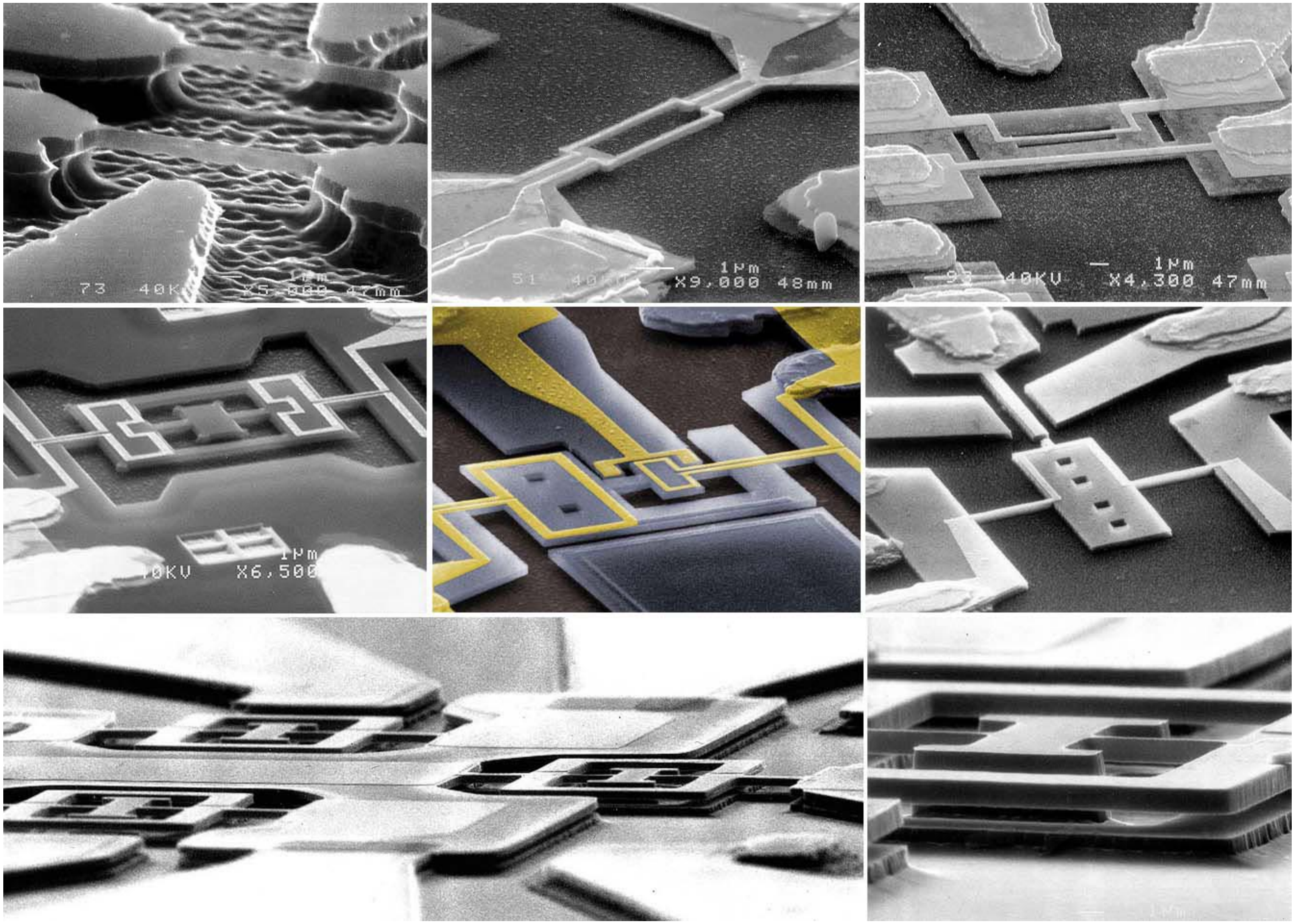
Noise, AFMs, and Nanomechanical Biosensors

with Mark Paul (Virginia Tech), and the Caltech BioNEMS Collaboration

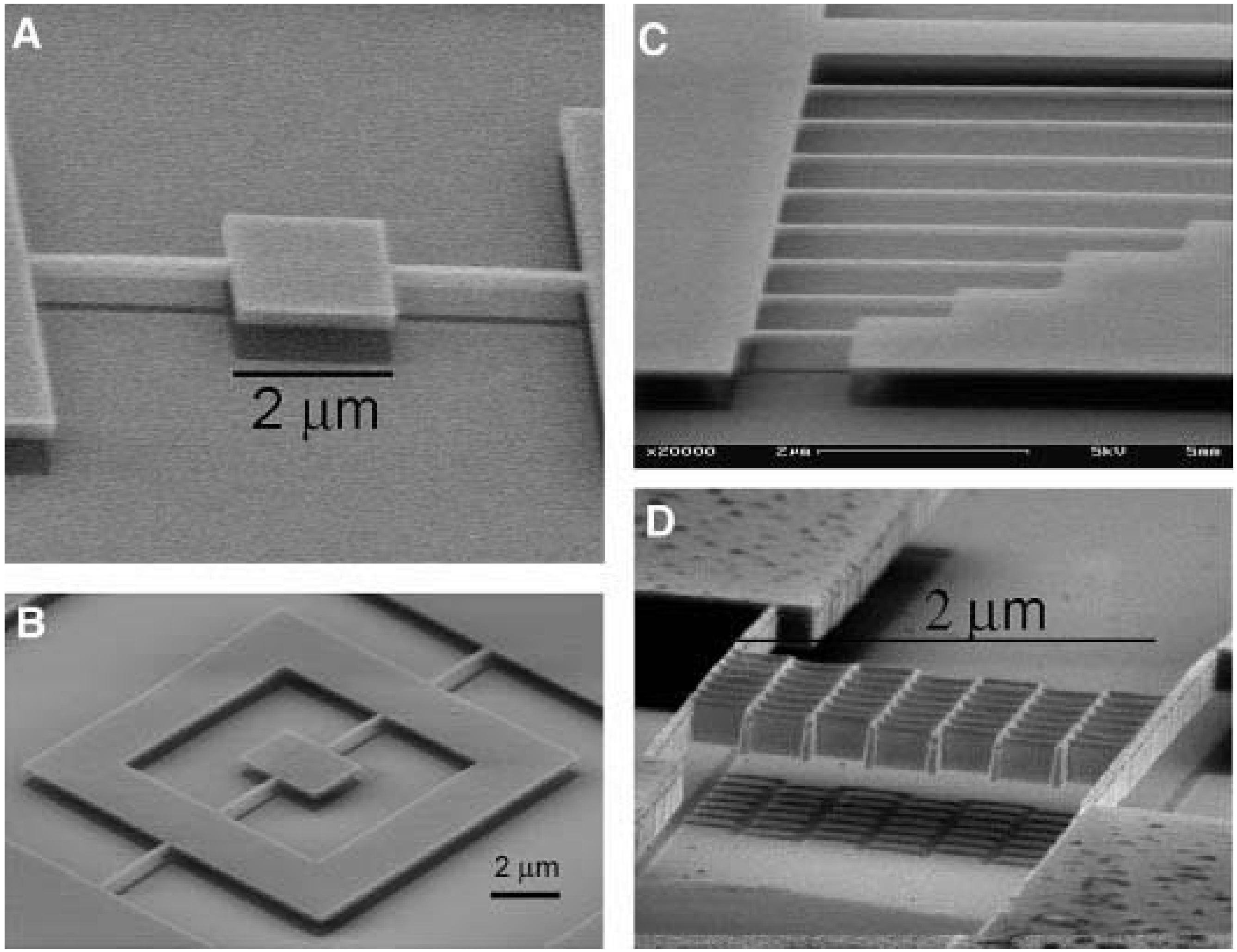
Support: DARPA

Outline

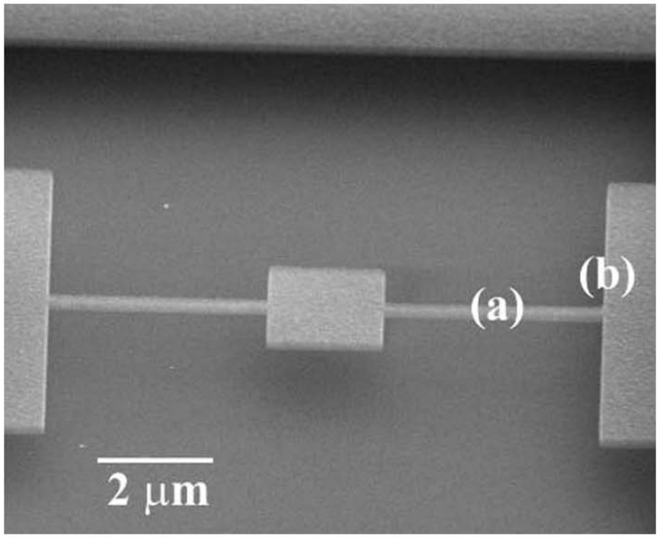
- Motivation: MEMS and NEMS
- BioNEMS: Fluctuations in the linear regime

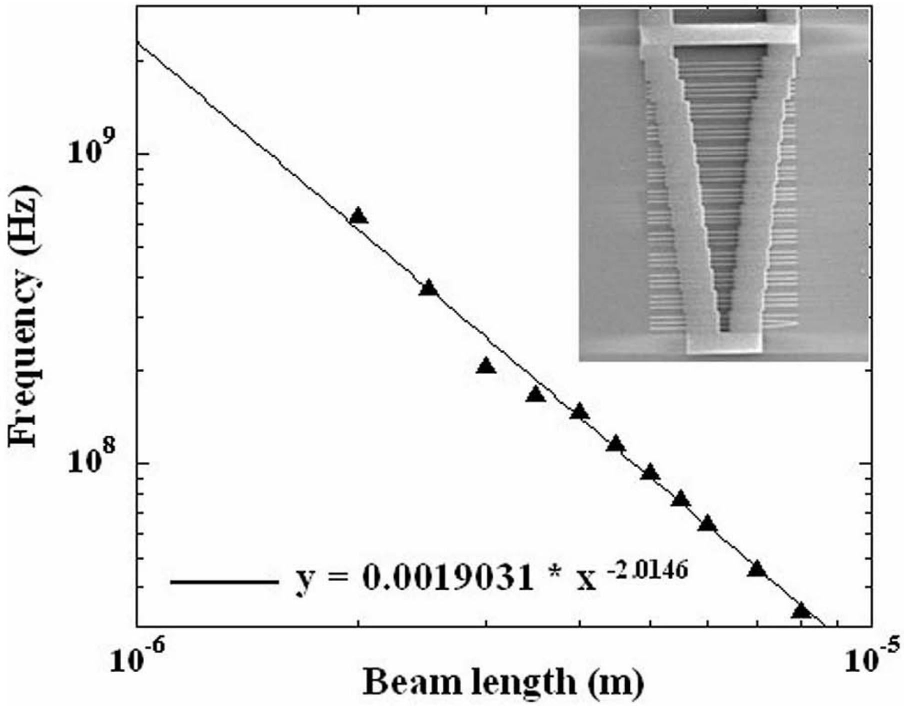


[From M. R. Roukes, Caltech]



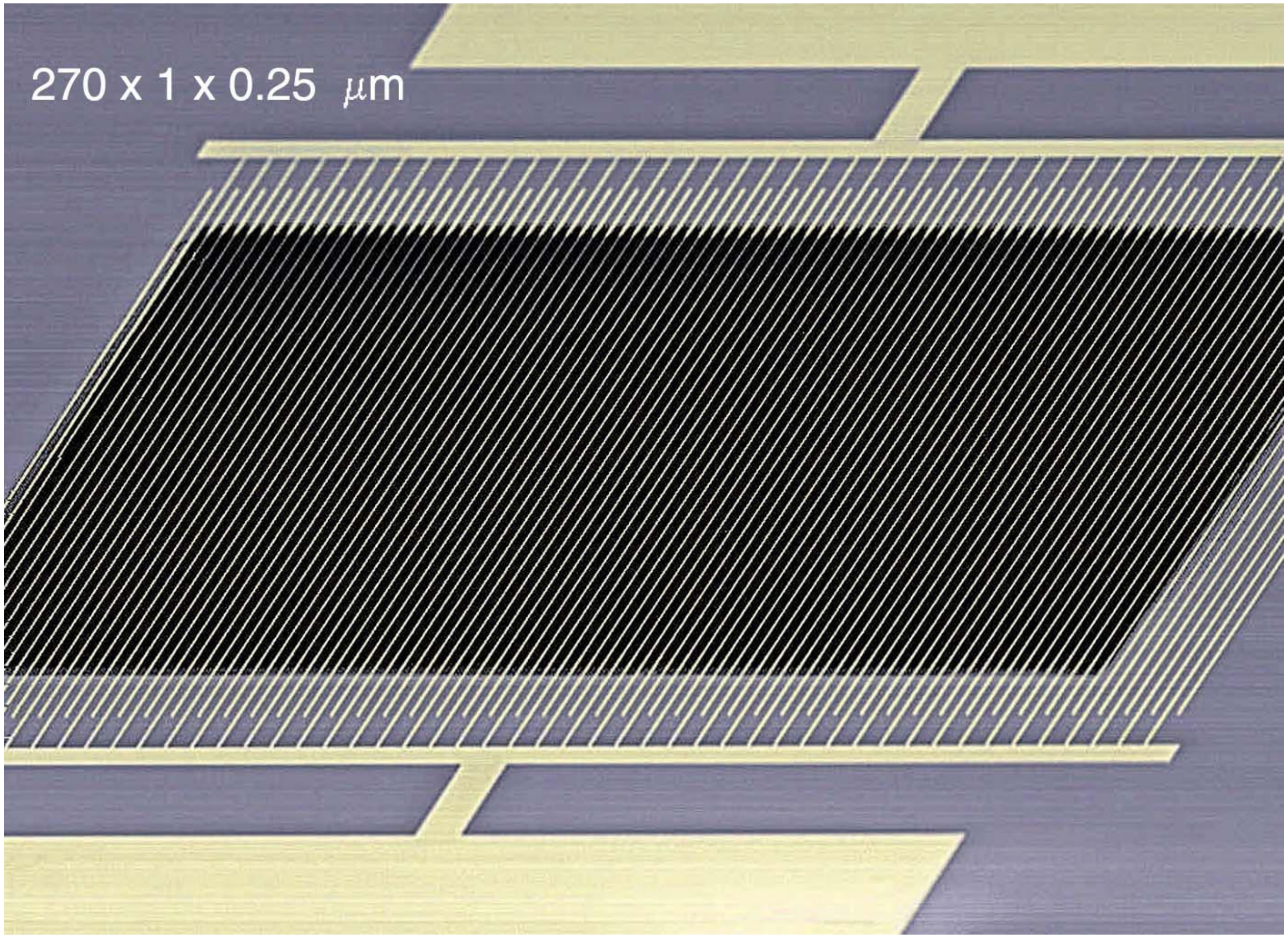
Single crystal silicon [From Craighead, Science **290**, 1532 (2000)]





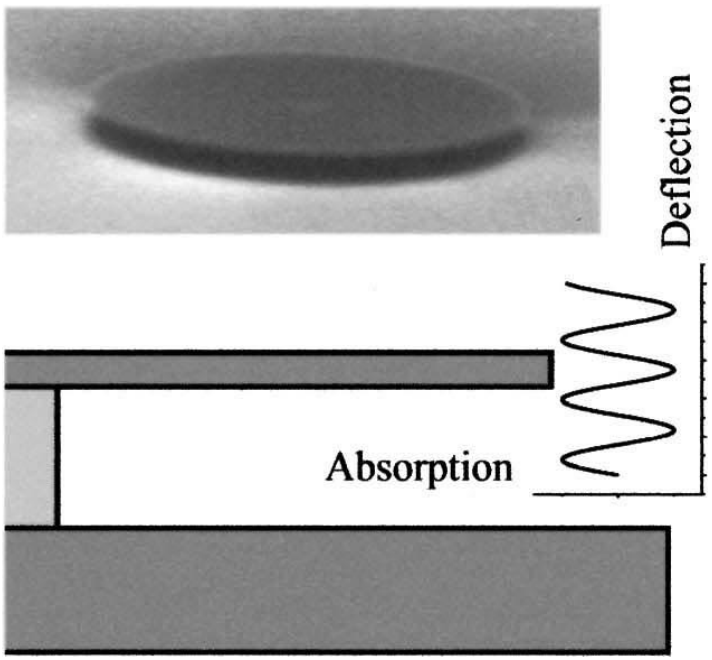
Diamond Film [From Sekaric et al., Appl. Phys. Lett. **81**, 4445 (2002)]

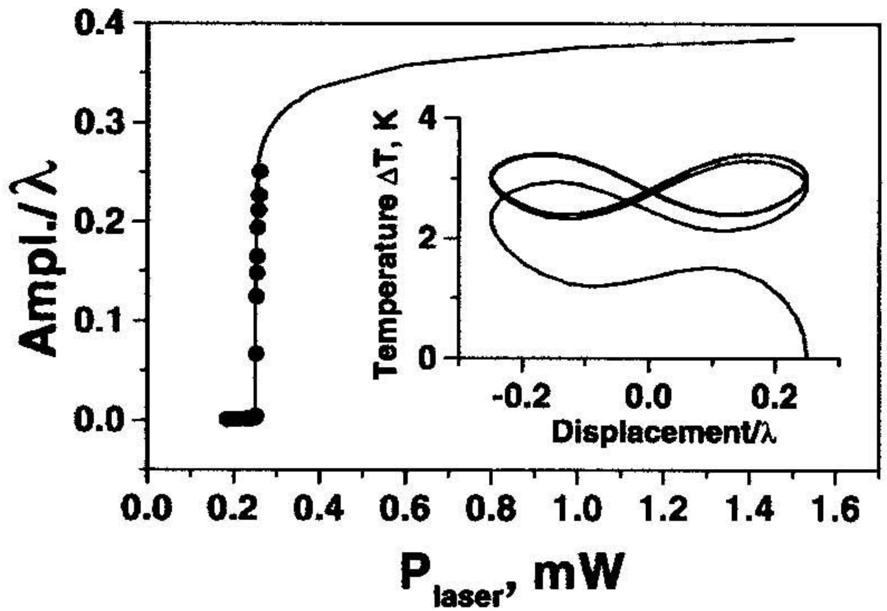
Array of μ-scale oscillators



[From Buks and Roukes J. MEMS. **11**, 802 (2002)]

Self-Oscillations





[Zalalutdinov et al., Appl. Phys. Lett. **79**, 695 (2001)]

MicroElectroMechanical Systems and NEMS

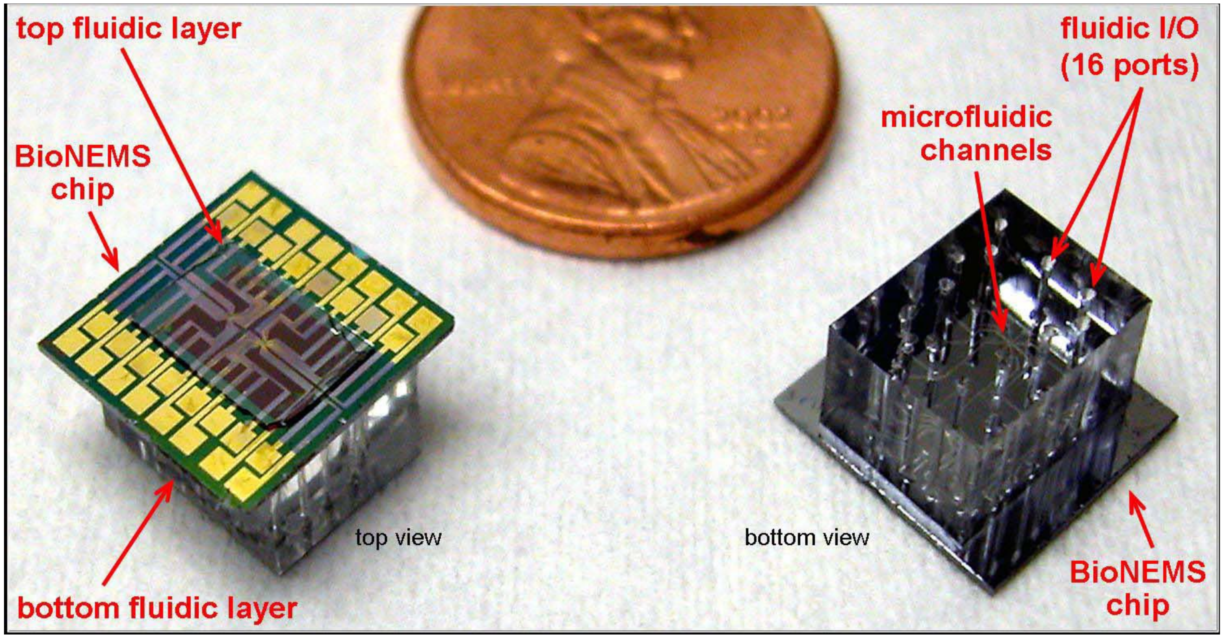
Tiny mechanical oscillators:

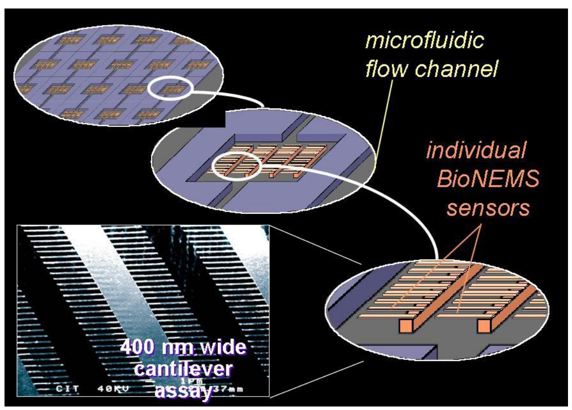
- driven, dissipative $\Rightarrow$ nonequilibrium
- nonlinear
- collective (arrays)
- noisy
- (potentially) quantum

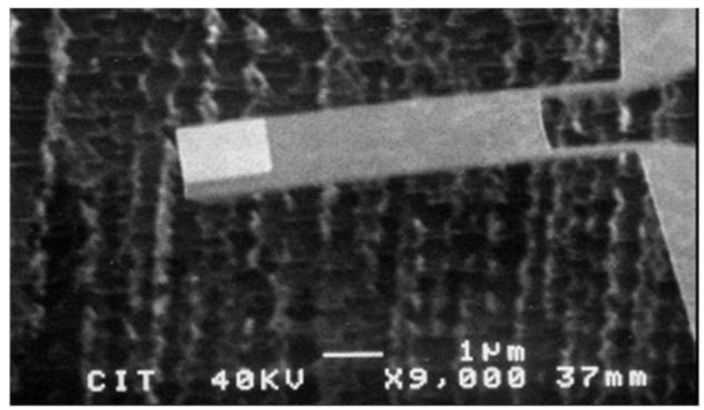
Goals

- Apply knowledge from statistical mechanics, nonlinear dynamics, pattern formation etc. to technologically important questions
- Investigate stochastic and nonlinear dynamics, and pattern formation in new regimes

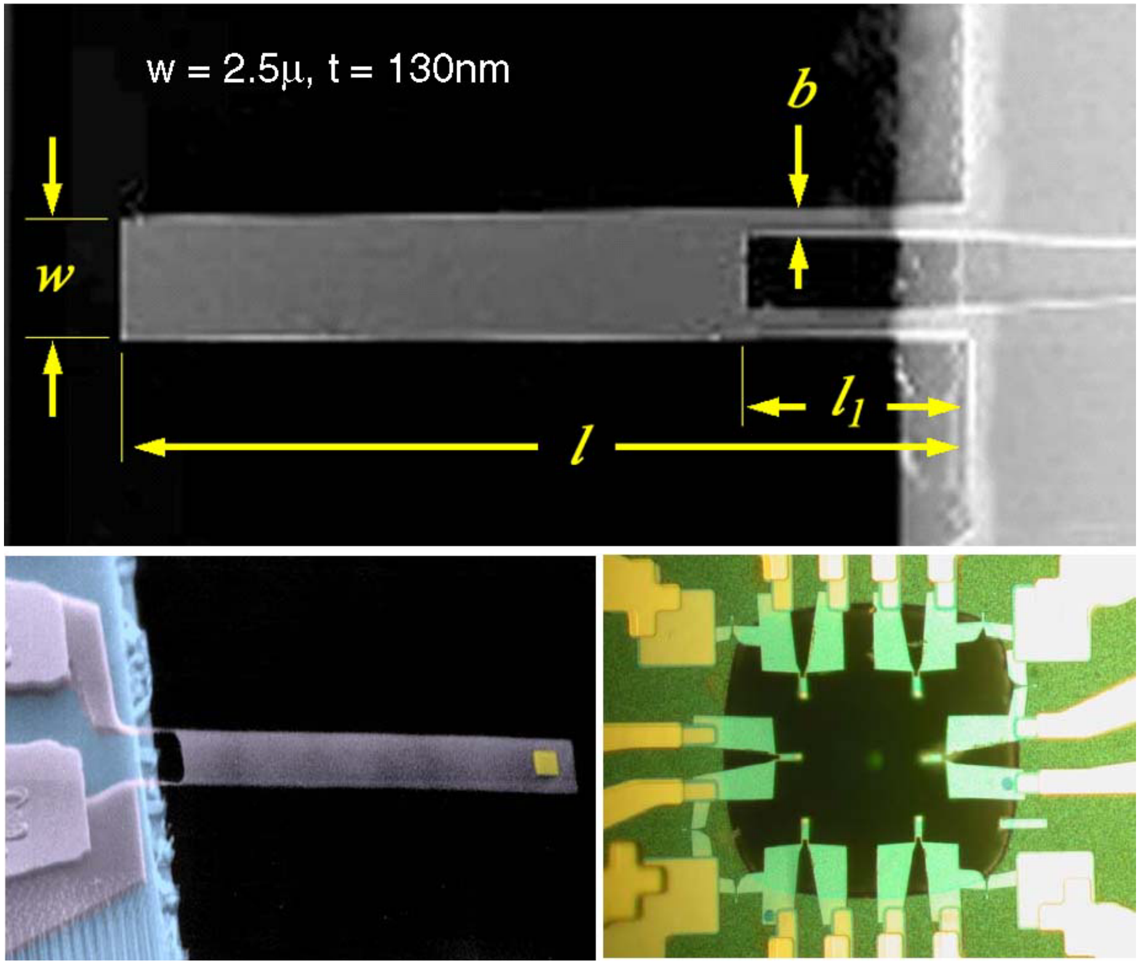
BioNEMS - Single BioMolecule Detector/Probe





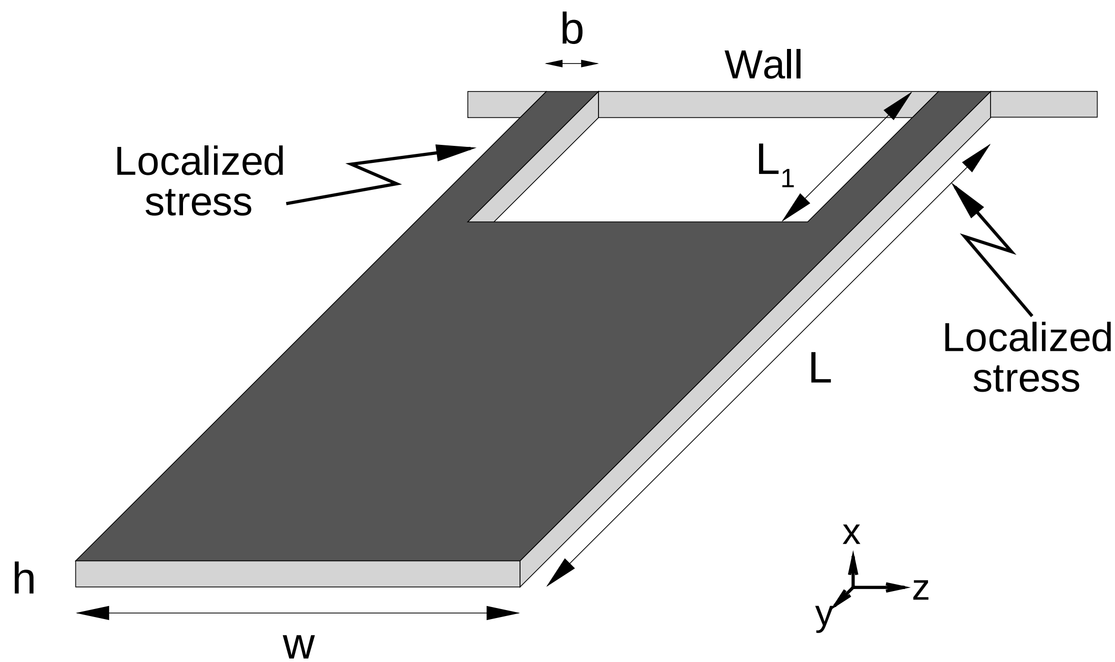


BioNEMS Prototype



(Arlett et. al, Nobel Symposium 131, August 2005)

Example Design Parameters

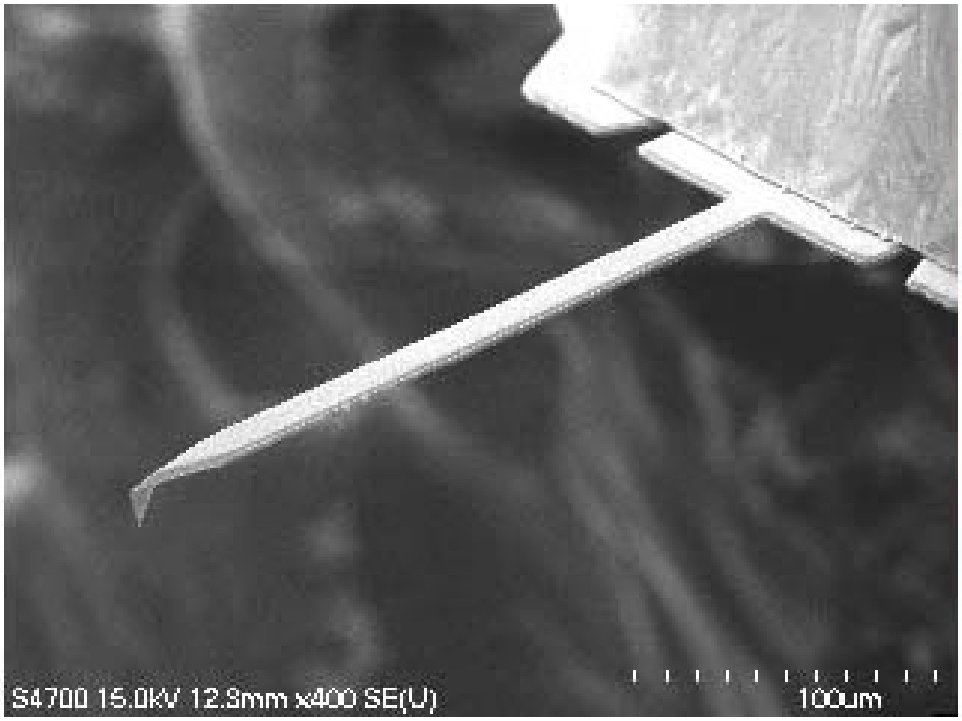


Dimensions: $L = 3\mu$, $w = 100$nm, $t = 30$nm, $L_1 = 0.6\mu$, $b = 33$nm

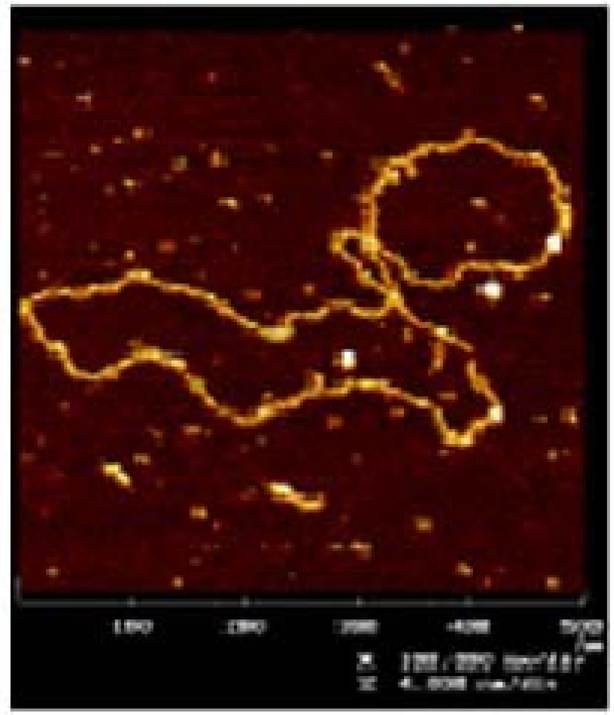
Material: $\rho = 2230$Kg/m^3, $E = 1.25 \times 10^{11}$N/m^2

Results: Spring constant $K = 8.7$mN/m; vacuum frequency $\nu_0 \sim 6$MHz

Atomic Force Microscopy (AFM)



Commercial AFM cantilever (Olympus)



DNA molecule in water

Noise in micro-cantilevers

Thermal fluctuations (Brownian motion) important for:

- BioNEMS: detection scheme
- AFM: calibration

Goals:

- Correct formulation of fluctuations for analytic calculations
- Practical scheme for numerical calculations of realistic geometries

Previous approach (Sader 1998)

- Model molecular collisions with cantilever as white noise force uniformly distributed along cantilever
- Calculate modal response $\tilde{x}_n(\omega)$ for periodic driving force $\tilde{F}(\omega)$ (resonance curves)
  - ⋆ interesting frequency dependent mass loading and damping from coupling to fluid
- Calculate fluctuation of tip displacement as sum of mode responses for constant $|\tilde{F}(\omega)|^2$

Problems

This approaches is formally incorrect and hard to implement for realistic geometries and strong damping:

- Noise force is not white
- Noise force is not uniformly distributed along surface
- Mode fluctuations are not in general independent
- Difficult to calculate coupled elastic-fluid modes, and many needed for strong damping

Fluid Dynamics Issues

$$\frac{\partial \vec{u}}{\partial t} + \vec{u} \cdot \vec{\nabla} \vec{u} = -\vec{\nabla} p + \nu \nabla^2 \vec{u},$$
$$\vec{\nabla} \cdot \vec{u} = 0$$

with ν the kinematic viscosity η/ρ.

Fluid dynamics is (relatively) easy if we can neglect the inertial terms.

For typical BioNEMS/AFM:

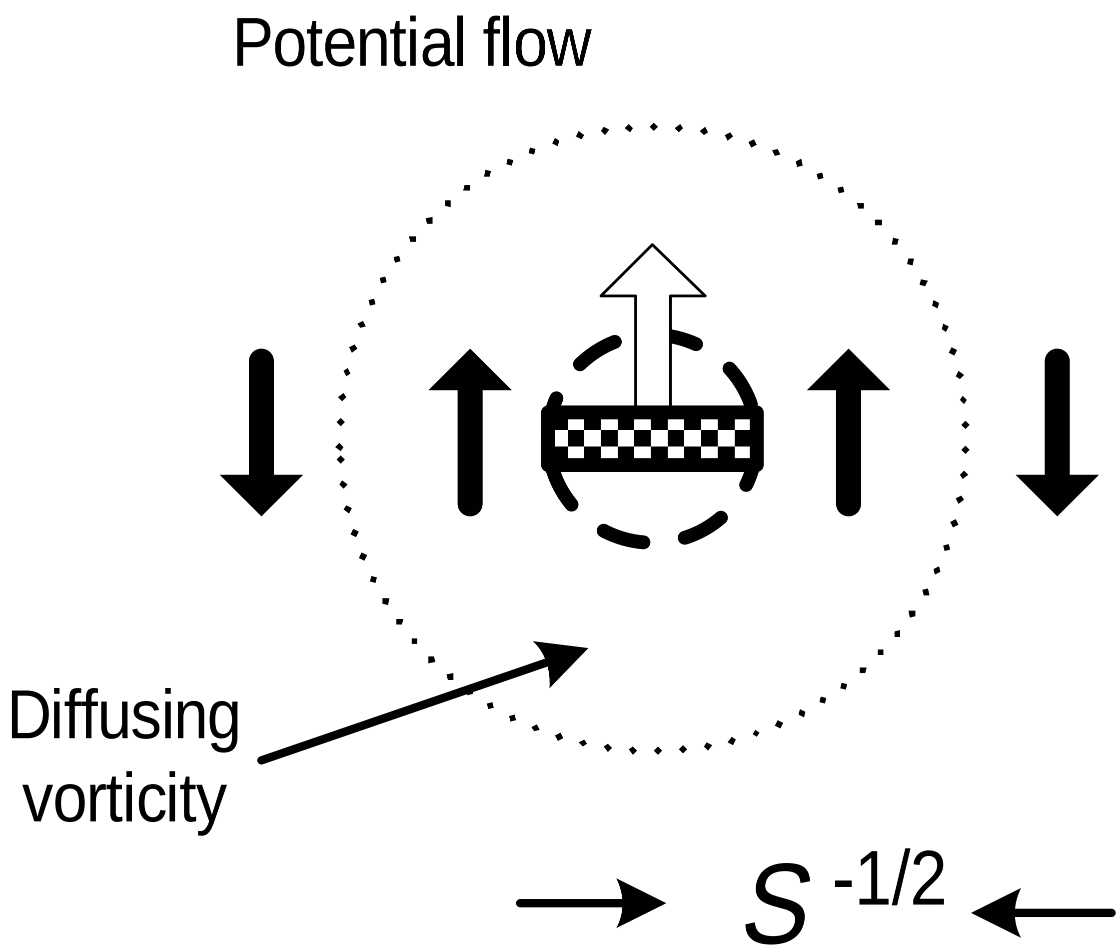
- $\vec{u} \cdot \vec{\nabla} \vec{u} = O(u^2)$ is negligible because of tiny oscillation amplitudes
- Important parameter is the Strouhal number

$$\boxed{\mathcal{S} = \frac{\omega w^2}{4\nu} \approx 1.6}$$

ω	frequency	$2\pi \times 1$ MHz
w	width	1μ
ν	kinematic viscosity	10^{-6} m^{2}s^{-1}

Low Reynolds number flow: linear ...but can't take $\mathcal{S} = 0$

Simple Picture (Sader)



Stokes Theory

Viscous force on sphere of radius a moving with speed v is

$$F/v = 6\pi\rho\nu a$$

Viscous force per unit length of cylinder of radius a is given by

$$\gamma = F/v = \pi\rho\nu \times \mathcal{S}\,\mathrm{Im}\,\Gamma(\mathcal{S})$$

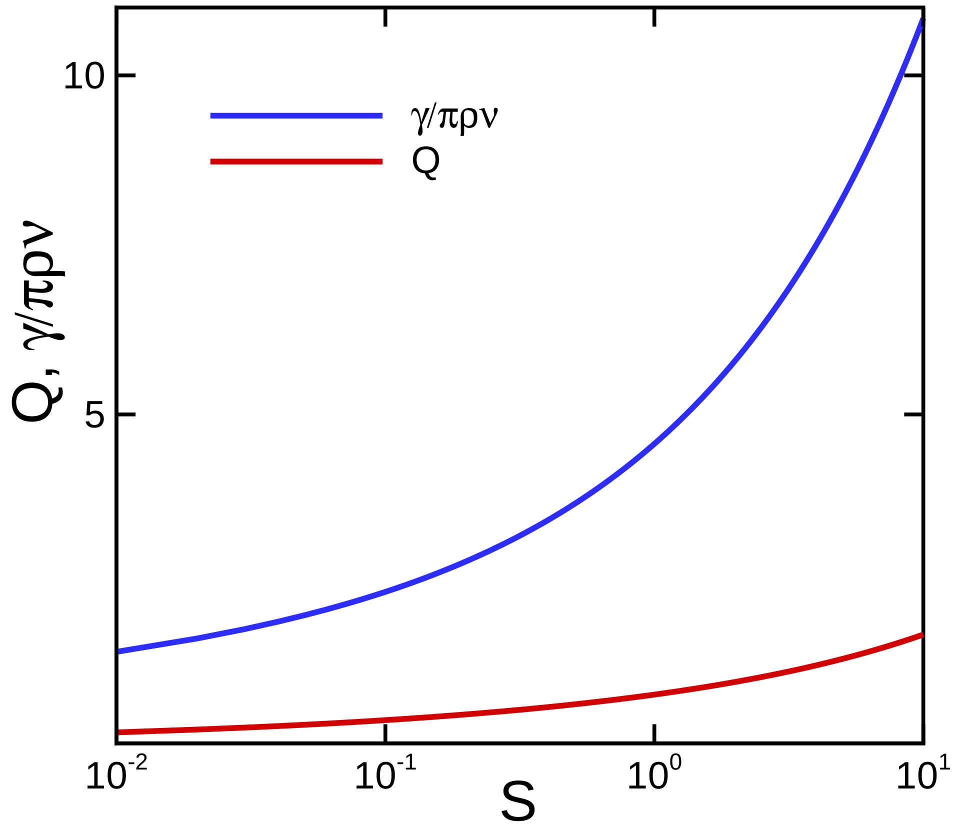
with

$$\Gamma(\mathcal{S}) = 1 + \frac{4iK_1(-i\sqrt{i\mathcal{S}})}{\sqrt{i\mathcal{S}}K_0(-i\sqrt{i\mathcal{S}})}$$

Effective mass per unit length from fluid

$$M = \pi a^2\rho\,\mathrm{Re}\,\Gamma(\mathcal{S}) \Longrightarrow Q \simeq \frac{\mathrm{Re}\,\Gamma(\mathcal{S})}{\mathrm{Im}\,\Gamma(\mathcal{S})}$$

(Other parameter $\mathcal{T} = \frac{\pi}{4}\frac{\rho}{\rho_s}\frac{w}{t} = \frac{\text{mass of cylinder of fluid}}{\text{mass of cantilever}} \sim 2$)



For small $\mathcal{S}$: $$\mathcal{S}\Gamma(\mathcal{S}) \to \frac{-4i}{\frac{1}{2}\log\left(\frac{4}{\mathcal{S}}\right) - C_E + i\,\frac{\pi}{4}}$$

New approach: fluctuation-dissipation theorem

(Paul and MCC, 2004)

Equilibrium fluctuations can be related to the decay of a prepared initial condition

- (near equilibrium) thermodynamics: Onsager regression hypothesis
- statistical mechanics: fluctuation-dissipation theorem, linear response theory, Kubo formalism …

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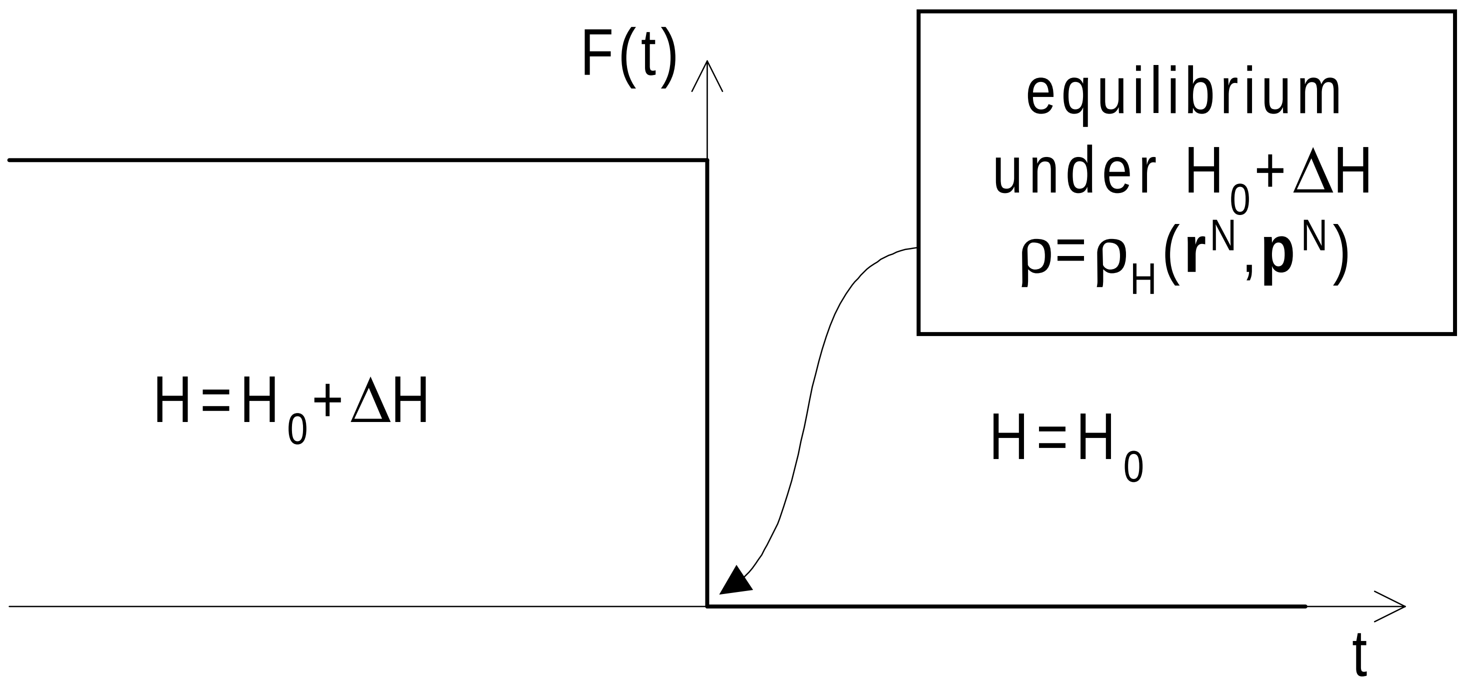
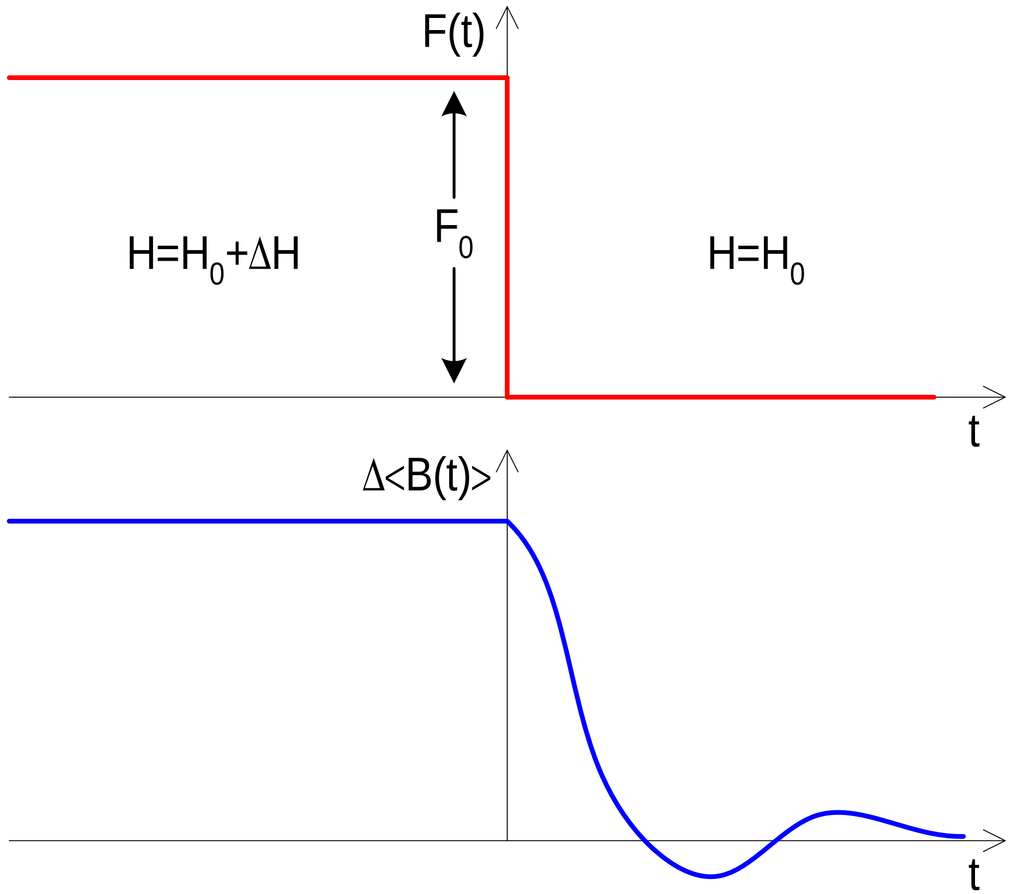
Consider Hamiltonian

$$H = H_0 - F(t)A$$

H_0	unperturbed Hamiltonian
$A(\mathbf{r}_1 \ldots \mathbf{r}_N, \mathbf{p}_1 \ldots \mathbf{p}_N)$	system observable
$F(t)$	(small) time dependent force


F(t)
equilibrium
under $H_0+\Delta H$
$\rho=\rho_H(\mathbf{r}^N,\mathbf{p}^N)$
$H=H_0+\Delta H$
$H=H_0$
t



$$\langle \delta B(t)\delta A(0)\rangle_{\mathrm{e}} = k_B T \frac{\Delta \langle B(t)\rangle}{F_0}$$

Derivation

(e.g. see “Introduction to Modern Statistical Mechanics” by *Chandler)*

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We can calculate averages in terms of the known distribution $\rho\left(\mathbf{r}^N, \mathbf{p}^N\right)$ at $t = 0$:

$$\langle B(t)\rangle = \int d\mathbf{r}^N d\mathbf{p}^N \rho\left(\mathbf{r}^N, \mathbf{p}^N\right) B\left(\mathbf{r}^N(t), \mathbf{p}^N(t)\right)$$

where $\mathbf{r}^N(t)$ is the phase space coordinate that evolves from the value $\mathbf{r}^N$ at $t = 0$.

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where $\mathbf{r}^N(t)$ is the phase space coordinate that evolves from the value $\mathbf{r}^N$ at $t = 0$.

We could equivalently follow the time evolution of ρ through Liouville's equation and instead evaluate

$$\langle B(t)\rangle = \int d\mathbf{r}^N d\mathbf{p}^N \rho\left(\mathbf{r}^N, \mathbf{p}^N, t\right) B\left(\mathbf{r}^N, \mathbf{p}^N\right)$$

but the first form is more convenient.

Derivation (cont.)

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$$\rho(\mathbf{r}^N, \mathbf{p}^N) = \frac{e^{-\beta(H_0+\Delta H)}}{\int d\mathbf{r}^N d\mathbf{p}^N e^{-\beta(H_0+\Delta H)}}$$

so that

$$\langle B\,(0)\rangle = \frac{Tr e^{-\beta(H_0+\Delta H)} B\left(\mathbf{r}^N, \mathbf{p}^N\right)}{Tr e^{-\beta(H_0+\Delta H)}}$$

writing $Tr \equiv \int d\mathbf{r}^N d\mathbf{p}^N$.

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For $t \ge 0$ we let $\mathbf{r}^N(t)$, $\mathbf{p}^N(t)$ for each member of the ensemble evolve under the Hamiltonian, now H_0, from its value $\mathbf{r}^N, \mathbf{p}^N$ at $t = 0$, so that

$$\langle B(t)\rangle = \frac{Tr\, e^{-\beta(H_0+\Delta H)} B\left(\mathbf{r}^N(t), \mathbf{p}^N(t)\right)}{Tr\, e^{-\beta(H_0+\Delta H)}}\ .$$

Note that the integral is over $\mathbf{r}^N, \mathbf{p}^N \equiv \mathbf{r}^N(0), \mathbf{p}^N(0)$, and $\Delta H = \Delta H\left(\mathbf{r}^N, \mathbf{p}^N\right)$ etc.

Derivation (cont.)

It is now a simple matter to expand the exponentials to first order in ΔH (F_0 small!)

$$\langle B(t)\rangle \simeq \frac{Tre^{-\beta H_0}(1-\beta\Delta H)B\left(\mathbf{r}^N(t),\mathbf{p}^N(t)\right)}{Tre^{-\beta H_0}(1-\beta\Delta H)}$$

to give

$$\langle B(t)\rangle = \langle B\rangle_0 - \beta\left[\langle \Delta H\ B(t)\rangle_0 - \langle B\rangle_0\langle\Delta H\rangle_0\right] + O\left(\Delta H\right)^2$$

where $<>_0$ denotes the average over the ensemble for an unperturbed system i.e. using $\rho_0 = e^{-\beta H_0}/Tre^{-\beta H_0}$.

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Finally writing $\delta B(t) = B(t) - \langle B\rangle_0$ etc., and noticing that putting in the form of ΔH

$$\Delta H = -F_0 A(\mathbf{r}^N,\mathbf{p}^N) = -F_0 A\left(0\right)$$

gives for the change in the measurement $\Delta\langle B(t)\rangle = \langle B(t)\rangle - \langle B\rangle_0$

$$\Delta\langle B(t)\rangle = \beta F_0\ \langle \delta A\left(0\right)\delta B(t)\rangle_0 \quad .$$

Application to single cantilever

Assume observable is tip displacement $X(t)$

- Apply small step force of strength F_0 to tip
- Calculate or simulate deterministic decay of $\Delta X(t)$ for $t > 0$. Then

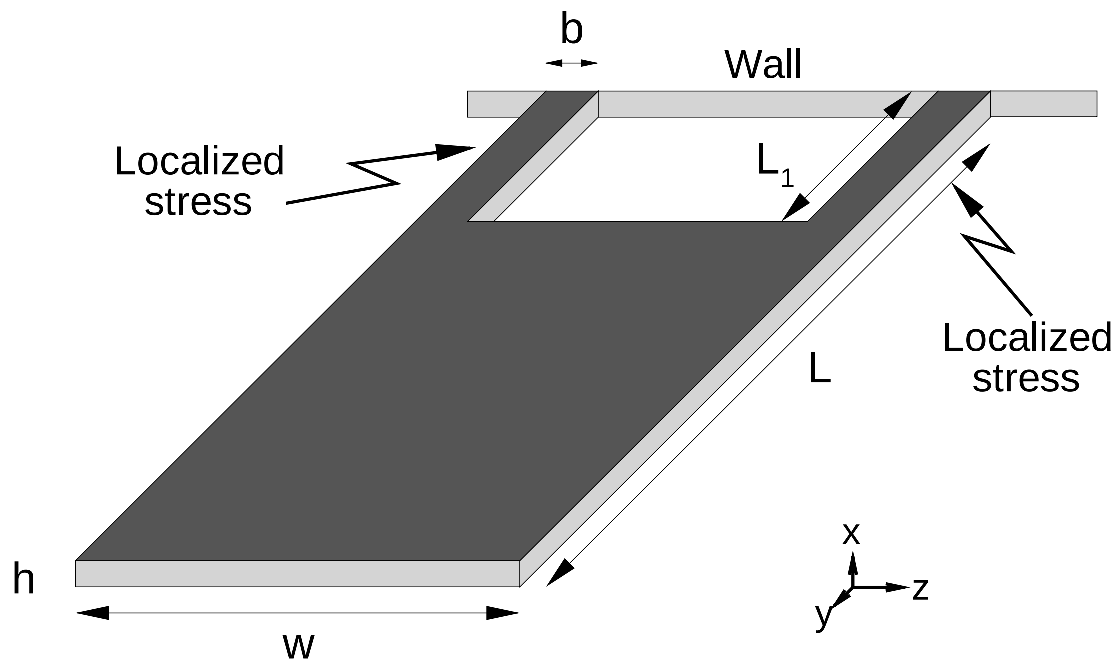
$$C_{XX}(t) = \langle \delta X(t) \delta X(0) \rangle_{\mathrm{e}} = k_B T \frac{\Delta X(t)}{F_0}$$

- Fourier transform of $C_{XX}(t)$ gives power spectrum of X fluctuations $G_X(\omega)$

Advantages

- Correct!
- Essentially no approximations in formulation
  - ◇ assume $\Delta \langle X(t) \rangle$ given by deterministic calculation
  - ◇ also in implementation assume continuum description
- Incorporates
  - ◇ full elastic-fluid coupling
  - ◇ non-white, spatially dependent noise
  - ◇ no assumption on independence of mode fluctuations
  - ◇ complex geometries
- Single numerical calculation over decay time gives complete power spectrum
- Can be modified for other measurement protocols by appropriate choice of conjugate force
  - ◇ AFM: deflection of light (angle near tip)
  - ◇ BioNEMS: curvature near pivot (piezoresistivity)

Single cantilever



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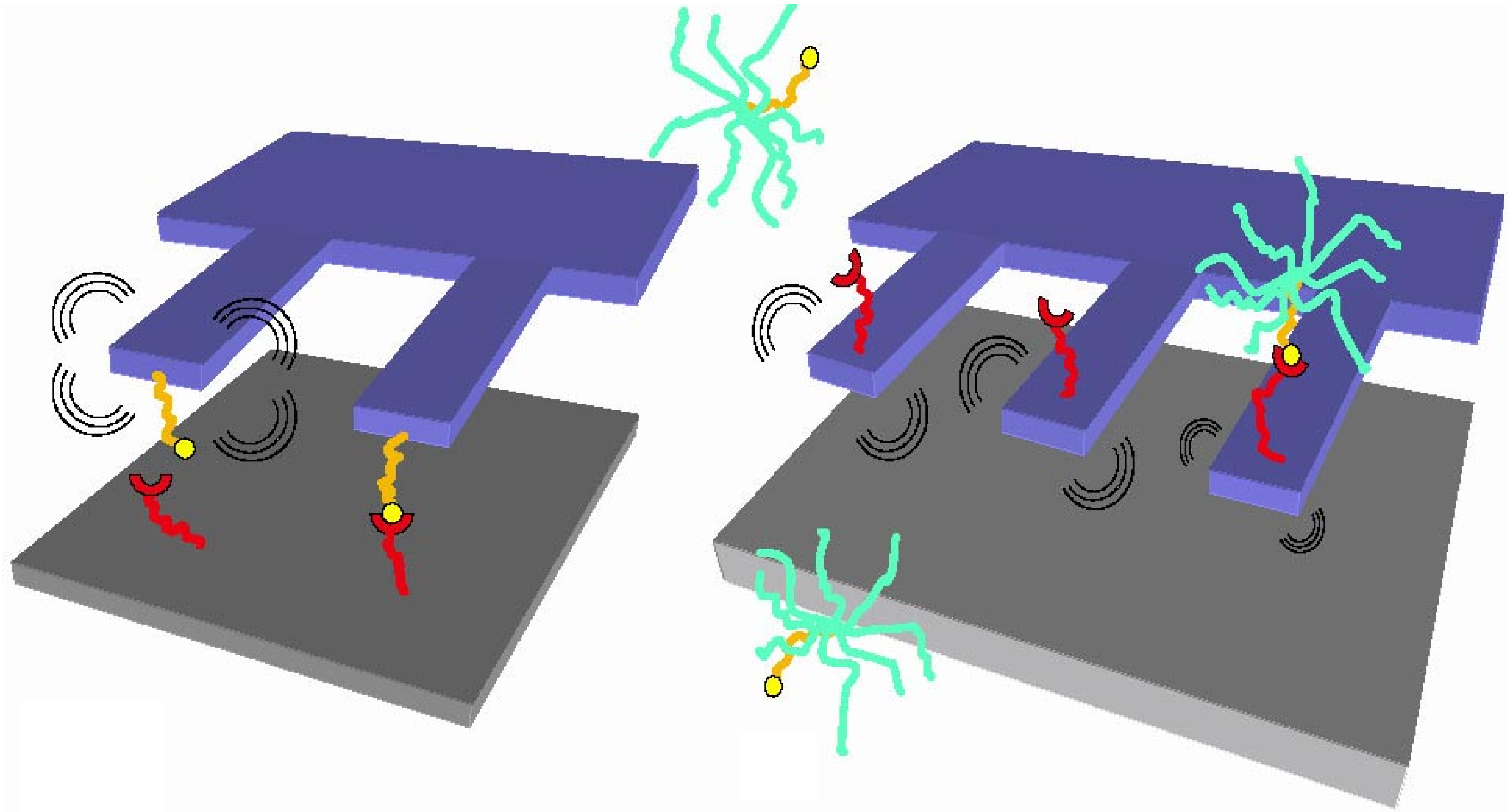
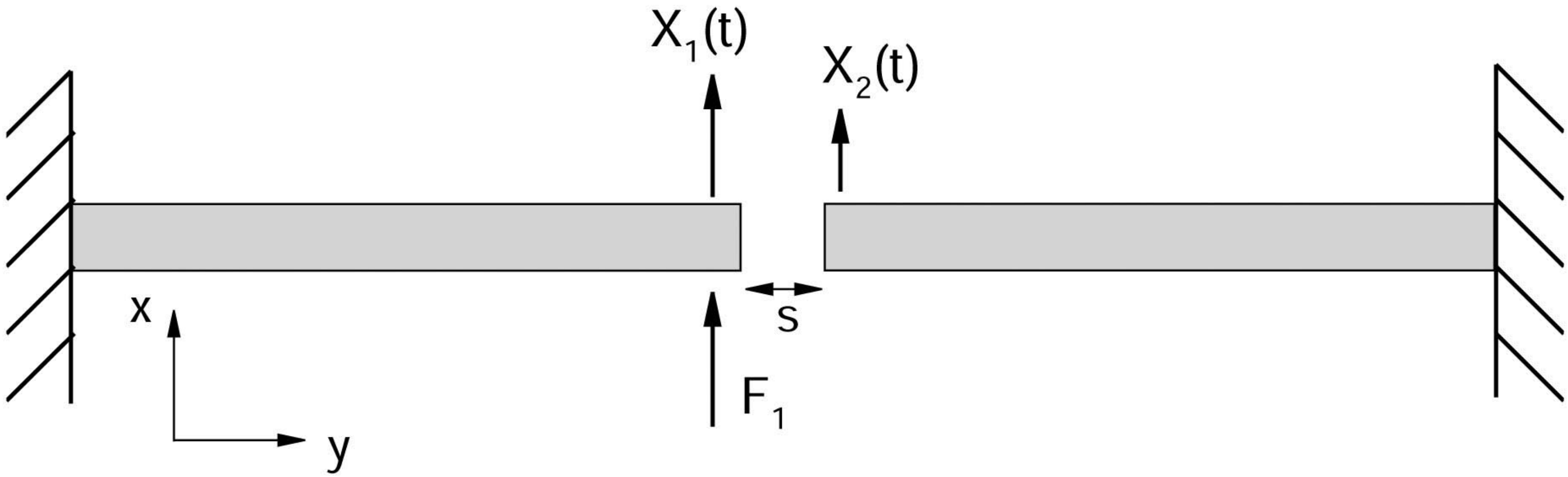
Device schematic



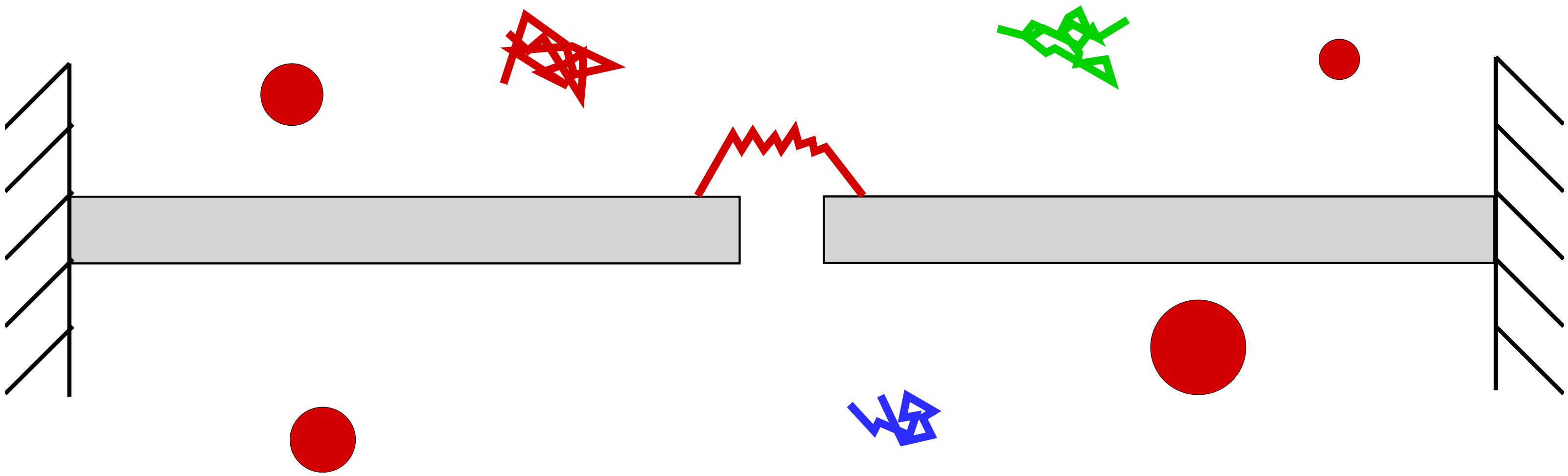
Adjacent cantilevers



Correlation of Brownian fluctuations

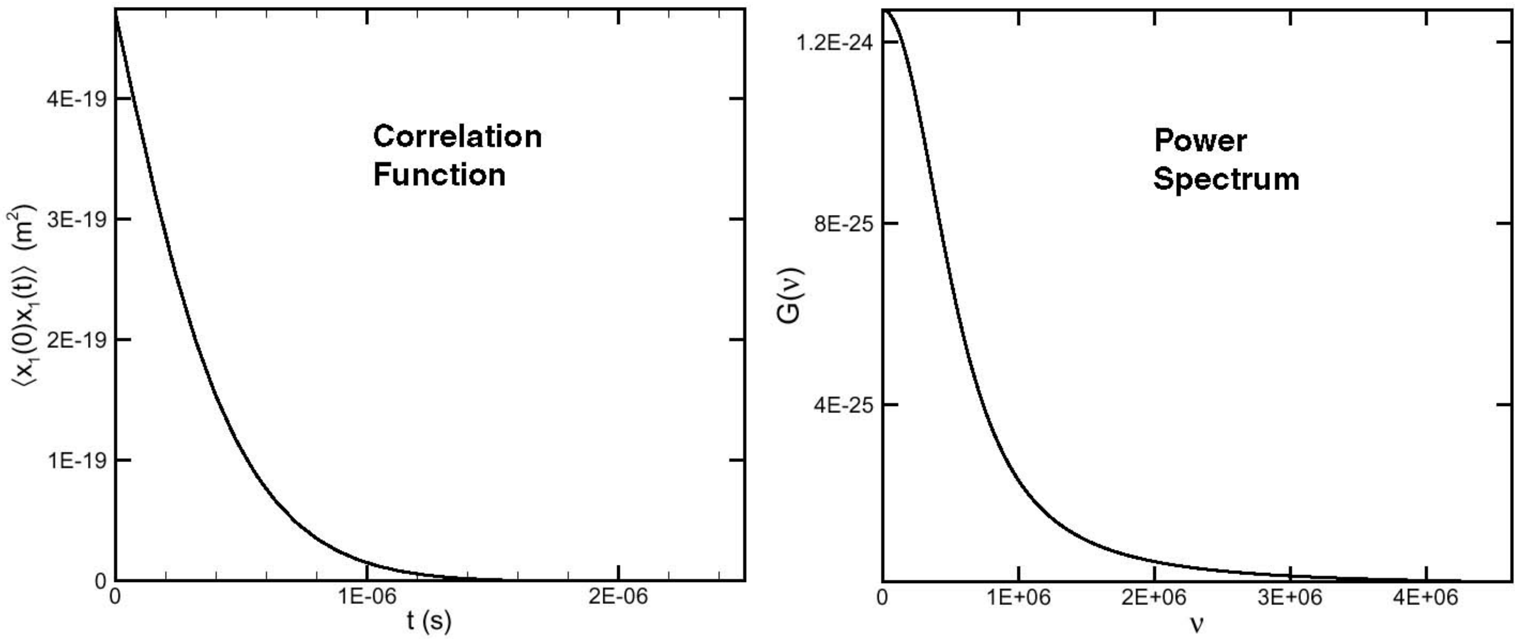
$$\langle \delta X_2(t)\delta X_1(0)\rangle_{\rm e} = k_B T \frac{\Delta X_2(t)}{F_1}$$

Device schematic



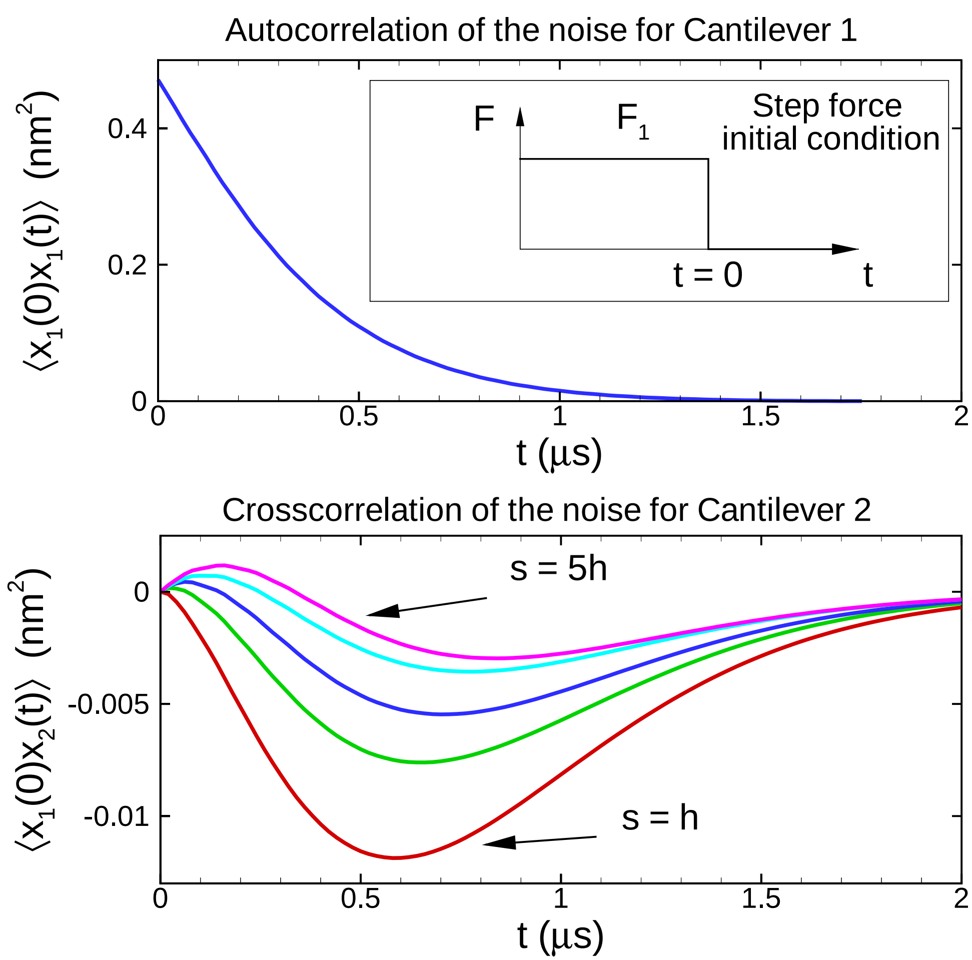
Results: single cantilever

3d Elastic-fluid code from CFD Research Corporation

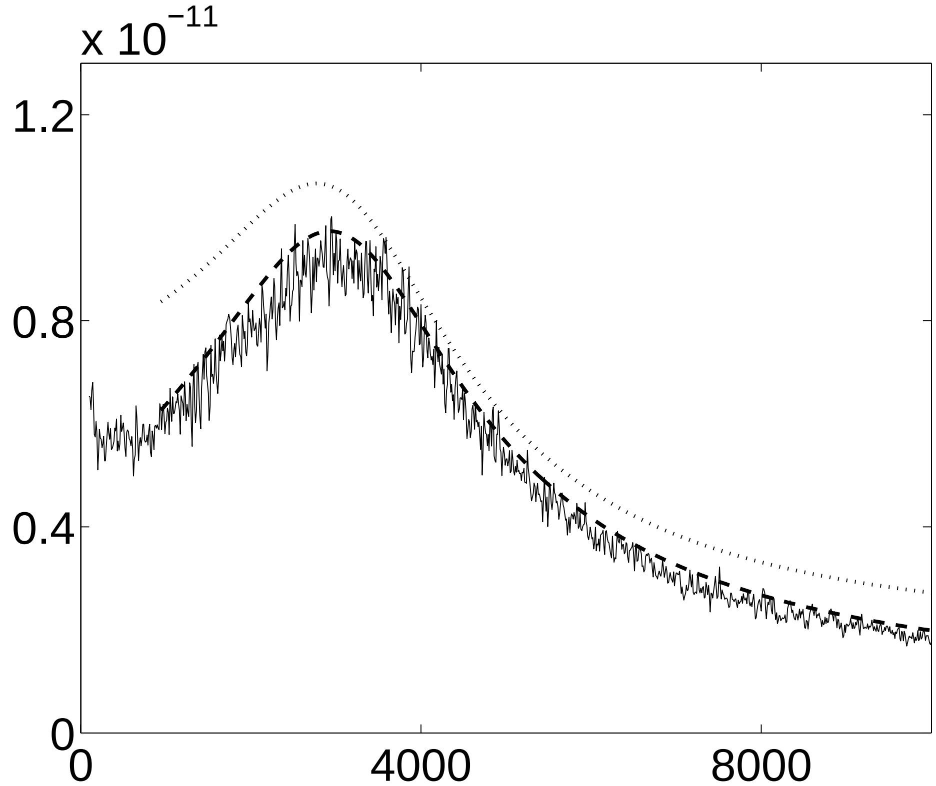


1μs force sensitivity: $K\sqrt{G_X(\nu) \times 1MHz} \sim 7pN$

Results: adjacent cantilevers



Comparison with AFM experiments

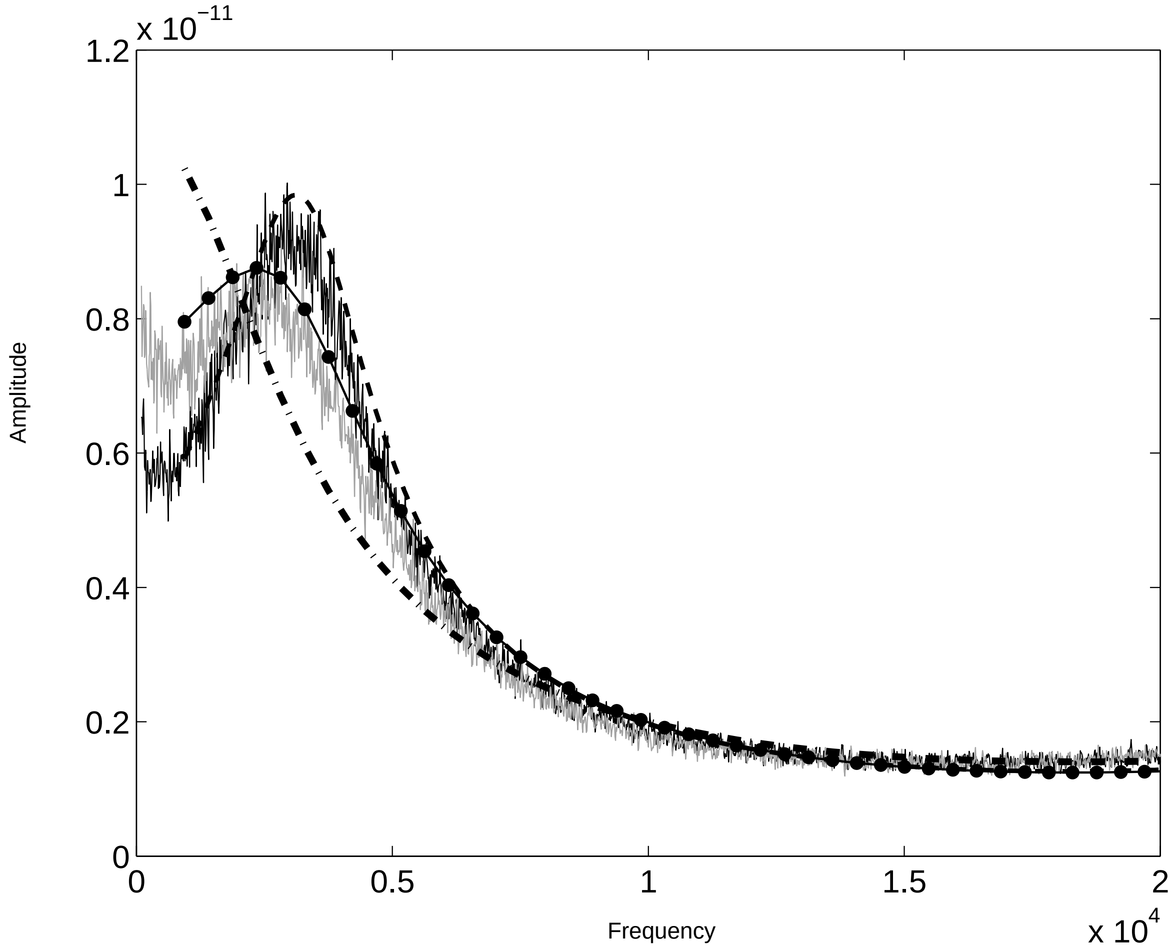


$232.4\mu \times 20.11\mu \times 0.573\mu$ Asylum Research AFM (Clarke et al., 2005)

Dashed line: calculations from fluctuation-dissipation approach

Dotted line: calculations from Sader (1998) approach

Wall effects



Conclusions

I've described one aspect of theoretically modelling micron and submicron scale oscillators

- Linear fluctuations in solution [Paul and MCC, Phys. Rev. Lett. **92**, 235501 (2004)]

Other areas of interest:

- Nonlinear collective effects of parametrically driven high-Q arrays [Lifshitz and MCC, Phys. Rev. **B67**, 134302 (2003)]
- Analysis of a QND scheme to measure the discrete levels in quantum harmonic oscillator [Santamore, Doherty, and MCC, Phys. Rev. **B70**, 144301 (2004)]
- Synchronization due to nonlinear frequency pulling and reactive coupling [MCC, Zumdieck, Lifshitz, and Rogers, Phys. Rev. Lett. **93**, 224101 (2004)]
- Noise induced transitions between driven (nonequilibrium) states
  - ⋆ Single nonlinear oscillator [cf. Aldridge and Cleland, Phys. Rev. Lett. **94**, 156403 (2005)]
  - ⋆ Collective states in arrays of oscillators