“Baseline Techniques in My Group”

And some concrete past examples

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Materials by Design Group, 10 Apr 2013

What do we do?

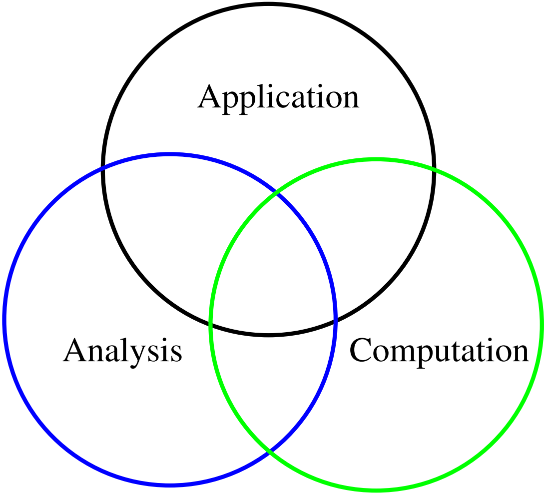
- Jeff Chadwick (CS): Fast structured direct solvers for PDEs
- Erdal Yilmaz (AEP): MEMS micro-gyro simulation
- Amanda Hood (CAM): Nonlinear eigenvalues, resonances
- Colin Ponce (CS): Network analysis, power grid tomography

Outline

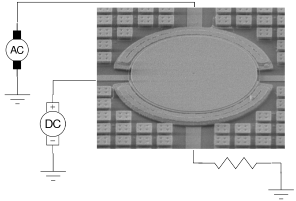
Outline

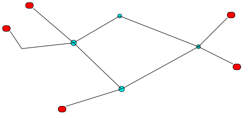
1. Possible materials connections
2. Resonant MEMS
3. Anchor losses and disk resonators
4. Thermoelastic losses and beam resonators
5. Elastic wave gyros
6. Conclusion

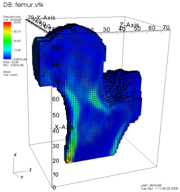
The Computational Science & Engineering Picture



The Computational Science & Engineering Picture







Application modeling

Analysis ⟷ Algorithms and software

$\rho \ddot{u} = \nabla \cdot \sigma$

$Ax = b$

$Ax = \lambda x$

HiQLab, Matscat, ...

Model reduction methods

Structured linear solvers

Useful Expertise? (I): Software

- Writing codes fast
  - High-level tools for writing/enabling simulations (matexpr, luasym, SUGAR, HiQLab, AxFEM, ...)
  - Interface tools to “glue together” codes (MATFEAP, FEAPMEX, MWrap, ...)
- Writing fast codes
  - CS 5220: Applications of Parallel Computers (S14)
  - Some of this is the usual fast solver work
  - Also cloud computing for science

Useful Expertise? (II): Numerical Methods

- Major theme: novel eigenvalue problems
  - Some familiar from physics – nearly degenerate modes, estimators for eigenvalue density
  - Nonlinear eigenvalue problems and resonances
  - Model reduction is closely related!
- Major theme: *structure-preserving* methods
  - Symmetry preservation for model reduction and eigencomputations
  - Fast PDE solvers and low-rank blocks
  - Fast eigensolvers (linear and nonlinear)
  - Parameter-dependent solvers

Useful Expertise? (III): Computational Mechanics

- Continuum level and network level
  - Same ingredients: balance law + constitutive eq + kinematic assumption (for discretization)
  - Beam / circuit theory just assumes more about kinematics!
- Mostly static, quasi-static, or time-harmonic
- Several codes (SUGAR, HiQLab, AxFEM, FEAP)

Useful Expertise? (IV): Network Analysis

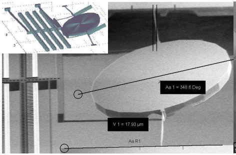
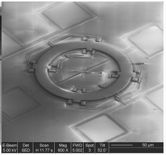
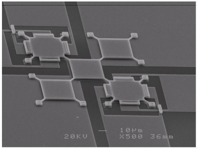
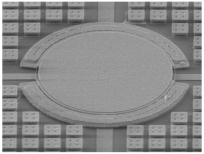
- Several instances:
  - Circuits / MEMS systems (SUGAR)
  - Computer network tomography
  - Social network analysis (clustering)
  - Line failures in power grids
- All turns into linear algebra...

Possible flow

- Inputs:
  - Quasi-continuum models of transport within CNT (BTE?)
  - Constitutive elements: source terms, hopping across junctions
  - Sample geometry and compositions of CNT networks
- Tasks:
  - Fast solvers for detailed simulations on network
  - Model reduction for expensive constitutive elements
  - Sensitivity analysis (check model reduction, assumptions)
  - Model fitting?
  - Reduced model for predicting overall charge transport?
- Output: objective functions for Peter and Jeff?

Outline

A Favorite Application: MEMS

I've worked on this for a while:

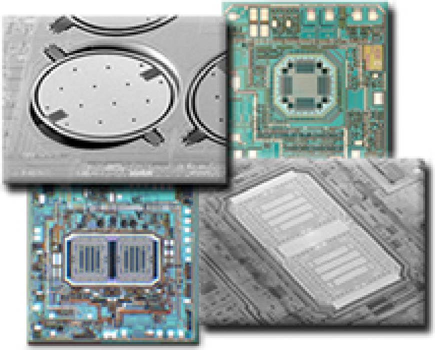
- SUGAR (early 2000s) – SPICE for MEMS
- HiQLab (2006) – high-Q mechanical resonator device modeling
- AxFEM (2012) – solid-wave gyro device modeling

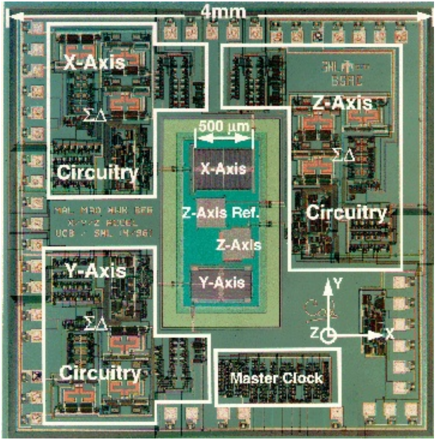
Goal today: two illustrative snapshots.

MEMS Basics

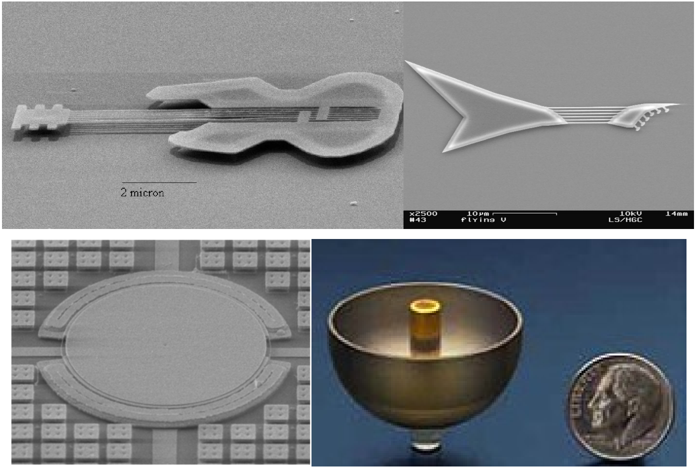
- Micro-Electro-Mechanical Systems
  - Chemical, fluid, thermal, optical (MECFTOMS?)
- Applications:
  - Sensors (inertial, chemical, pressure)
  - Ink jet printers, biolab chips
  - Radio devices: cell phones, inventory tags, pico radio
- Use integrated circuit (IC) fabrication technology
- Tiny, but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

Where are MEMS used?



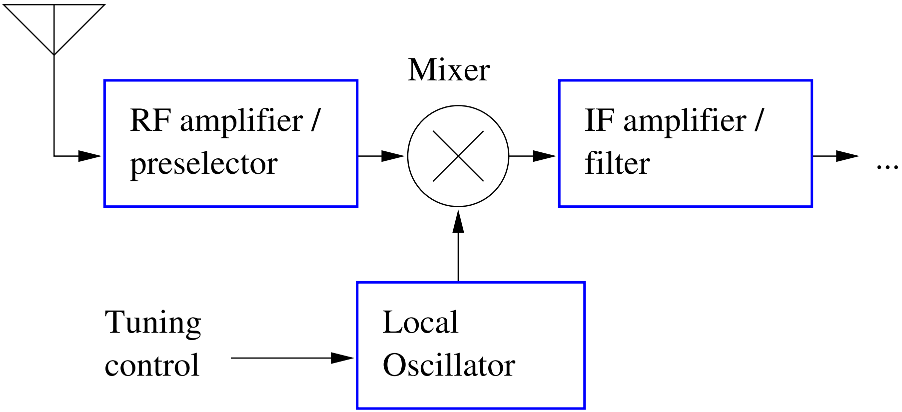


My favorite applications



Why you should care, too!

The Mechanical Cell Phone



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

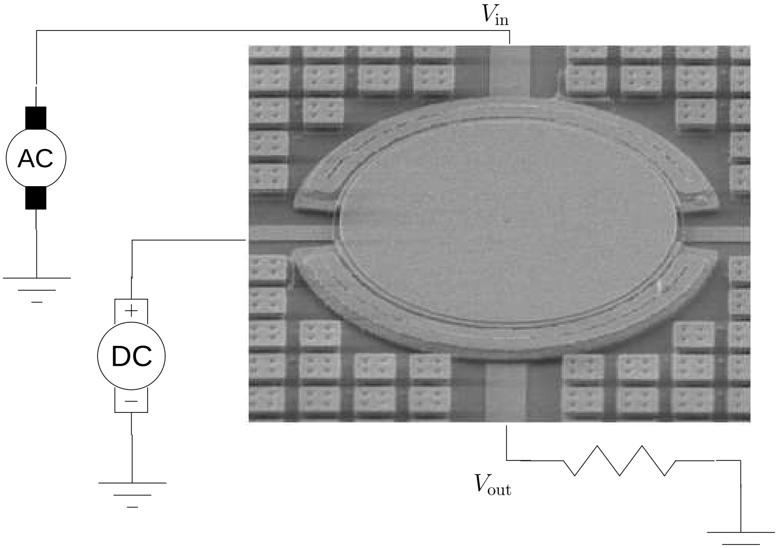
Ultimate Success

"Calling Dick Tracy!"

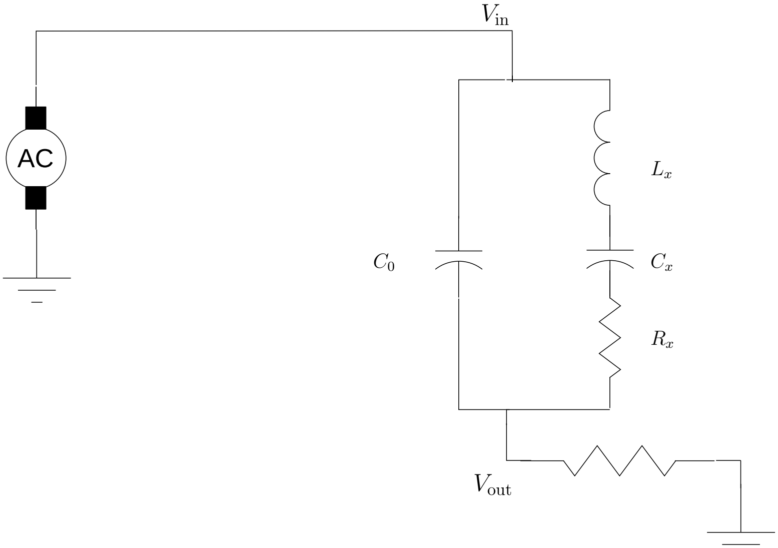
Computational Challenges

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

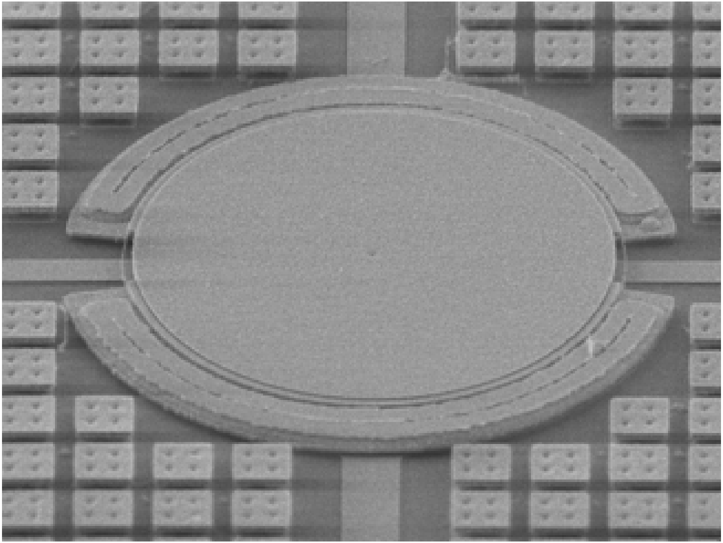
Ideally, would like:

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

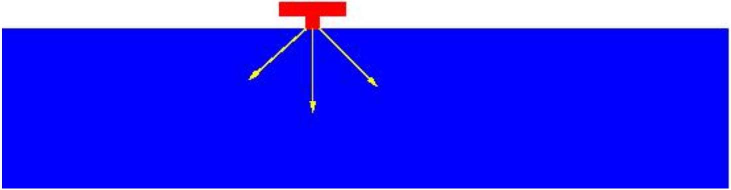
We aren't there yet.

Outline

Disk Resonator Simulations



Damping Mechanisms

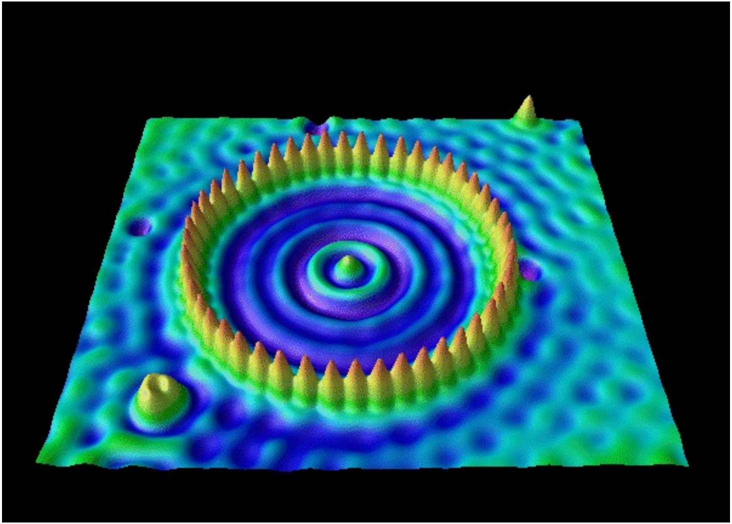


Possible loss mechanisms:

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

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

Resonances in Physics



Resonances and Literature

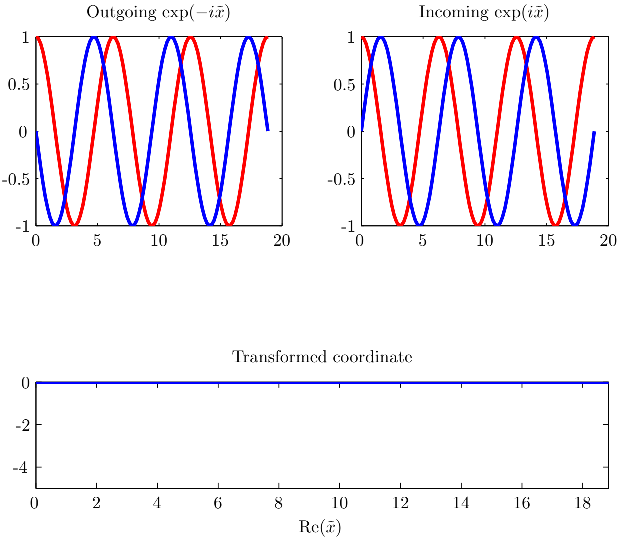
In bells of frost I heard the resonance die.

– 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



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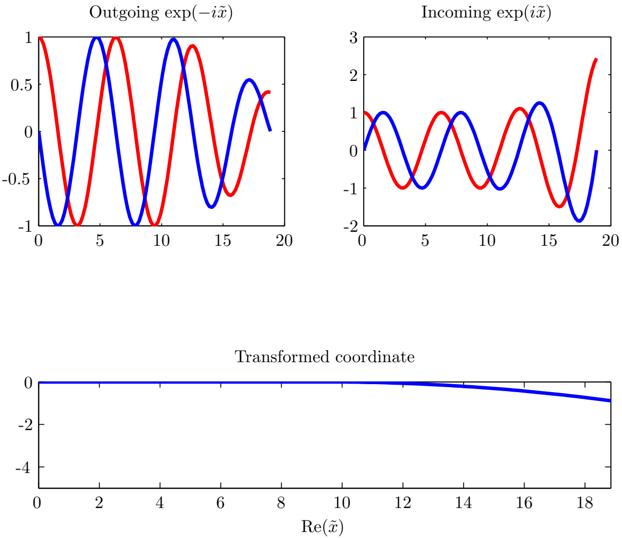

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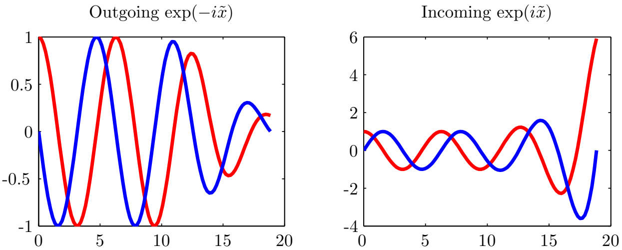

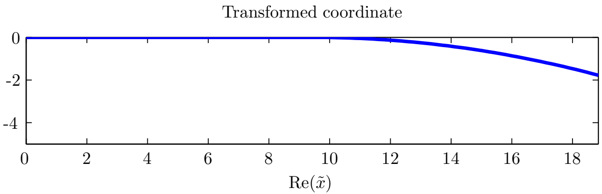

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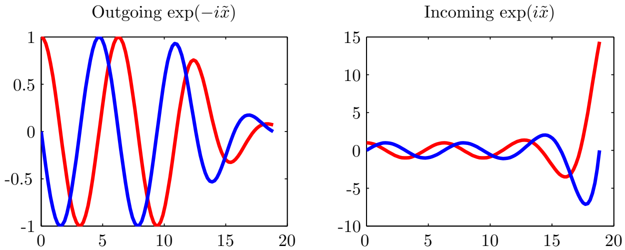

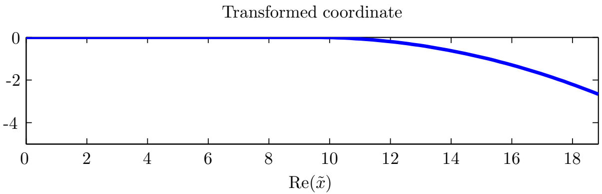

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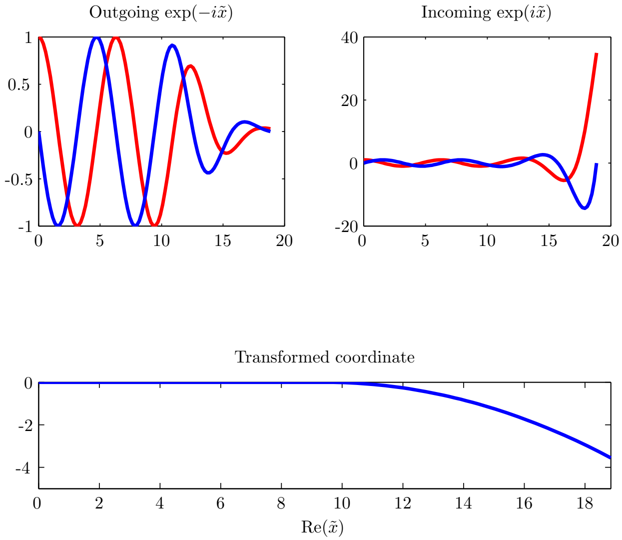

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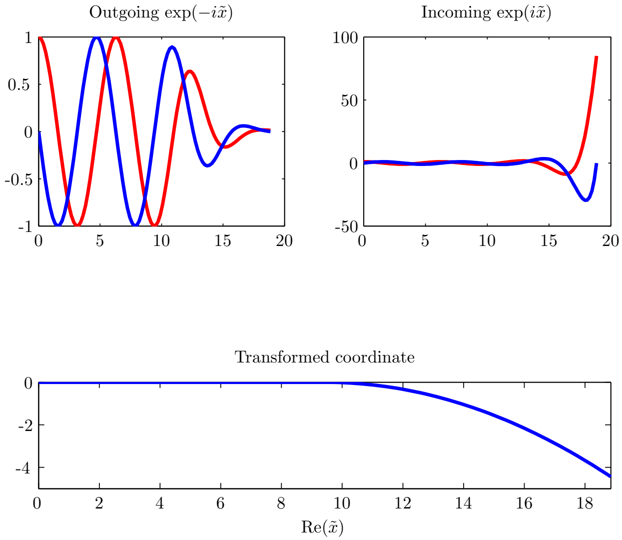
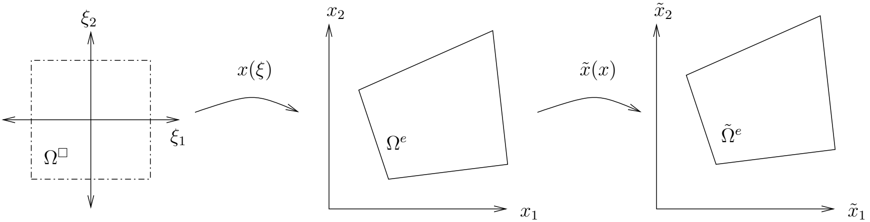
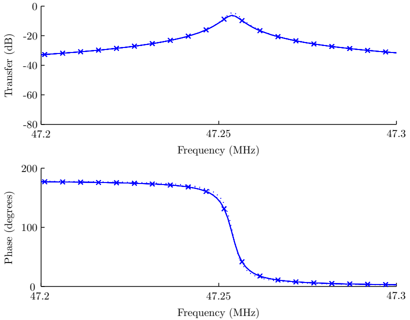


Finite Element Implementation



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!

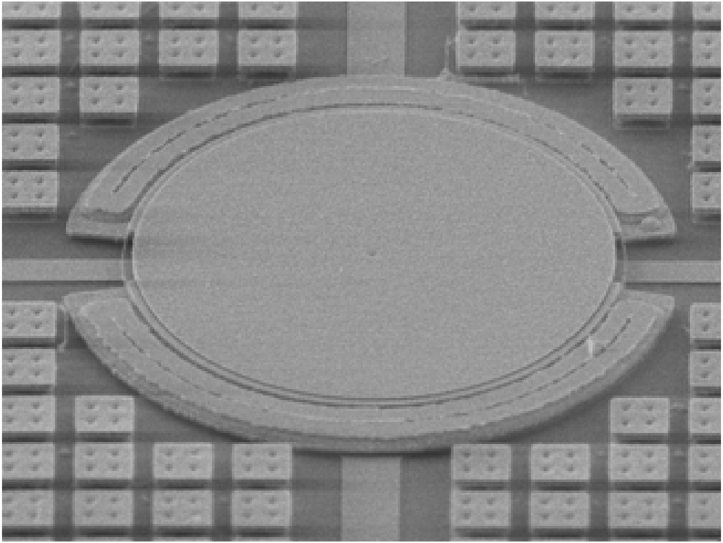
Accurate Model Reduction

- Build new projection basis from V:

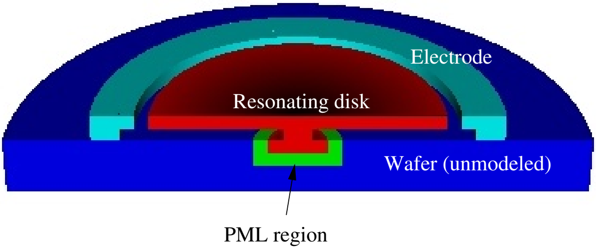
$$W = \mathrm{orth}[\mathrm{Re}(V), \mathrm{Im}(V)]$$

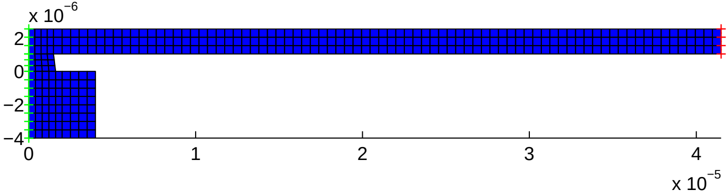
- $\mathrm{span}(W)$ contains both $\mathcal{K}_n$ and $\bar{\mathcal{K}}_n$
  $\implies$ double digits correct vs. projection with V
- W is a real-valued basis
  $\implies$ projected system is complex symmetric

Disk Resonator Simulations



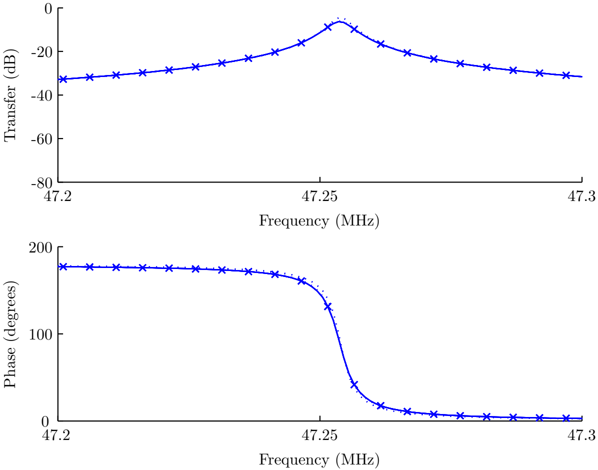
Disk Resonator Mesh





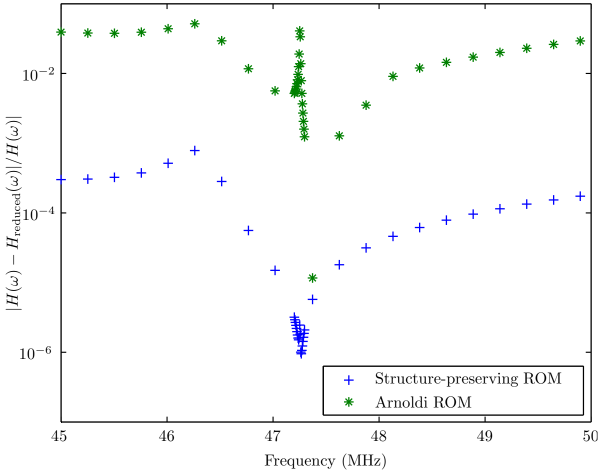
Axisymmetric model, bicubic, $\approx 10^4$ nodal points at convergence

Model Reduction Accuracy



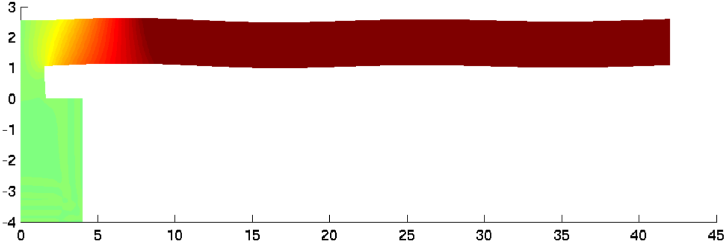
Results from ROM (solid and dotted lines) nearly indistinguishable from full model (crosses)

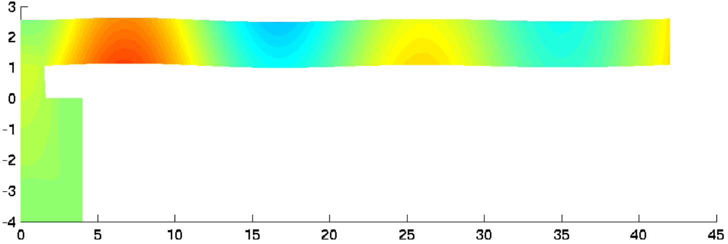
Model Reduction Accuracy



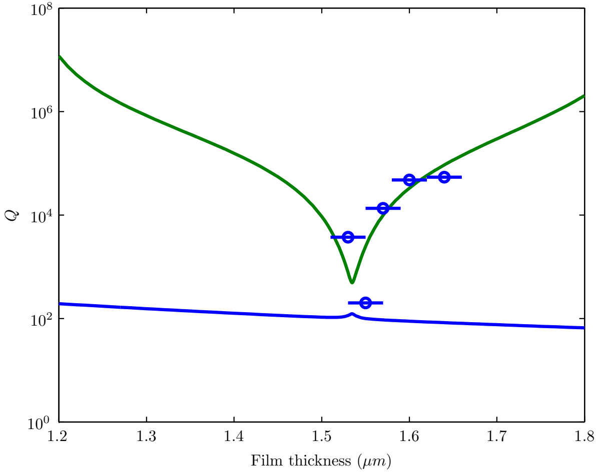
Preserve structure $\implies$
get twice the correct digits

Response of the Disk Resonator



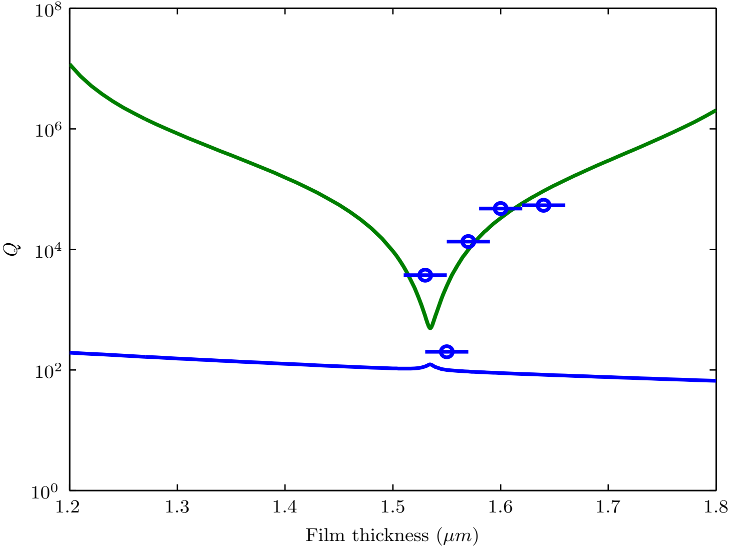


Variation in Quality of Resonance



Simulation and lab measurements vs. disk thickness

Explanation of Q Variation



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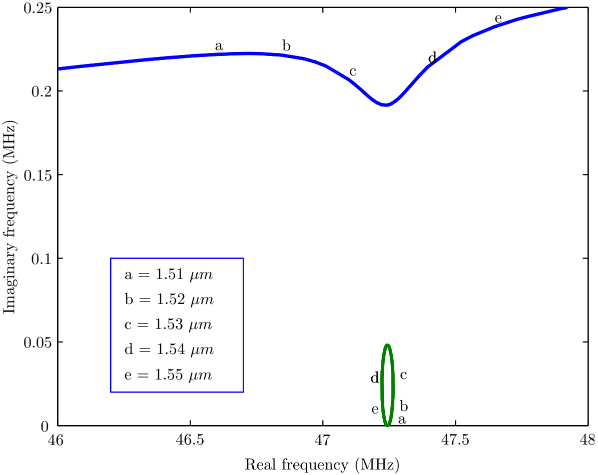
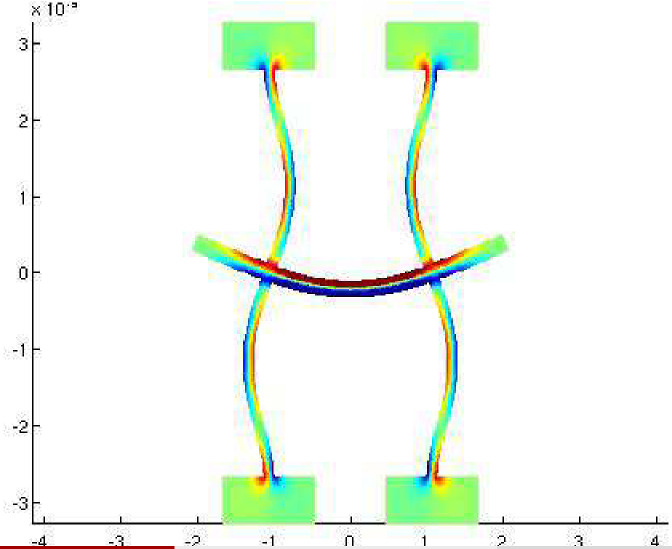


Interaction of two nearby eigenmodes

Outline

Thermoelastic Damping (TED)



Thermoelastic Damping (TED)

u is displacement and $T = T_0 + \theta$ is temperature

$$
\begin{aligned}
\sigma &= C\epsilon - \beta\theta 1 \\
\rho \ddot{u} &= \nabla \cdot \sigma \\
\rho c_v \dot{\theta} &= \nabla \cdot (\kappa \nabla \theta) - \beta T_0 \operatorname{tr}(\dot{\epsilon})
\end{aligned}
$$

- Coupling between temperature and volumetric strain:
  - Compression and expansion $\implies$ heating and cooling
  - Heat diffusion $\implies$ mechanical damping
  - Not often an important factor at the macro scale
  - Recognized source of damping in microresonators
- Zener: semi-analytical approximation for TED in beams
- We consider the fully coupled system

Nondimensionalized Equations

Continuum equations:

$$\begin{aligned} \sigma &= \hat{C}\epsilon - \xi\theta 1 \\ \ddot{u} &= \nabla \cdot \sigma \\ \dot{\theta} &= \eta \nabla^2 \theta - \operatorname{tr}(\dot{\epsilon}) \end{aligned}$$

Discrete equations:

$$\begin{aligned} M_{uu}\ddot{u} + K_{uu}u &= \xi K_{u\theta}\theta + f \\ C_{\theta\theta}\ddot{\theta} + \eta K_{\theta\theta}\theta &= -C_{\theta u}\dot{u} \end{aligned}$$

- Micron-scale poly-Si devices: ξ and η are $\sim 10^{-4}$.
- Linearize about $\xi = 0$

Perturbative Mode Calculation

Discretized mode equation:

$$\begin{aligned}(-\omega^2 M_{uu} + K_{uu})u &= \xi K_{u\theta}\theta \\ (i\omega C_{\theta\theta} + \eta K_{\theta\theta})\theta &= -i\omega C_{\theta u} u\end{aligned}$$

First approximation about $\xi = 0$:

$$\begin{aligned}(-\omega_0^2 M_{uu} + K_{uu})u_0 &= 0 \\ (i\omega_0 C_{\theta\theta} + \eta K_{\theta\theta})\theta_0 &= -i\omega_0 C_{\theta u} u_0\end{aligned}$$

First-order correction in ξ:

$$-\delta(\omega^2) M_{uu} u_0 + (-\omega_0^2 M_{uu} + K_{uu})\delta u = \xi K_{u\theta}\theta_0$$

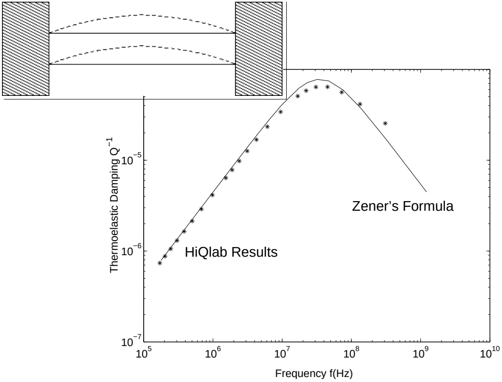
Multiply by u_0^T:

$$\delta(\omega^2) = -\xi \left(\frac{u_0^T K_{u\theta}\theta_0}{u_0^T M_{uu} u_0} \right)$$

Zener's Model

1. Clarence Zener investigated TED in late 30s-early 40s.
2. Model for beams common in MEMS literature.
3. “Method of orthogonal thermodynamic potentials” == perturbation method + a variational method.

Comparison to Zener's Model



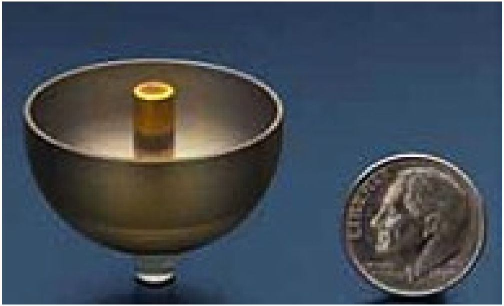
- Comparison of fully coupled simulation to Zener approximation over a range of frequencies
- Real and imaginary parts after first-order correction agree to about three digits with Arnoldi

Outline

Bryan's Experiment

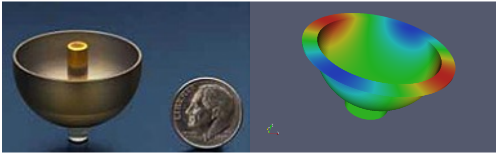
"On the beats in the vibrations of a revolving cylinder or bell"
by G. H. Bryan, 1890

A Small Application



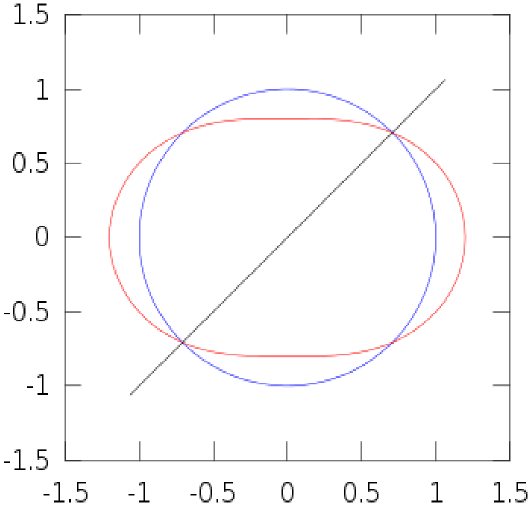
Northrup-Grummond HRG

Current example: Micro-HRG / GOBLiT / OMG

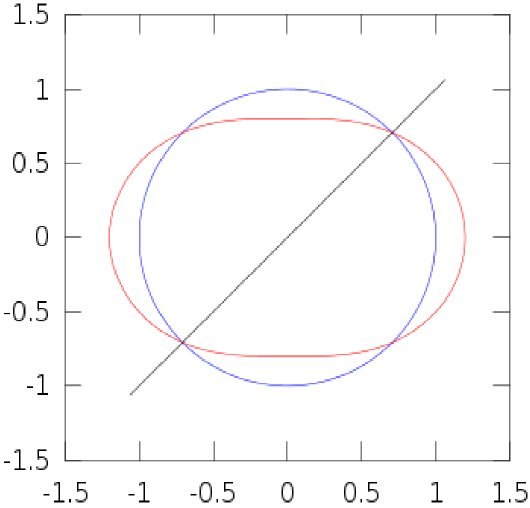


- Goal: Cheap, small (1mm) HRG
- Collaborator roles:
  - Basic design
  - Fabrication
  - Measurement
- Our part:
  - Detailed physics
  - Fast software
  - Sensitivity
  - Design optimization

How It Works



How It Works



Goal state

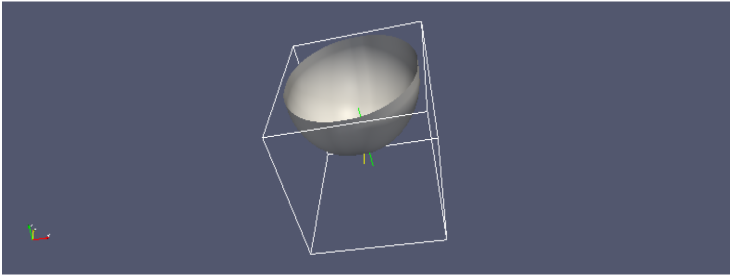
We want to compute:

- 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!

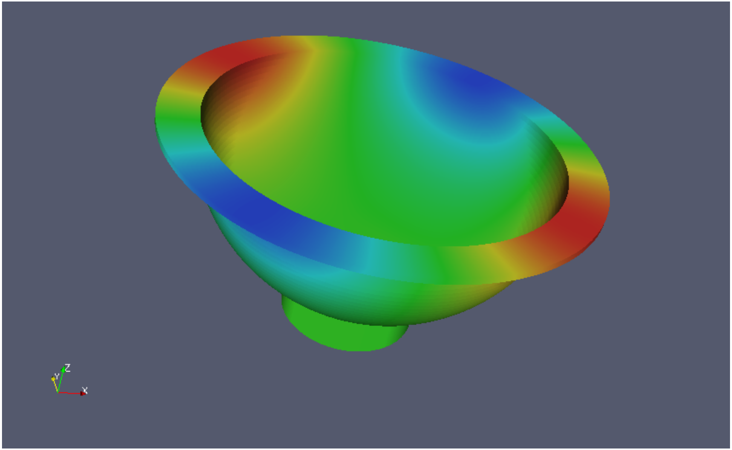
- Axisymmetric geometry $\implies$ 3D to 2D via Fourier
- Perturbed geometry $\implies$ interactions for different wave numbers

Getting the Geometry

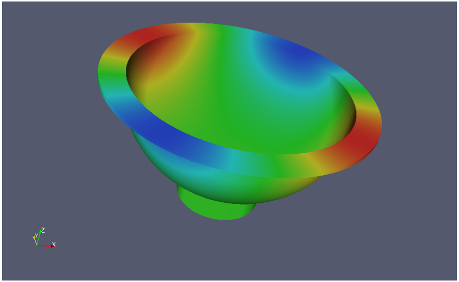


- Simple isotropic etch modeling fails – 1mm is *huge*!
- Working on better simulator (reaction-diffusion).
- For now, take idealized geometries on faith...

Full Dynamics



Essential Dynamics



Dynamics in 2D subspace of degenerate modes:

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

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

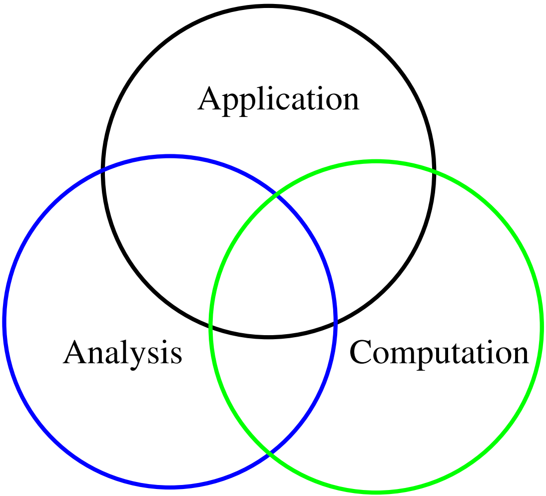
$$\delta(\omega^2) = \frac{u_0^T \, G(\omega_0) \, u_0}{u_0^T M_{mm} u_0}.$$

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

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