Computer Aided Design of Micro-Electro-Mechanical Systems

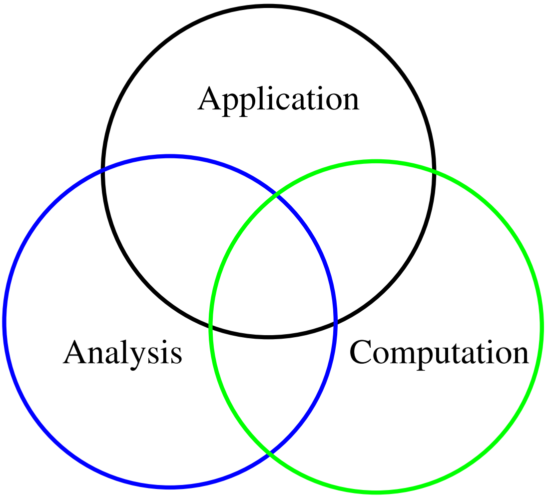
From Eigenvalues to Devices

David Bindel

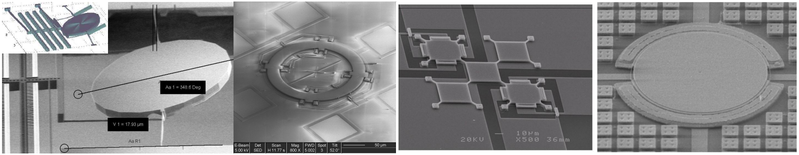
Department of Computer Science
Cornell University

Duke University, 4 Apr 2013

The Computational Science & Engineering Picture



A Favorite Application: MEMS



I've worked on this for a while:

- SUGAR (early 2000s) – SPICE for MEMS
- HiQLab (2006) – high-Q mechanical resonator device modeling
- AxFEM (2012) – solid-wave gyro device modeling

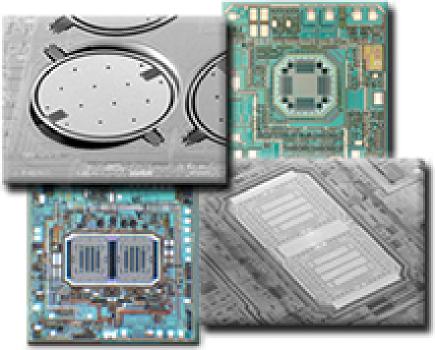
Goal today: two illustrative snapshots.

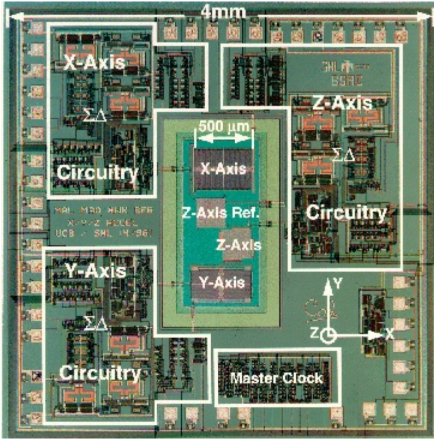
Outline

MEMS Basics

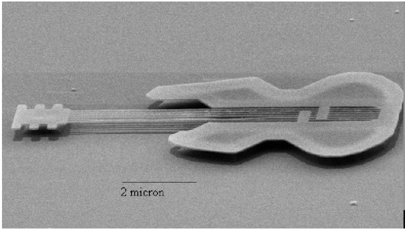
- Micro-Electro-Mechanical Systems
  - Chemical, fluid, thermal, optical (MECFTOMS?)
- Applications:
  - Sensors (inertial, chemical, pressure)
  - Ink jet printers, biolab chips
  - Radio devices: cell phones, inventory tags, pico radio
- Use integrated circuit (IC) fabrication technology
- Tiny, but still classical physics

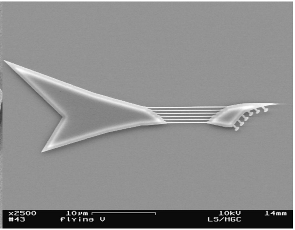
Where are MEMS used?

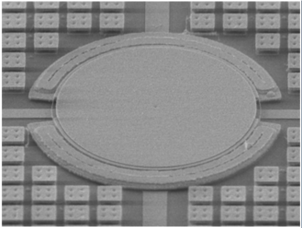


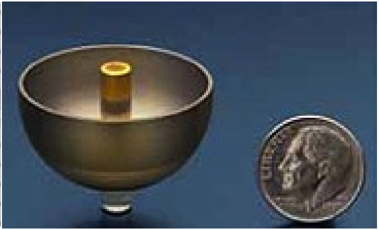


My favorite applications



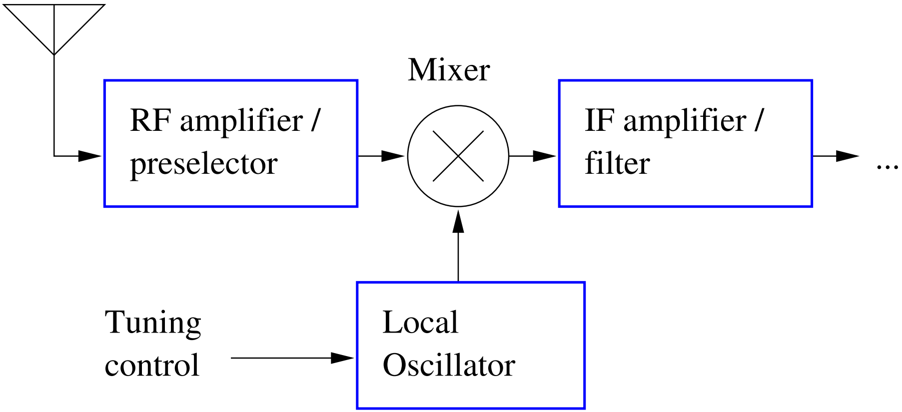






Why you should care, too!

The Mechanical Cell Phone



- ...and lots of mechanical sensors, too!

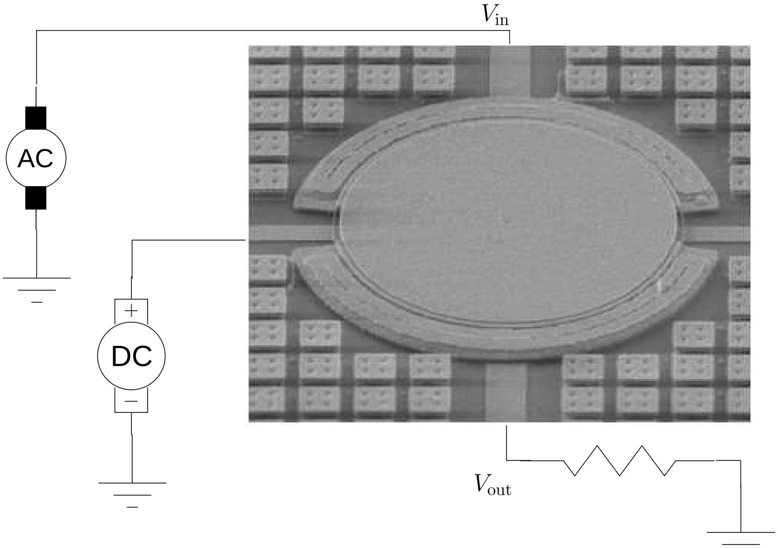
Ultimate Success

"Calling Dick Tracy!"

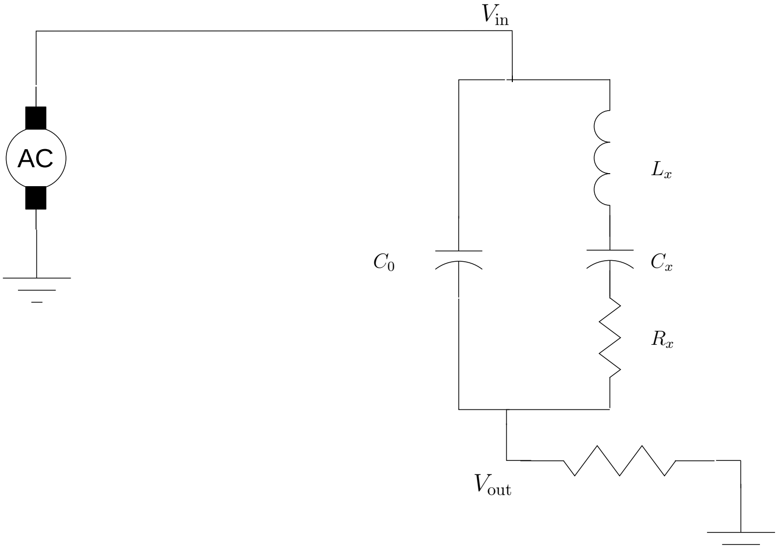
Computational Challenges

Devices are fun – but I'm not a device designer.
Why am I in this?

Model System



The Circuit Designer View



Electromechanical Model

Balance laws (KCL and BLM):

$$\begin{aligned} \frac{d}{dt}\left(C(u)V\right) + GV &= I_{\text{external}} \\ Mu_{tt} + Ku - \nabla_u \left(\frac{1}{2} V^* C(u) V\right) &= F_{\text{external}} \end{aligned}$$

Linearize about static equilibium (V_0, u_0):

$$\begin{aligned} C(u_0)\,\delta V_t + G\,\delta V + \left(\nabla_u C(u_0) \cdot \delta u_t\right) V_0 &= \delta I_{\text{external}} \\ M\,\delta u_{tt} + \tilde{K}\,\delta u + \nabla_u \left(V_0^* C(u_0)\,\delta V\right) &= \delta F_{\text{external}} \end{aligned}$$

where

$$\tilde{K} = K - \frac{1}{2} \frac{\partial^2}{\partial u^2} \left(V_0^* C(u_0) V_0\right)$$

Electromechanical Model

Assume time-harmonic steady state, no external forces:

$$\begin{bmatrix} i\omega C + G & i\omega B \\ -B^T & \tilde{K} - \omega^2 M \end{bmatrix} \begin{bmatrix} \delta\hat{V} \\ \delta\hat{u} \end{bmatrix} = \begin{bmatrix} \delta\hat{I}_{\text{external}} \\ 0 \end{bmatrix}$$

Eliminate the mechanical terms:

$$\begin{aligned} Y(\omega)\,\delta\hat{V} &= \delta\hat{I}_{\text{external}} \\ Y(\omega) &= i\omega C + G + i\omega H(\omega) \\ H(\omega) &= B^T(\tilde{K} - \omega^2 M)^{-1} B \end{aligned}$$

Goal: Understand electromechanical piece ($i\omega H(\omega)$).

- As a function of geometry and operating point
- Preferably as a simple circuit

Damping and Q

Designers want high *quality of resonance* (Q)

- Dimensionless damping in a one-dof system

$$\frac{d^2u}{dt^2} + Q^{-1}\frac{du}{dt} + u = F(t)$$

- For a resonant mode with frequency $\omega \in \mathbb{C}$:

$$Q := \frac{|\omega|}{2\,\mathrm{Im}(\omega)} = \frac{\text{Stored energy}}{\text{Energy loss per radian}}$$

To understand Q, we need damping models!

The Designer's Dream

Reality is messy:

- Coupled physics
- ... some poorly understood (damping)
- ... subject to fabrication errors

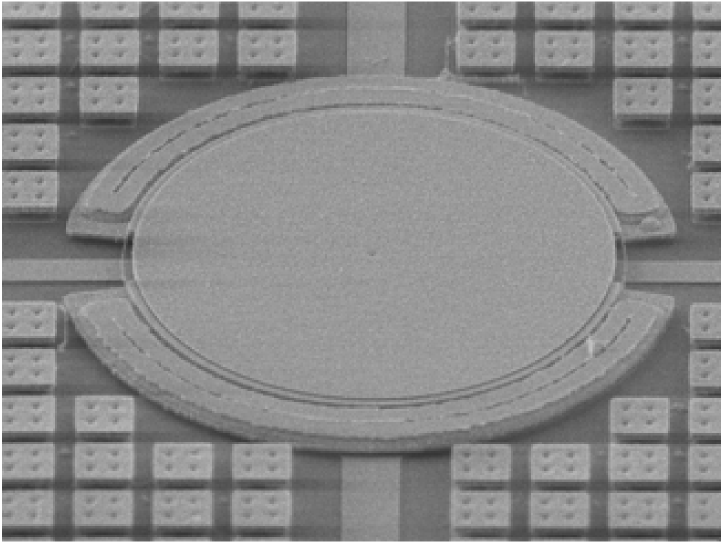
Ideally, would like:

- Simple models for behavioral simulation
- Parameterized for design optimization
- Including all relevant physics
- With reasonably fast and accurate set-up

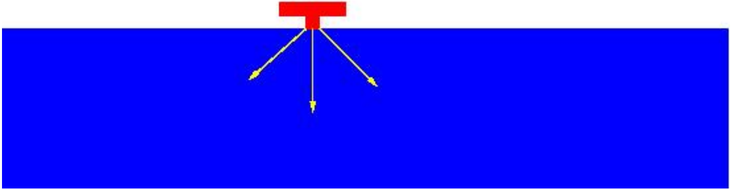
We aren't there yet.

Outline

Disk Resonator Simulations



Damping Mechanisms

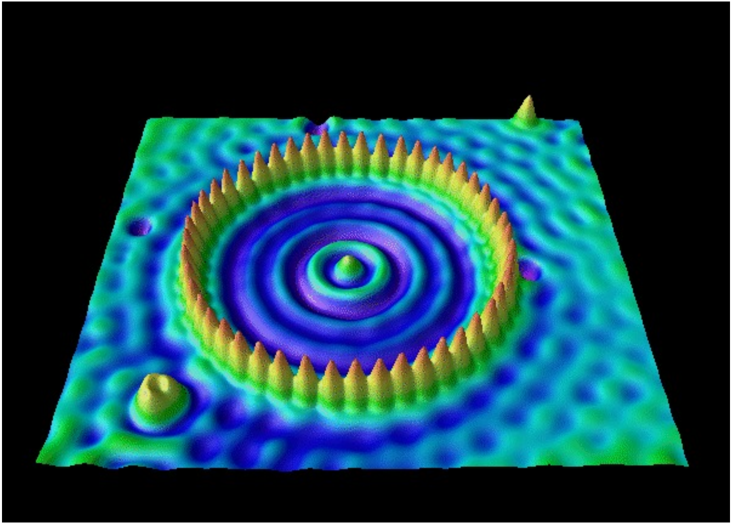


Possible loss mechanisms:

- Fluid damping
- Material losses
- Thermoelastic damping
- Anchor loss

Model substrate as semi-infinite $\Longrightarrow$ resonances!

Resonances in Physics



Resonances and Literature

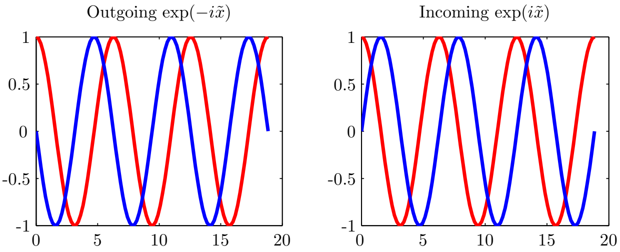
In bells of frost I heard the resonance die.

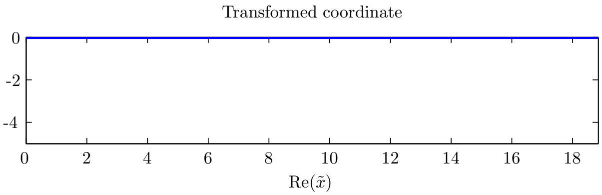
– Li Bai (translated by Vikram Seth)

Perfectly Matched Layers

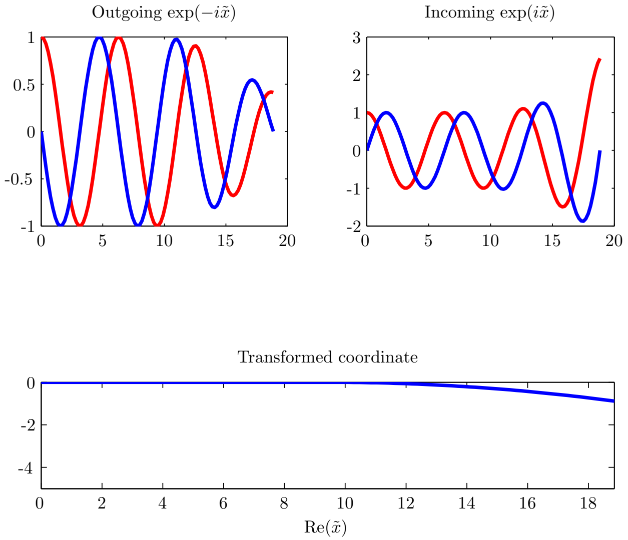
- Complex coordinate transformation
- Generates a “perfectly matched” absorbing layer
- Idea works with general linear wave equations
    - Electromagnetics (Berengér, 1994)
    - Quantum mechanics – *exterior complex scaling* (Simon, 1979)
    - Elasticity in standard finite element framework (Basu and Chopra, 2003)
    - Works great for MEMS, too! (Bindel and Govindjee, 2005)

Model Problem Illustrated

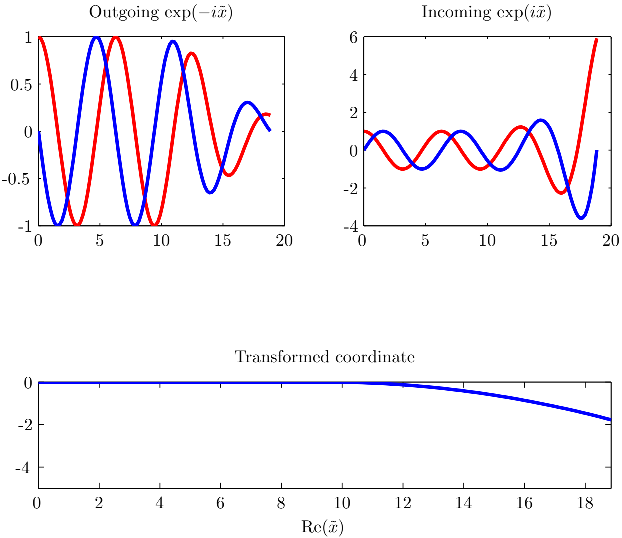




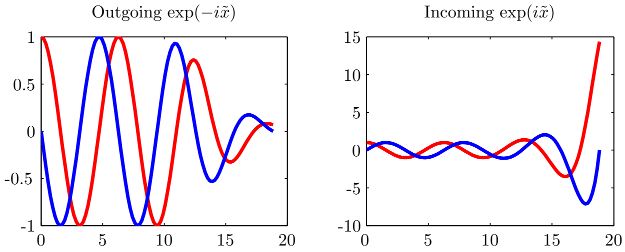
Model Problem Illustrated

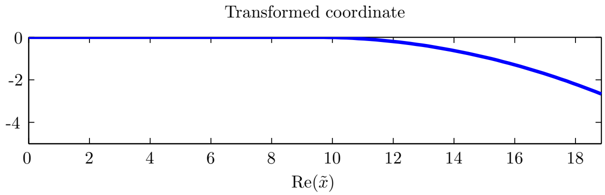


Model Problem Illustrated

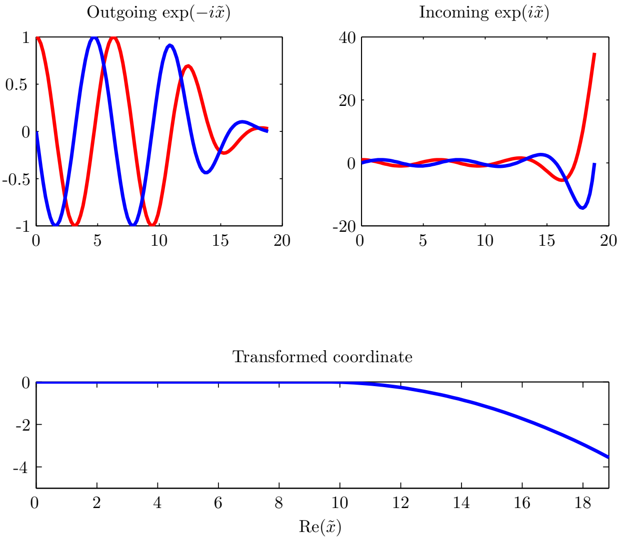


Model Problem Illustrated

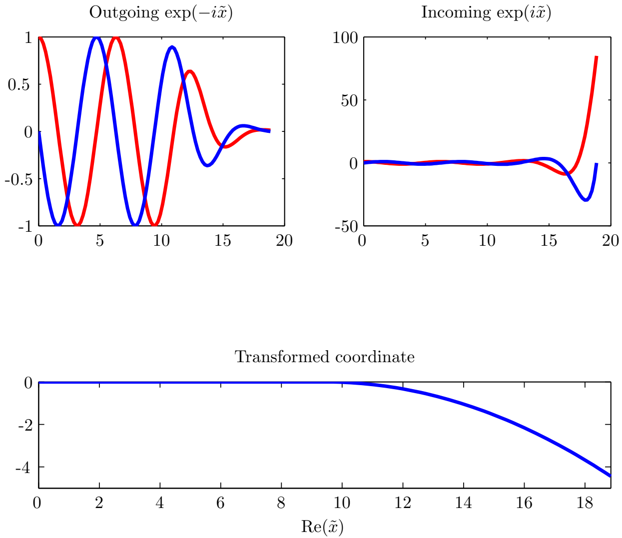




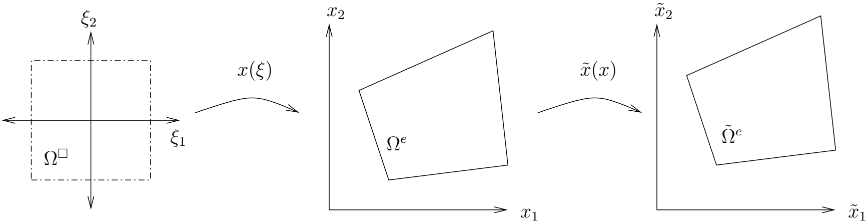
Model Problem Illustrated



Model Problem Illustrated

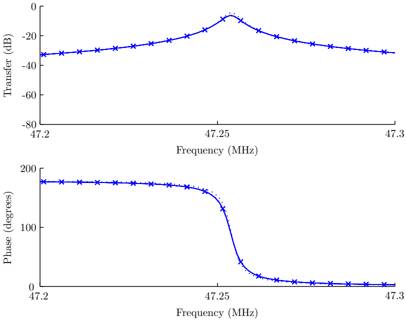


Finite Element Implementation



Matrices are *complex symmetric*

Eigenvalues and Model Reduction



Goal: understand $H(\omega)$:

$$H(\omega) = B^T (K - \omega^2 M)^{-1} B$$

Look at

- Poles of H (eigenvalues)
- Bode plots of H

Model reduction: Replace $H(\omega)$ by cheaper $\hat{H}(\omega)$.

Approximation from Subspaces

A general recipe for large-scale numerical approximation:

1. A subspace $\mathcal{V}$ containing good approximations.
2. A criterion for “optimal” approximations in $\mathcal{V}$.

Basic building block for eigensolvers and model reduction!

Better subspaces, better criteria, better answers.

Variational Principles

- Variational form for complex symmetric eigenproblems:
  - Hermitian (Rayleigh quotient):

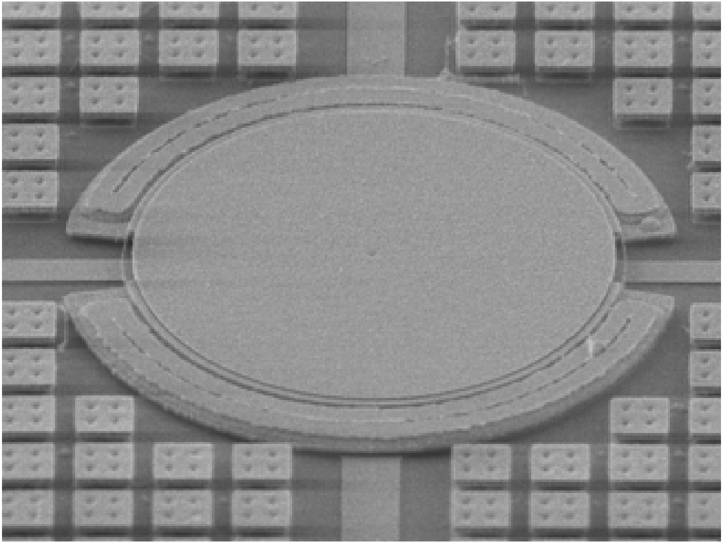
$$\rho(v) = \frac{v^* K v}{v^* M v}$$

  - Complex symmetric (modified Rayleigh quotient):

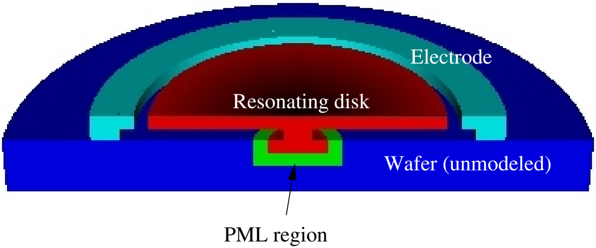
$$\theta(v) = \frac{v^T K v}{v^T M v}$$

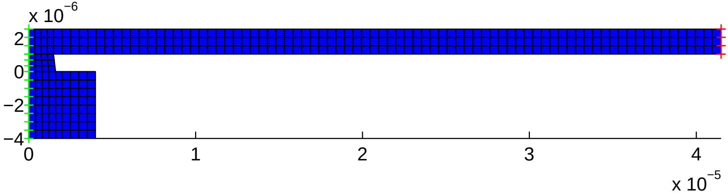
- First-order accurate eigenvectors $\implies$ Second-order accurate eigenvalues.
- Good for model reduction, too!

Disk Resonator Simulations



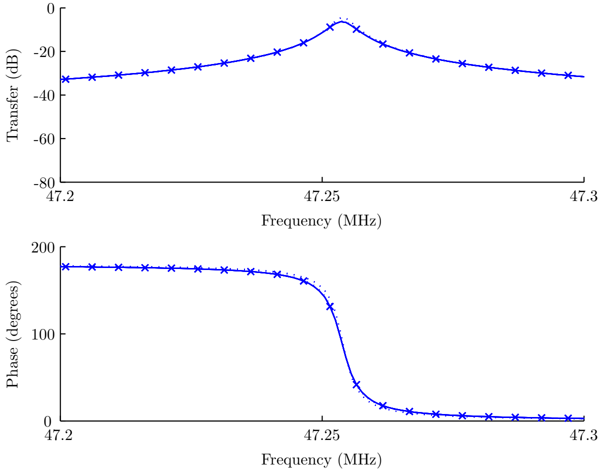
Disk Resonator Mesh





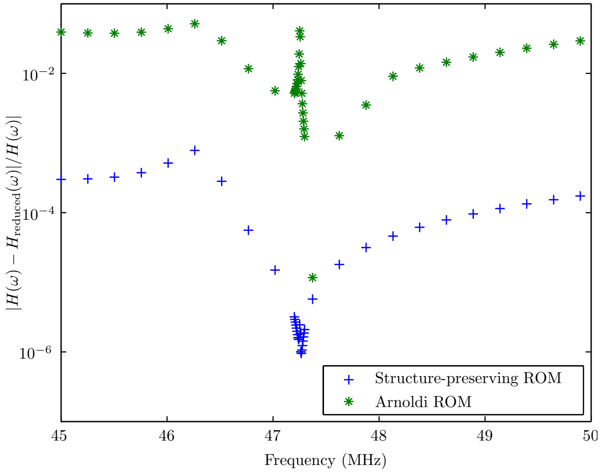
Axisymmetric model, bicubic, $\approx 10^4$ nodal points at convergence

Model Reduction Accuracy



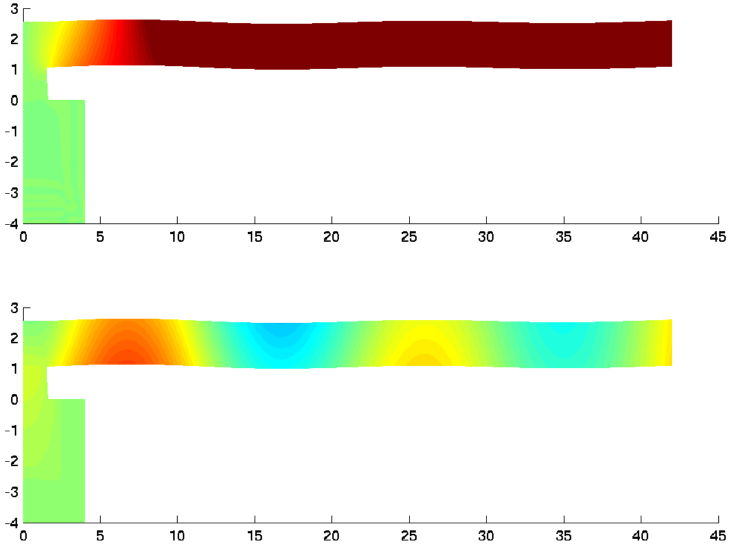
Results from ROM (solid and dotted lines) nearly indistinguishable from full model (crosses)

Model Reduction Accuracy

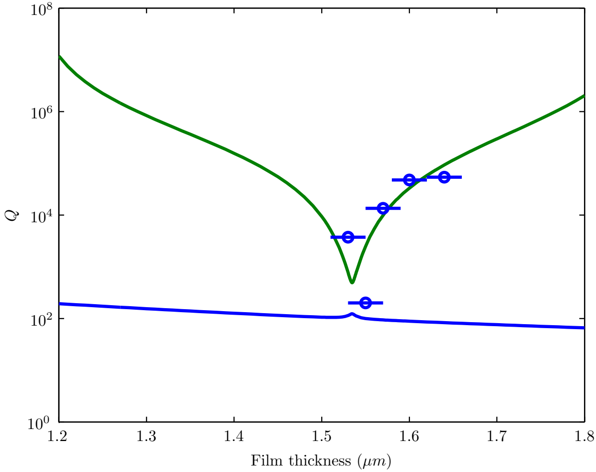


Preserve structure $\Longrightarrow$
get twice the correct digits

Response of the Disk Resonator

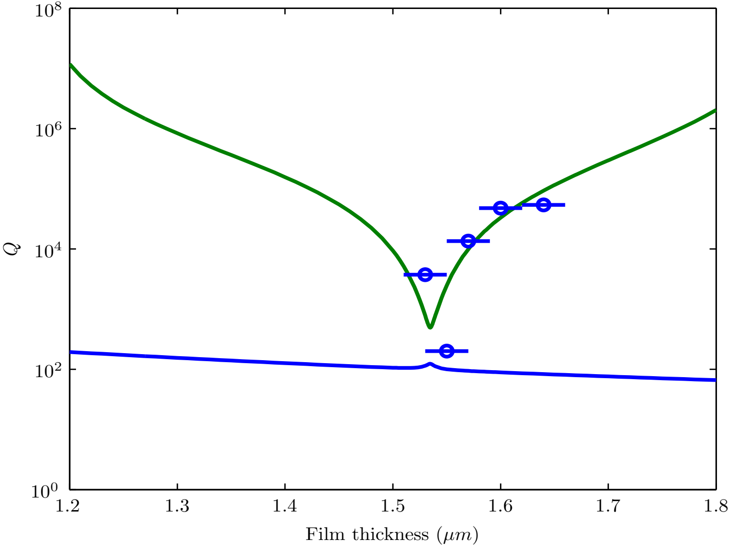


Variation in Quality of Resonance

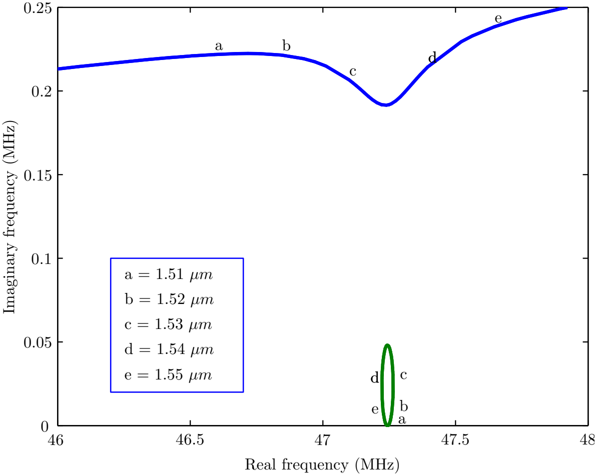


Simulation and lab measurements vs. disk thickness

Explanation of Q Variation



Explanation of Q Variation



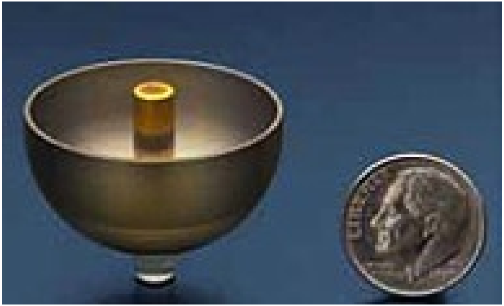
Interaction of two nearby eigenmodes

Outline

Bryan's Experiment

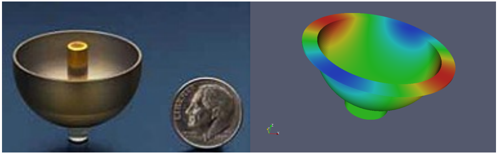
"On the beats in the vibrations of a revolving cylinder or bell"
by G. H. Bryan, 1890

A Small Application



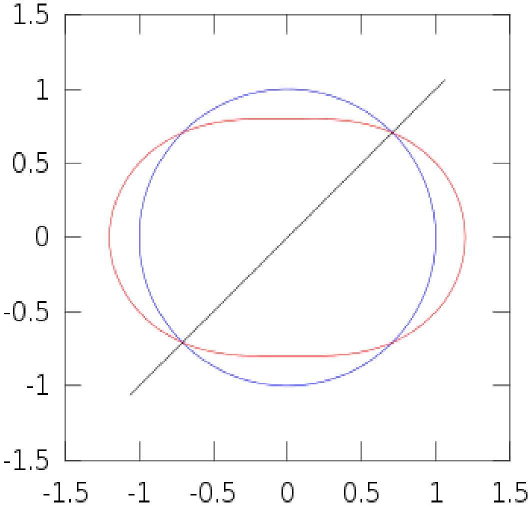
Northrup-Grummond HRG

Current example: Micro-HRG / GOBLiT / OMG

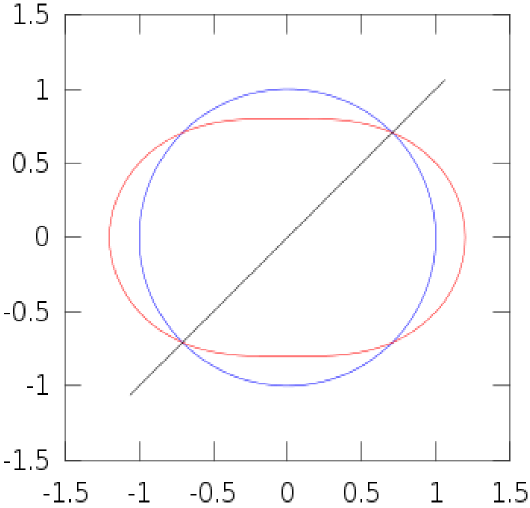


- Goal: Cheap, small (1mm) HRG
- Collaborator roles:
  - Basic design
  - Fabrication
  - Measurement
- Our part:
  - Detailed physics
  - Fast software
  - Sensitivity
  - Design optimization

How It Works



How It Works



Goal state

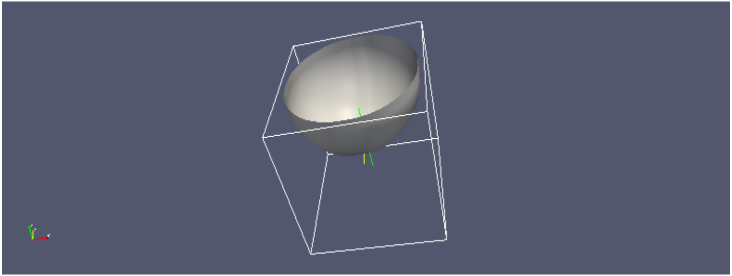
We want to compute:

- Geometry
- Fundamental frequencies
- Angular gain (Bryan's factor)
- Damping (thermoelastic, radiation, material)
- Sensitivities of everything
- Effects of symmetry breaking

For speed and accuracy: use structure!

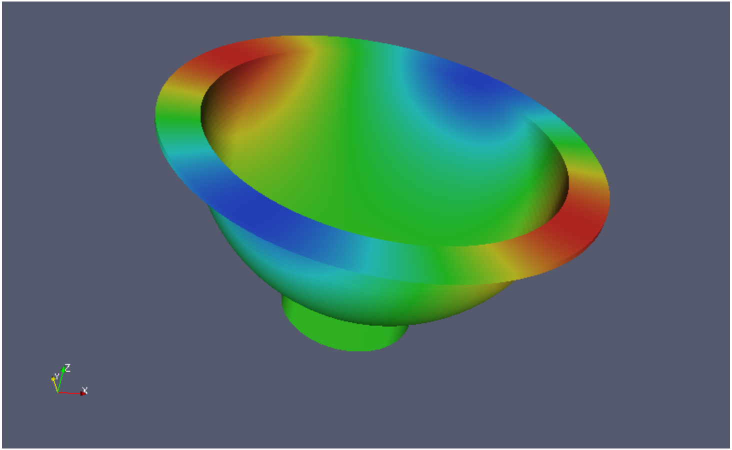
- Axisymmetric geometry $\implies$ 3D to 2D via Fourier
- Perturbed geometry $\implies$ interactions for different wave numbers

Getting the Geometry

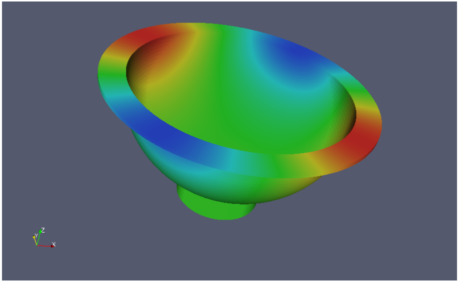


- Simple isotropic etch modeling fails – 1mm is *huge*!
- Working on better simulator (reaction-diffusion).
- For now, take idealized geometries on faith...

Full Dynamics



Essential Dynamics



Dynamics in 2D subspace of degenerate modes:

$$\left(-\omega^2 mI + 2i\omega\Omega g J + kI\right) c = 0$$

Scaled gain g is *Bryan's factor*

$$\mathrm{BF} = \frac{\text{Angular rate of pattern relative to body}}{\text{Angular rate of vibrating body}}$$

If no parameters in the world were very large or very small, science would reduce to an exhaustive list of everything.

– Nick Trefethen

Fourier Picture

Write displacement fields as Fourier series:

$$\mathbf{u} = \sum_{m=0}^{\infty} \left(\begin{bmatrix} u_{mr}(r,z)\cos(m\theta) \\ u_{m\theta}(r,z)\sin(m\theta) \\ u_{mz}(r,z)\cos(m\theta) \end{bmatrix} + \begin{bmatrix} -u'_{mr}(r,z)\sin(m\theta) \\ u'_{m\theta}(r,z)\cos(m\theta) \\ -u'_{mz}(r,z)\sin(m\theta) \end{bmatrix} \right)$$

- Works whenever *geometry* is axisymmetric
- Treat non-axisymmetric geometries as mapped axisymmetric
  - Now *coefficients* in PDEs are non-axisymmetric
- Problems with different m decouple if *everything* axisymmetric

Fourier Picture

Perfect axisymmetry:

$$\begin{bmatrix} K_{11} & & & \\ & K_{22} & & \\ & & K_{33} & \\ & & & \ddots \end{bmatrix} - \omega^2 \begin{bmatrix} M_{11} & & & \\ & M_{22} & & \\ & & M_{33} & \\ & & & \ddots \end{bmatrix}$$

Fourier Picture

Broken symmetry (via coefficients):

$$\begin{bmatrix} K_{11} & \epsilon & \epsilon & \epsilon \\ \epsilon & K_{22} & \epsilon & \epsilon \\ \epsilon & \epsilon & K_{33} & \epsilon \\ \epsilon & \epsilon & \epsilon & \ddots \end{bmatrix} - \omega^2 \begin{bmatrix} M_{11} & \epsilon & \epsilon & \epsilon \\ \epsilon & M_{22} & \epsilon & \epsilon \\ \epsilon & \epsilon & M_{33} & \epsilon \\ \epsilon & \epsilon & \epsilon & \ddots \end{bmatrix}$$

Perturbing Fourier

Modes “near” azimuthal number m = nonlinear eigenvalues

$$\left(K_{mm} - \omega^2 M_{mm} + E_{mm}(\omega) \right) u = 0.$$

Need:

- Control on E_{mm}
  - Depends on frequency spacing
  - Depends on Fourier analysis of perturbation
- Perturbation theory for nonlinearly perturbed eigenproblems
  - For self-adjoint case, results similar to Lehmann intervals

First-order estimate: $(K_{mm} - \omega_0^2 M_{mm}) u_0 = 0$; then

$$\delta(\omega^2) = \frac{u_0^T E_{mm}(\omega_0) u_0}{u_0^T M_{mm} u_0}.$$

Perturbation and Radiation

Incorporating numerical radiation BCs gives:

$$\left(K - \omega^2 M + G(\omega) \right) u = 0.$$

Perturbation approach: ignore G to get (ω_0, u_0). Then

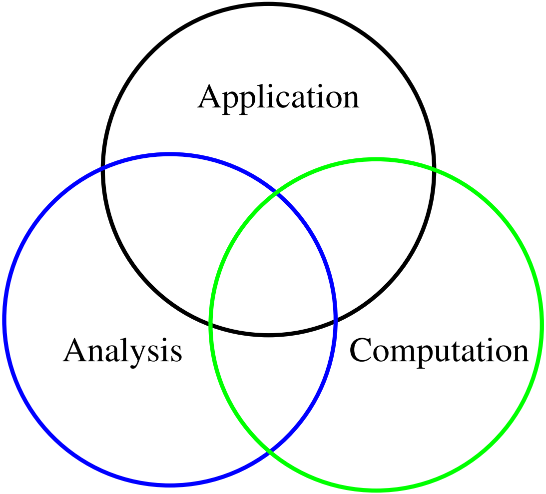
$$\delta(\omega^2) = \frac{u_0^T \, G(\omega_0) \, u_0}{u_0^T M_{mm} u_0}.$$

Works when BC has small *influence* (coefficients aren't small).

Also an approach to understanding sensitivity to BC!
... explains why PML works okay despite being inappropriate?

Outline

The Computational Science & Engineering Picture



Conclusions

The difference between art and science is that science is what we understand well enough to explain to a computer. Art is everything else.

Donald Knuth

The purpose of computing is insight, not numbers.

Richard Hamming

- Collaborators:
  - Disk: S. Govindjee, T. Koyama, S. Bhave, E. Quevy
  - HRG: S. Bhave, L. Fegely, E. Yilmaz
- Funding: DARPA MTO, Sloan Foundation