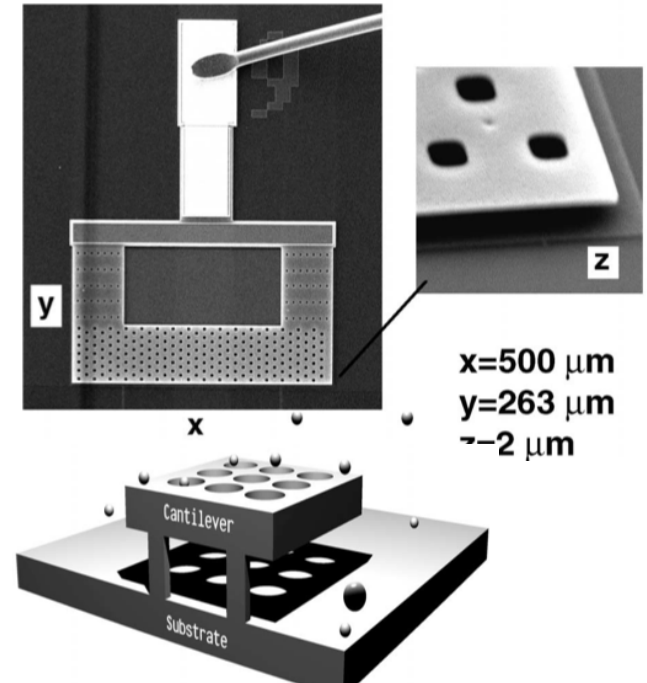
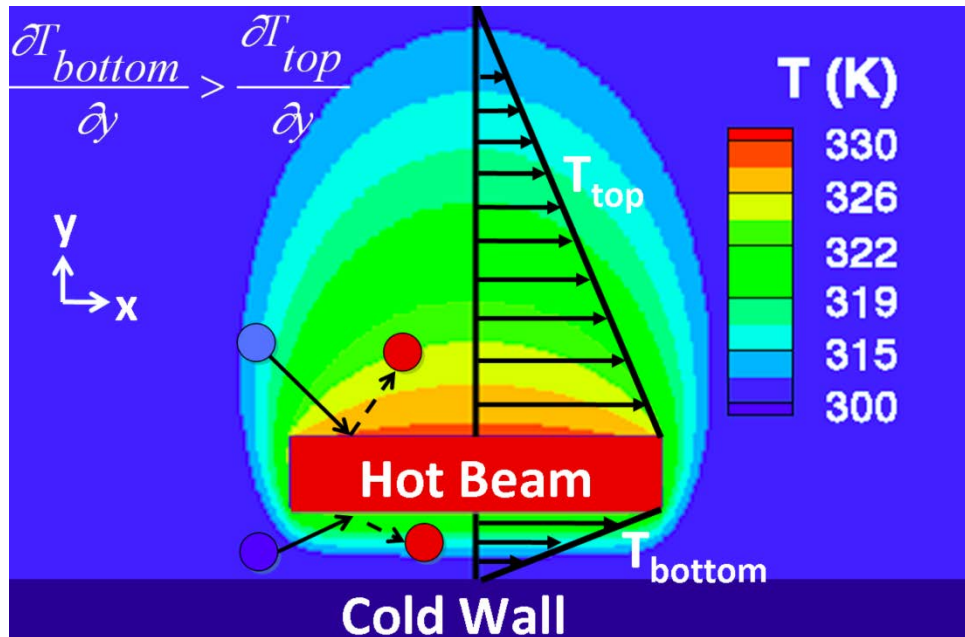


*Transpiration: Longitudinal*

$$U_{creep} \sim \lambda \cdot \frac{dT}{dx} = Kn \cdot \Delta T$$

# Kn force actuation

- Consequence of a thermal non-equilibrium between gas and solid
- Can be generated by resistive heating as well as optically Experimental data [Passian et al, PRL, 2003](#) measurements using heated AFM probes





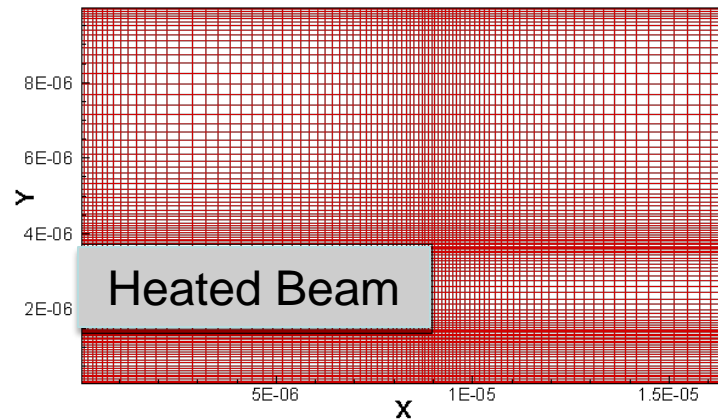
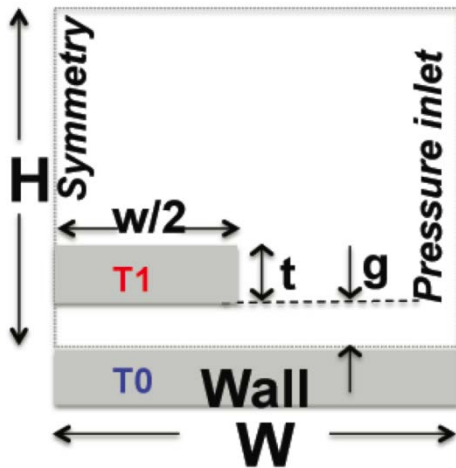
# Knudsen Force: Modeling Approach

2D quasi-stationary Boltzmann-ESBGK equation:

$$u \frac{\partial f}{\partial x} + v \frac{\partial f}{\partial y} = \frac{f_0 - f}{\tau}$$

$1/\tau$  – collision frequency  
 $f_0$  – Gaussian d.f.

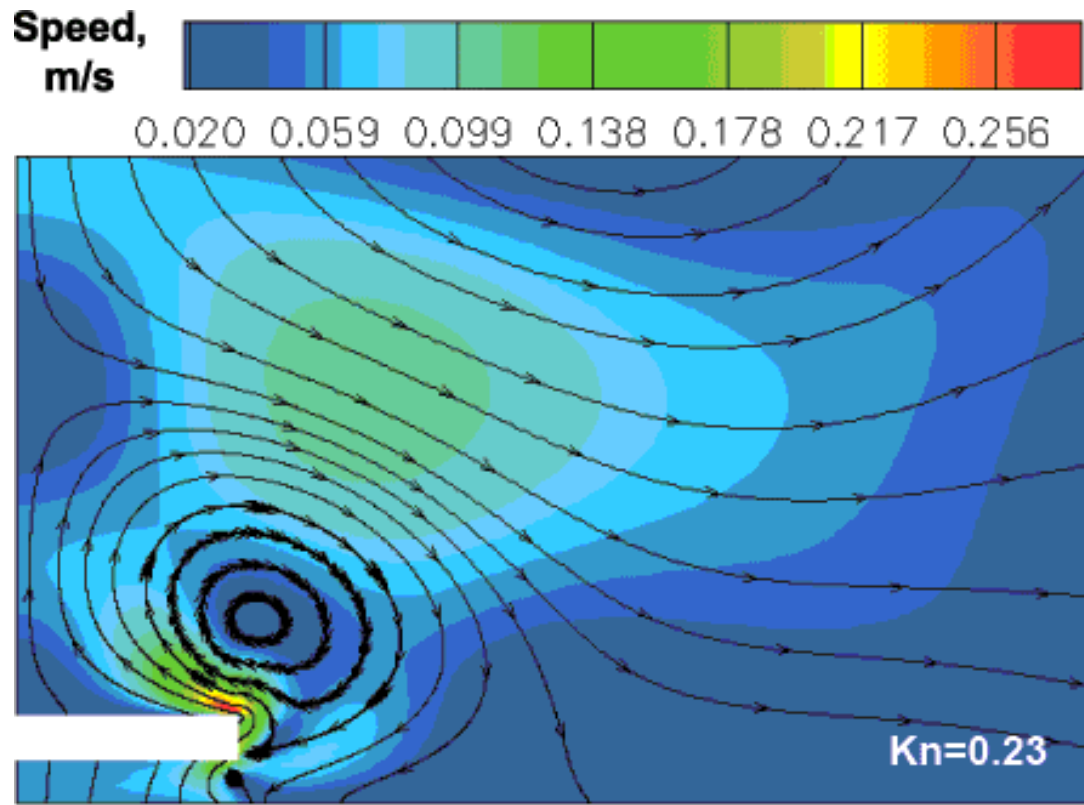
- 2<sup>nd</sup>-order upwind FVM scheme in physical space
- High order discrete ordinates in velocity space
- Typical Mesh:  $N=150 \times 150 \times 16 \times 64 = 23$  M; Memory:  $\approx 700$ MB;
- Simulations for planar geometry with equivalent front-to-side area ratio



Non-uniform grid

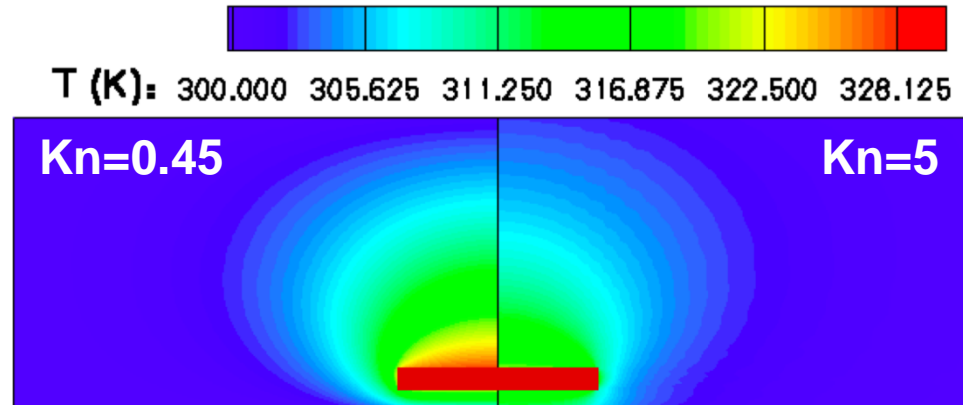
# Passian et al data: Simulation Results

- Velocity Contours and Streamlines:

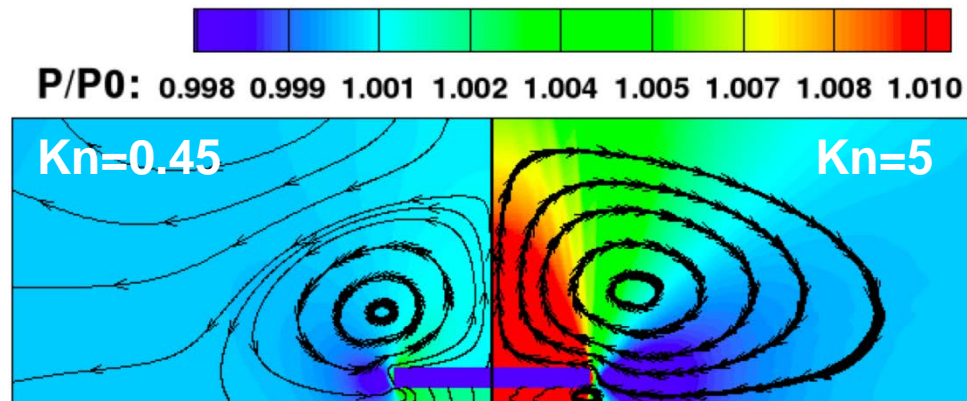


# Passian et al data: Simulation Results

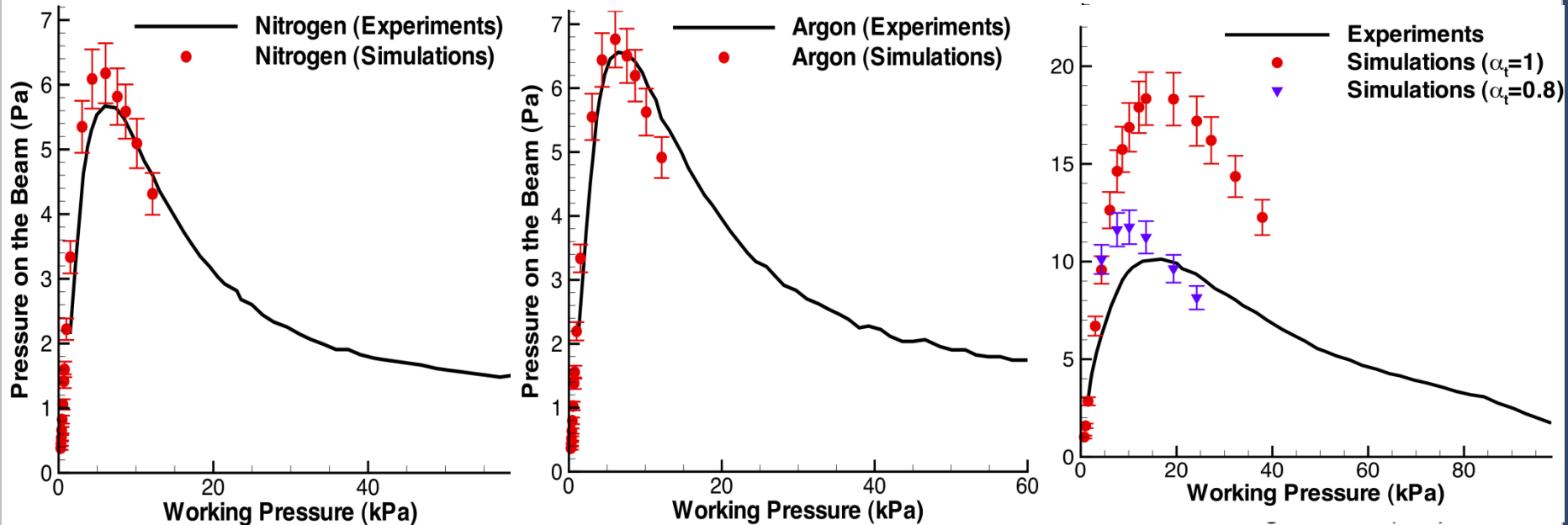
- Temperature Contours:



- Non-dimensional Pressure and Streamlines:



# Experimental Validation



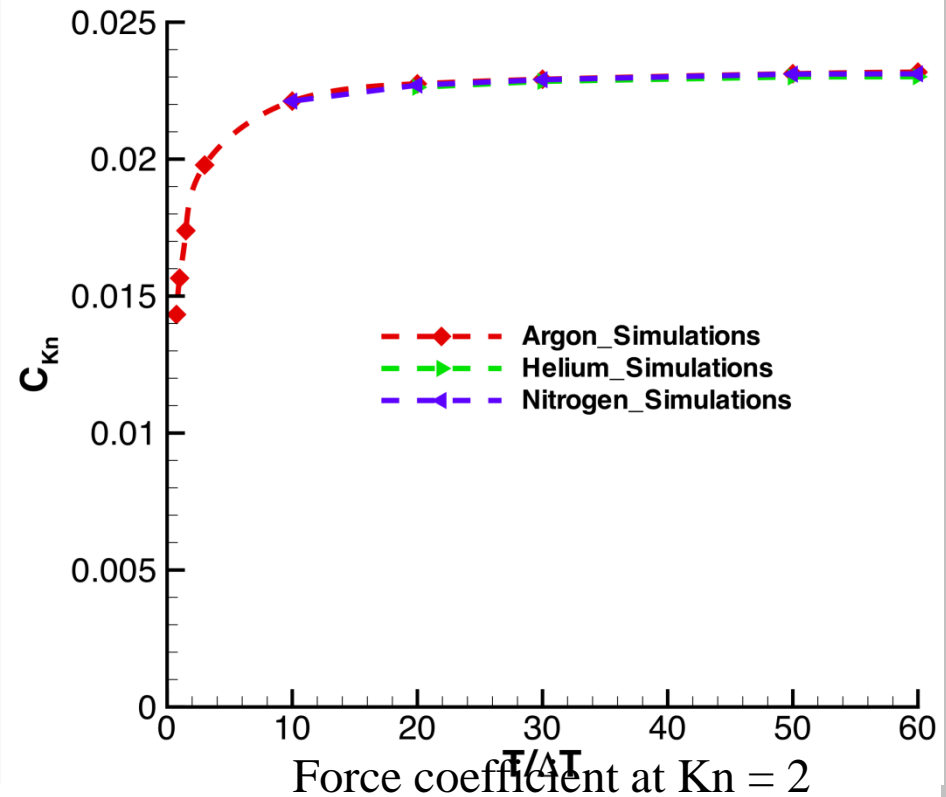
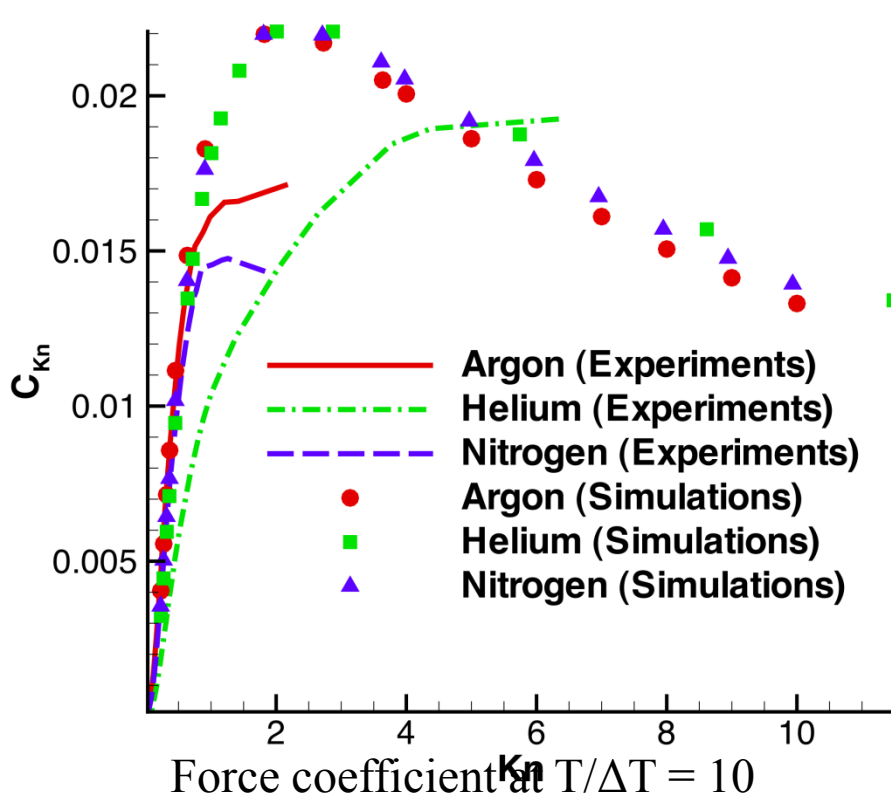
- Argon and Nitrogen simulations agree with experiments within 10%.
- Deviation for Helium is about 80% at the maximum of Knudsen force.

Nabeth, Chigullapalli, Alexeenko, *PRE*, 2011

# Compact Model for Kn Force

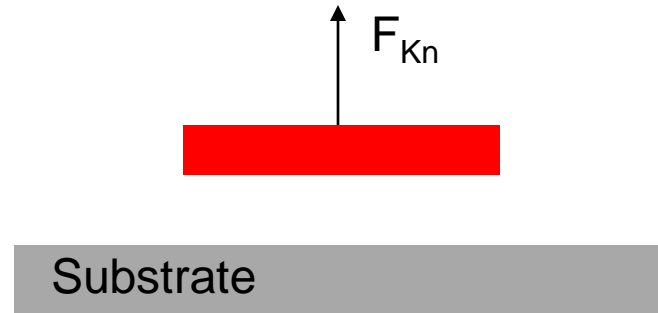
Closed-form model for non-dimensional Knudsen thermal force coefficient for uniformly heated beam:

$$C_{Kn}(Kn, \frac{T}{\Delta T}) = \frac{F'}{w\rho R\Delta T} = \frac{1 + D(\frac{T}{\Delta T})^d + E(\frac{T}{\Delta T})^e}{AKn^a + BKn^b + CKn^c}$$

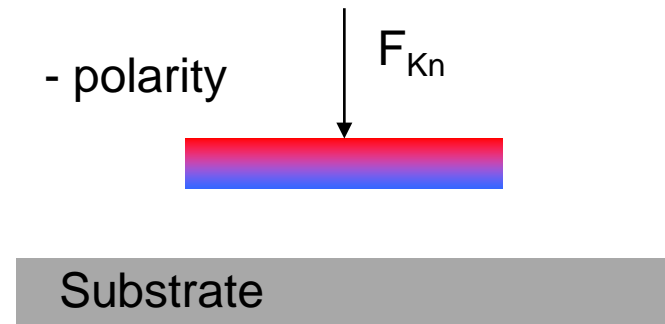
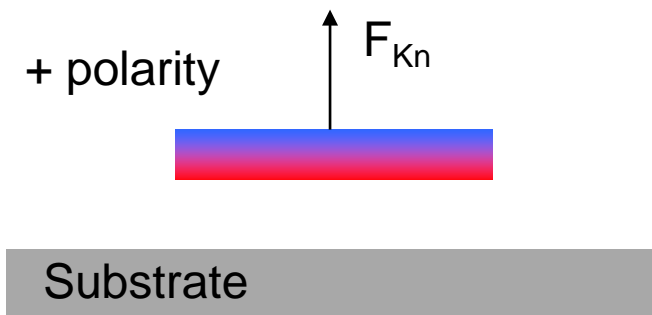


# Force Enhancement and Reversal

- Uniformly heated beam (Passian et al, 2003)



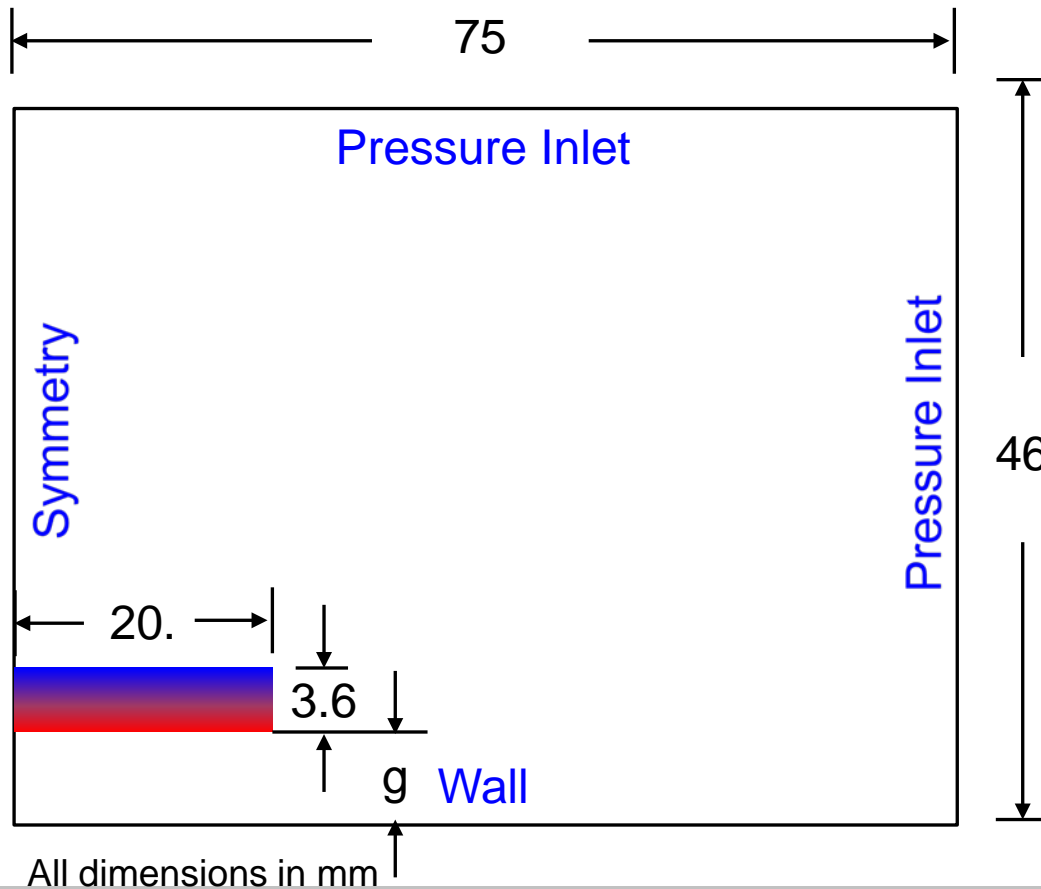
- Thermoelectric heating for bi-directional actuation (this work):



# Modeling the Knudsen Force

Simulate Knudsen force on suspended heating element using ES-BGK model

- 2D-2V finite volume solver with second-order upwind fluxes
- 8<sup>th</sup>-order Gauss-Hermite quadrature in velocity space



Parameter	Value
$P_{\text{ref}}$	298 – 12,522 Pa
$ \Delta T_b $	25 K
$T_{b,\text{mean}}$	326 K
$T_{\text{substrate}}$	298 K
$\Delta T_{b,s}$	26 K

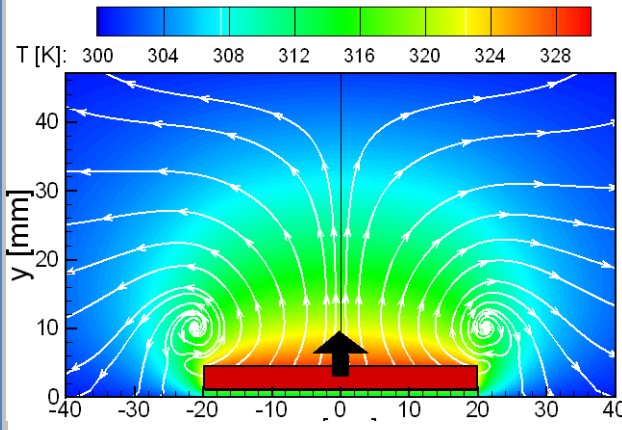
Richardson Extrapolation:  
160x160 mesh for force within 2%

# Simulation Results

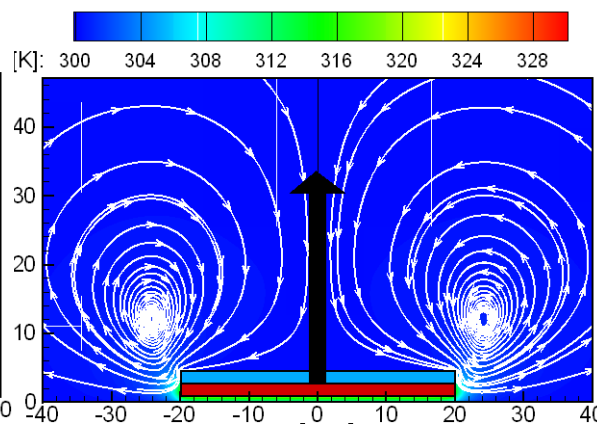
*Uniform Heating*

*Thermoelectric: Bottom-Up*

*Thermoelectric: Top-Down*

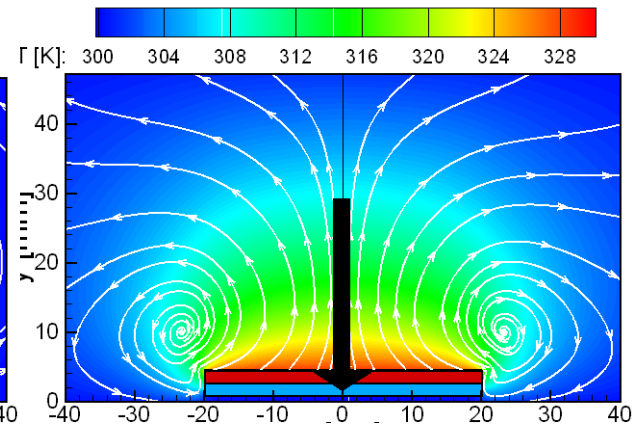


0.105% of  $p_0$



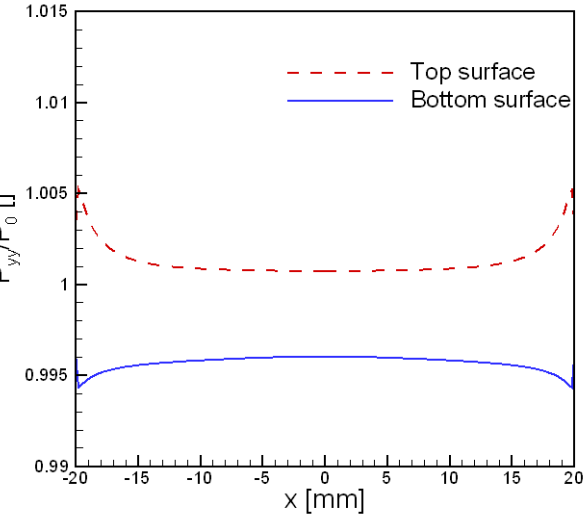
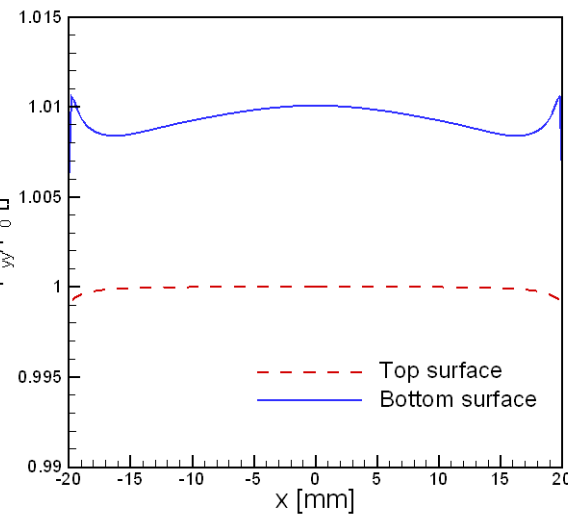
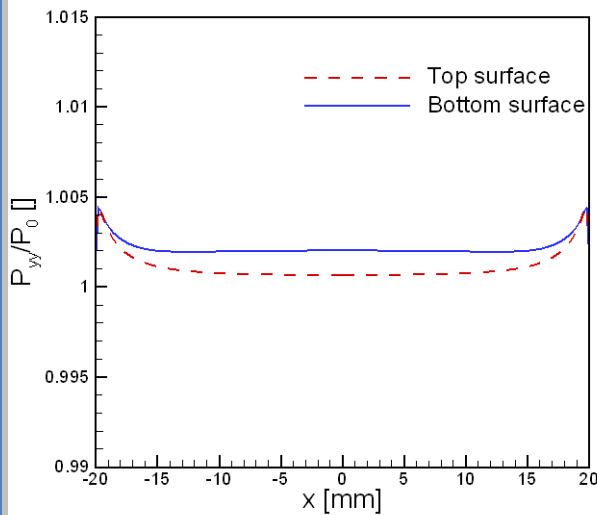
0.938% of  $p_0$

*X8.9 enhancement*



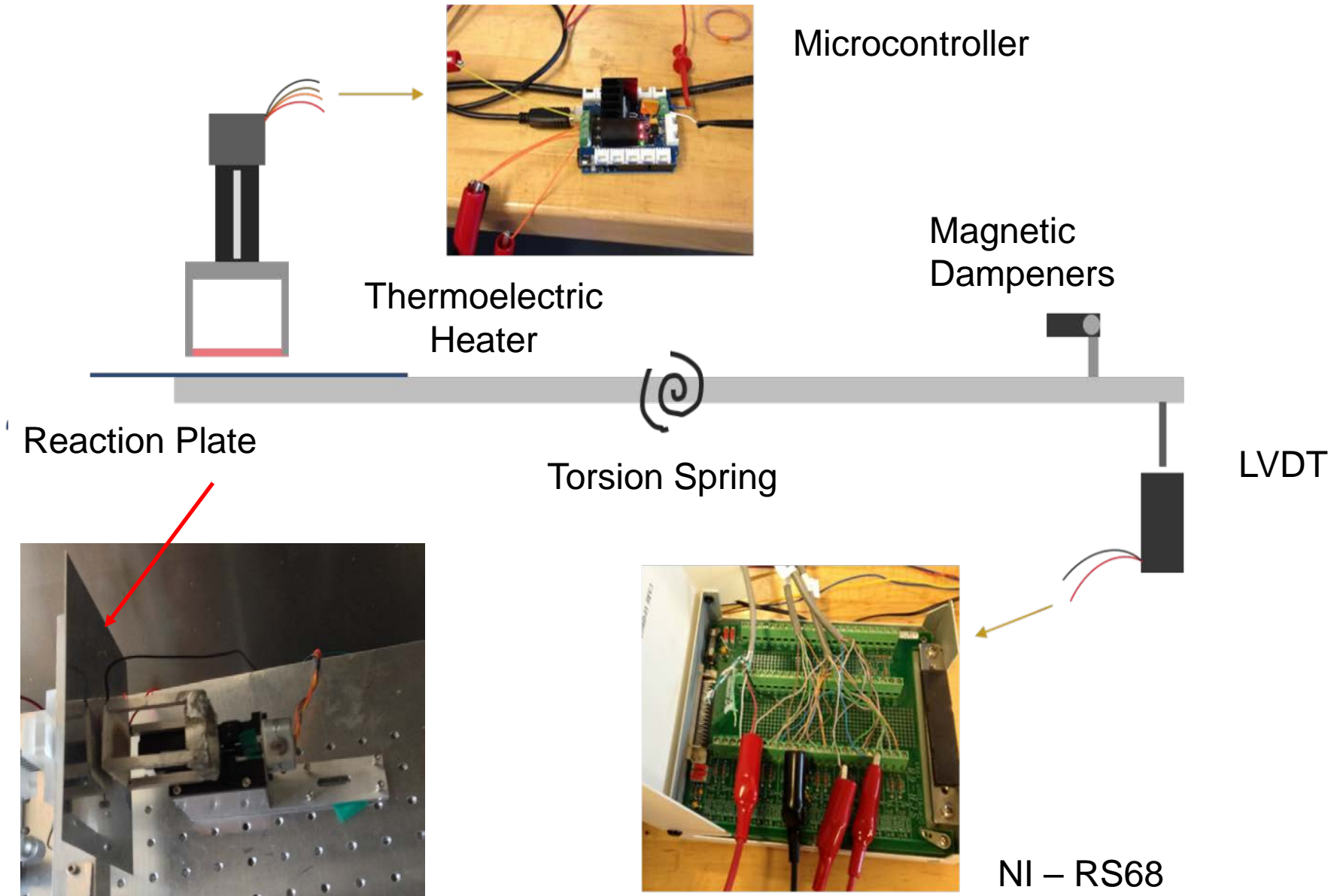
-0.557 % of  $p_0$

*X5.3 enhancement & reversal*





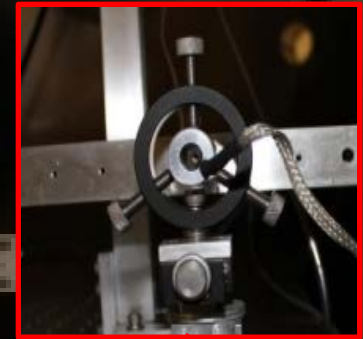
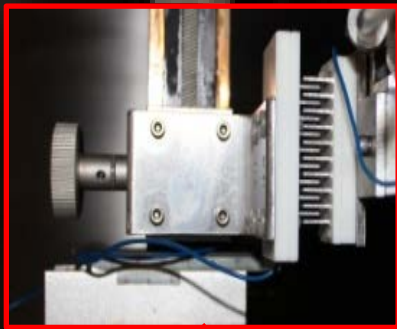
# Experimental Setup



# Experimental Setup

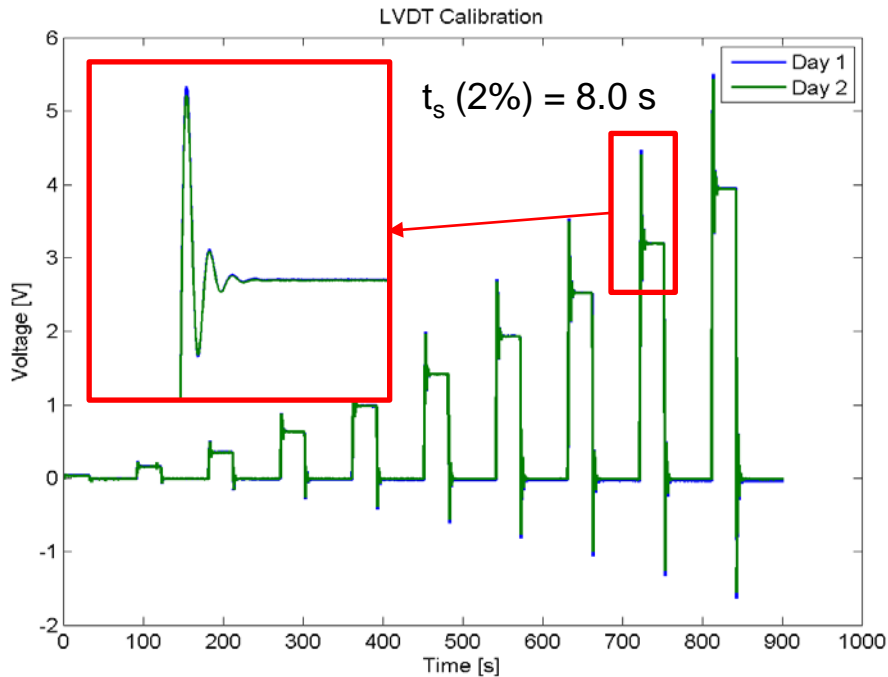
## Purdue LEAP MicroNewton Thrust Stand

Electrostatic Fins



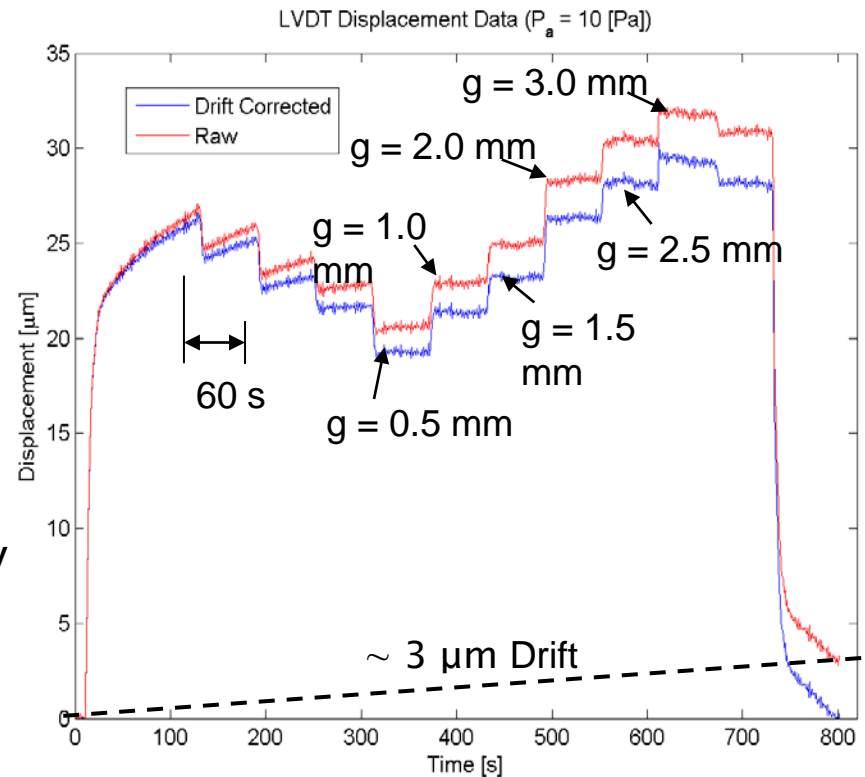
Force range: 10 to 800  $\mu\text{N}$   
Measurement Uncertainty: 1.0  $\mu\text{N}$

# Measurement Technique



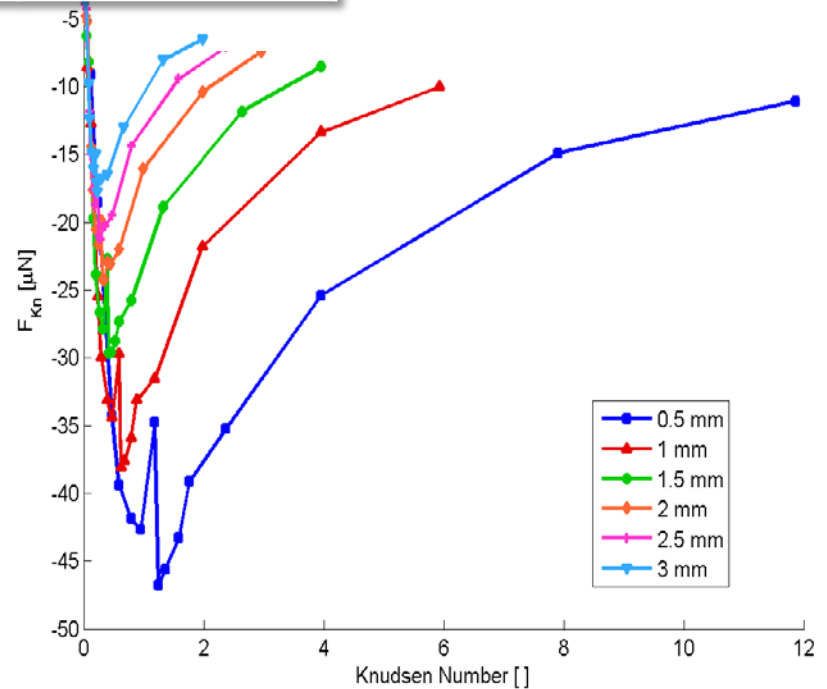
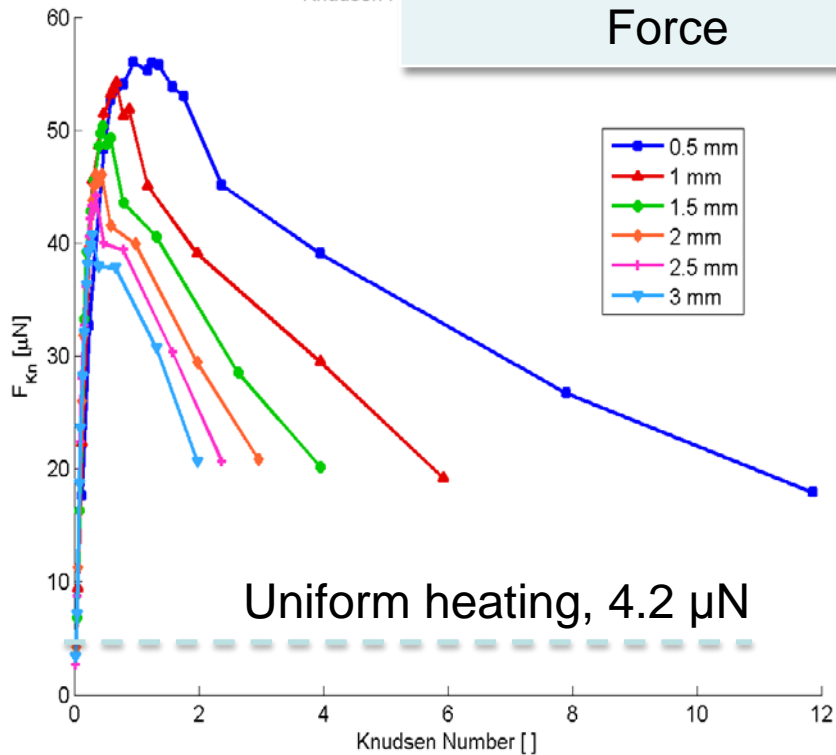
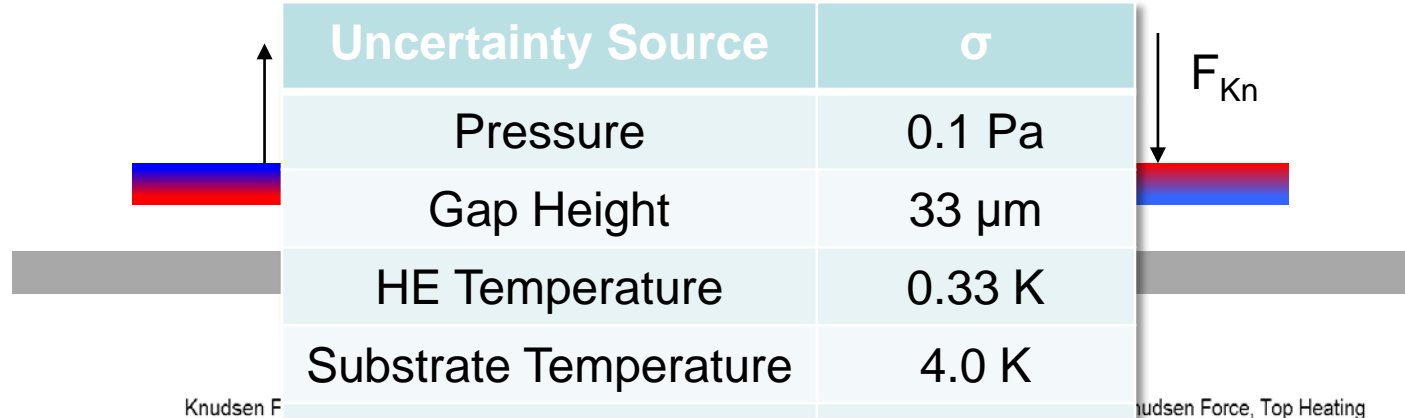
- Measure displacement of reaction plate
- Sweep 0.5 – 3.0 mm gap size at fixed pressure
  - Hold for 60 seconds to ensure steady state
  - Apply linear drift correction

- Calibration performed at the beginning of each test day
- Sweep 0 - 100 V, 30 seconds high, 60 seconds low
  - Evaluate force from LVDT voltage

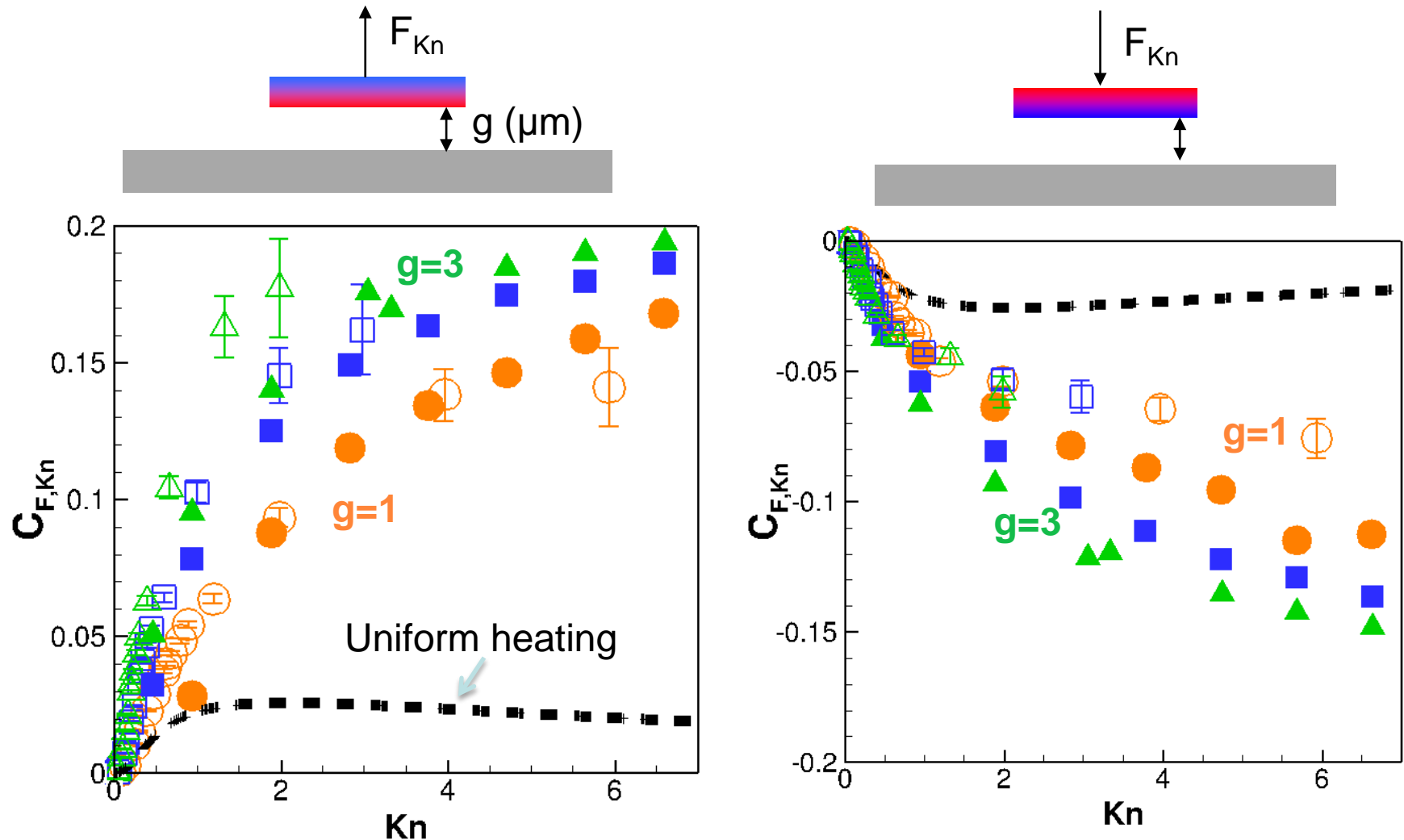


# Thermoelectric Kn force: Measurements

Uncertainty Source	$\sigma$
Pressure	0.1 Pa
Gap Height	33 $\mu\text{m}$
HE Temperature	0.33 K
Substrate Temperature	4.0 K
Force	1.8 $\mu\text{N}$



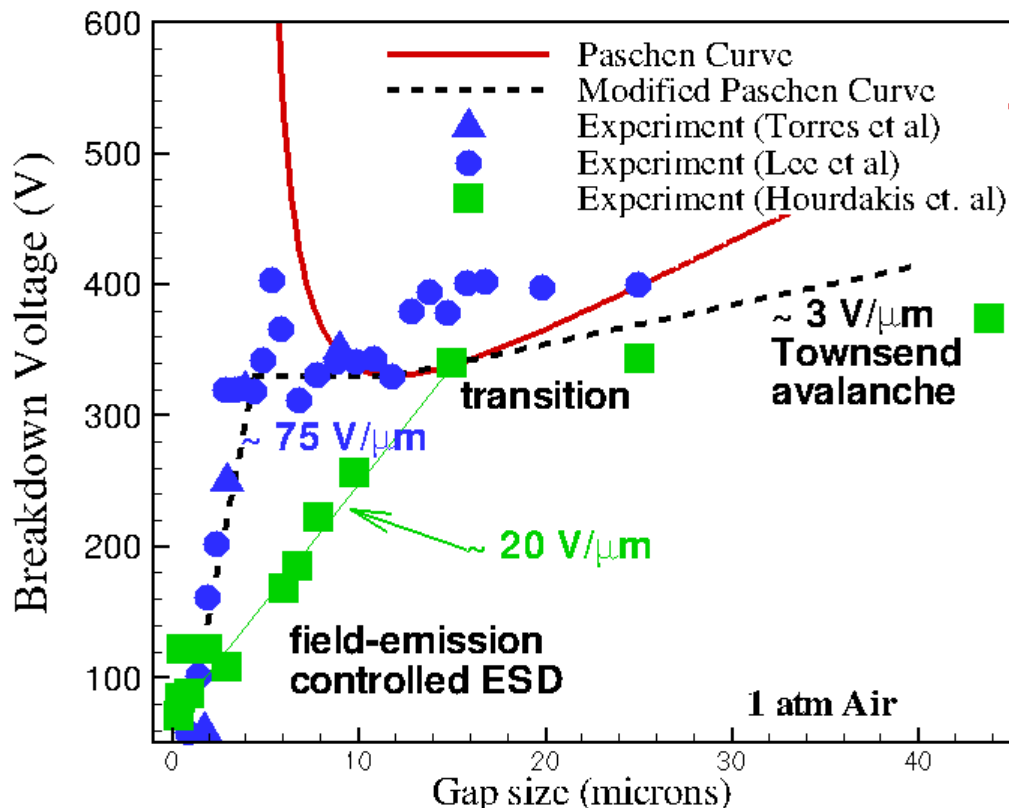
# Comparison of Modeling and Experiment



Maximum 36% error in  $C_{F,Kn}$  between simulation and experiment

- Difference likely due to 3D effects in experimental measurements
- Errors likely stem from model inputs related to the heating element

# Experiments: DC breakdown in microgaps



## Fowler-Nordheim field emission:

$$j_{fe} = \frac{A \beta^2 E^2}{\phi t^2(y)} \exp\left(\frac{-B \phi^{3/2} v(y)}{\beta E}\right)$$

$$A = \frac{e}{2\pi h} = 6.2E-6 \text{ A/eV}$$

$$B = \frac{4\kappa}{3} = 6.85E7$$

e – electron charge  
h – Planck's constant

$$\kappa = \sqrt{\frac{8\pi^2 m}{h^2}}$$

Field enhancement factor

$\beta = 1.5 - 100$ .

Depends on geometry and material.

Field-emission become dominant for  $E > 100 \text{ MV/m}$  or  $100 \text{ V}/\mu\text{m}$

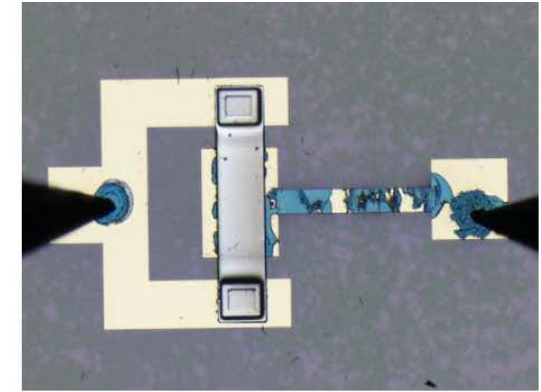
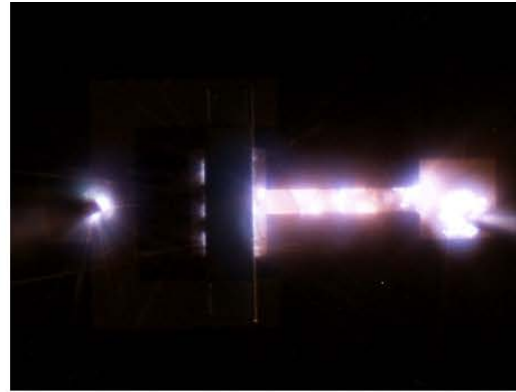
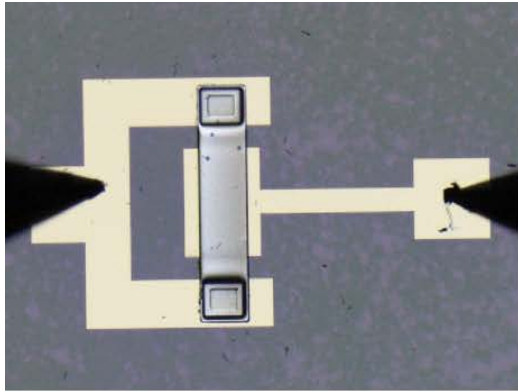
High  $\beta$

Low  $\beta$

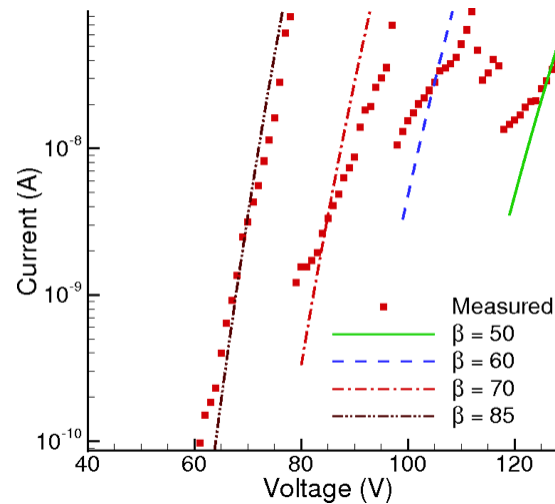
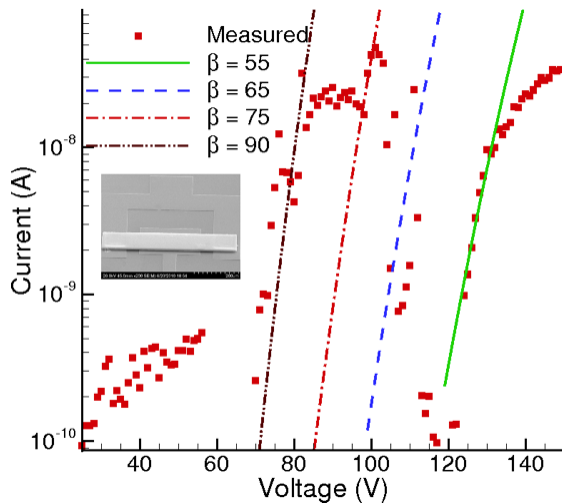
# MEMS microdischarges measurements

Example: Nickel RF MEMS capacitive switch

200 V DC



Garg et al, "Direct Measurement of Field Emission Current in Electrostatic MEMS", MEMS 2011



I-V measurements  
and PIC/MCC model:

Venkattraman, Garg,  
Peroulis, Alexeenko  
*APL*, 2012