# Computer-Aided Design for Micro-Electro-Mechanical Systems

## Eigenvalues, Energy Losses, and Dick Tracy Watches

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Caltech, 1 Feb 2006

# The Computational Science Picture



- Application modeling
  - Checkerboard resonator
  - Disk resonator
  - Shear ring resonator
- Mathematical analysis
  - Physical modeling and finite element technology
  - Structured eigenproblems and reduced-order models
  - Parameter-dependent eigenproblems
- Software engineering
  - HiQLab
  - SUGAR
  - FEAPMEX

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# Outline

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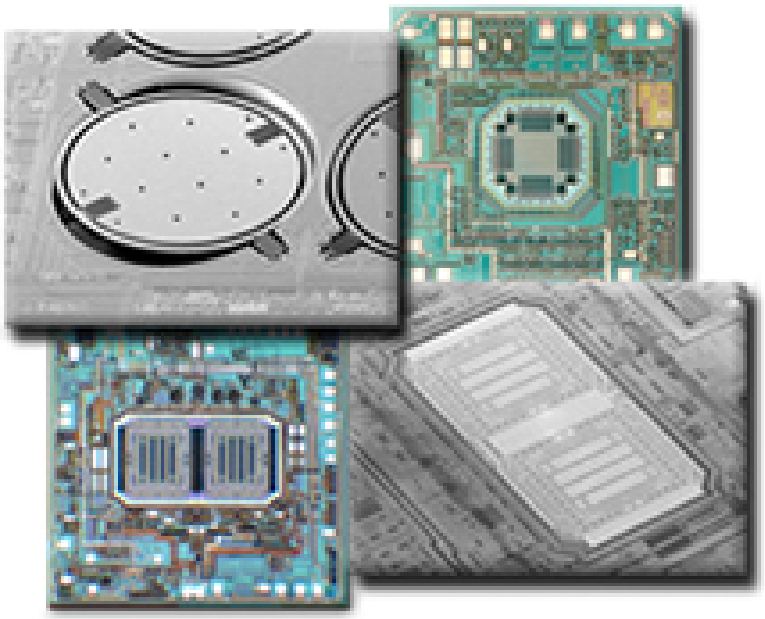
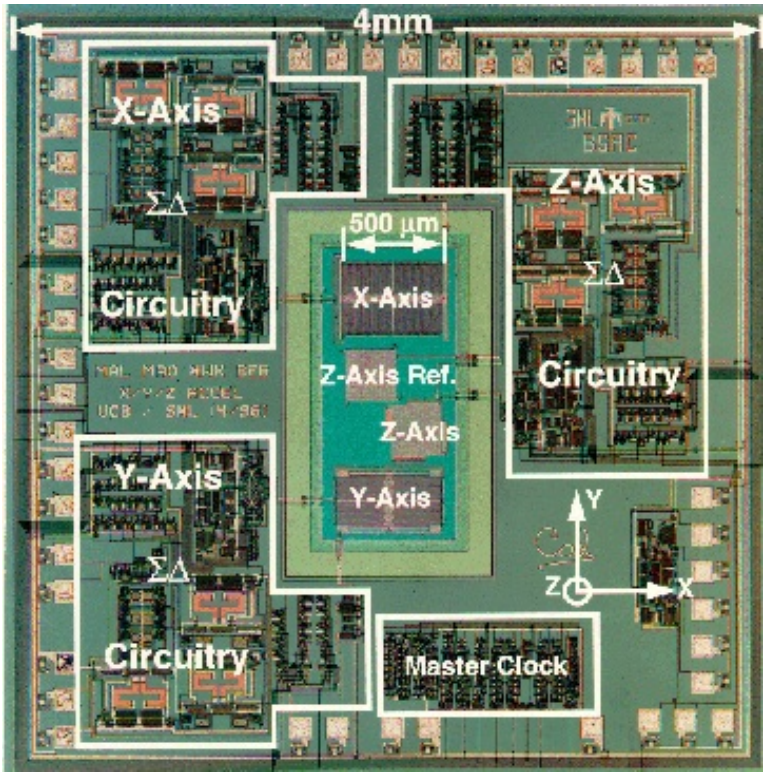
# What are MEMS?







# MEMS Basics

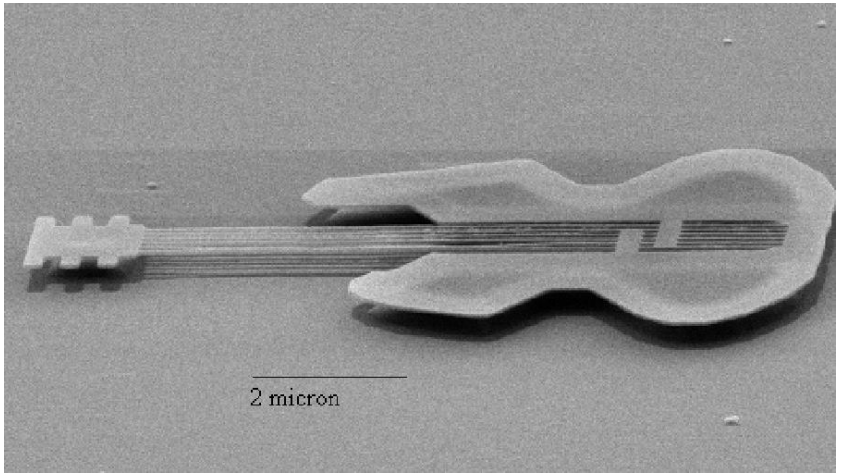


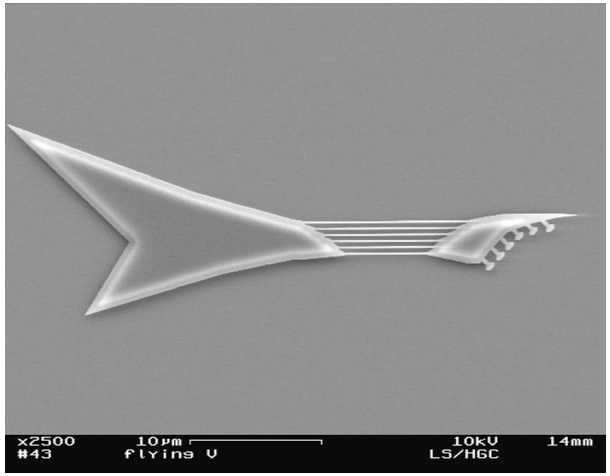


- Micro-Electro-Mechanical Systems
  - Chemical, fluid, thermal, optical (MECFTOMS?)
- Applications:
  - Sensors (inertial, chemical, pressure)
  - Ink jet printers, biolab chips
  - Radio devices: cell phones, inventory tags, pico radio
- Use integrated circuit (IC) fabrication technology
- Tiny, but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

# Radio-Frequency MEMS





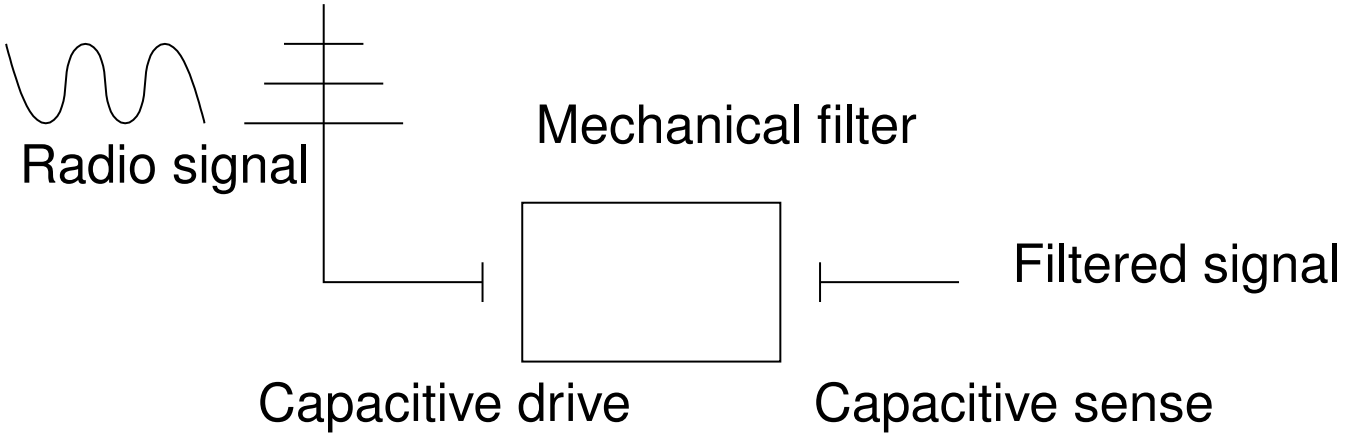




Microguitars from Cornell University (1997 and 2003)

- MHz-GHz mechanical resonators
- Impact: smaller, lower-power cell phones
- Other uses:
  - Sensing elements (e.g. chemical sensors)
  - Really high-pitch guitars

# Micromechanical Filters






- Mechanical high-frequency (high MHz-GHz) filter
  - Your cell phone is mechanical!
  - New MEMS filters can be integrated with circuitry
    $\Longrightarrow$ smaller and lower power

# Ultimate Success





"Calling Dick Tracy!"

# Designing Transfer Functions



Time domain:

$$\begin{aligned} Mu'' + Cu' + Ku &= b\phi(t) \\ y(t) &= p^T u \end{aligned}$$

Frequency domain:

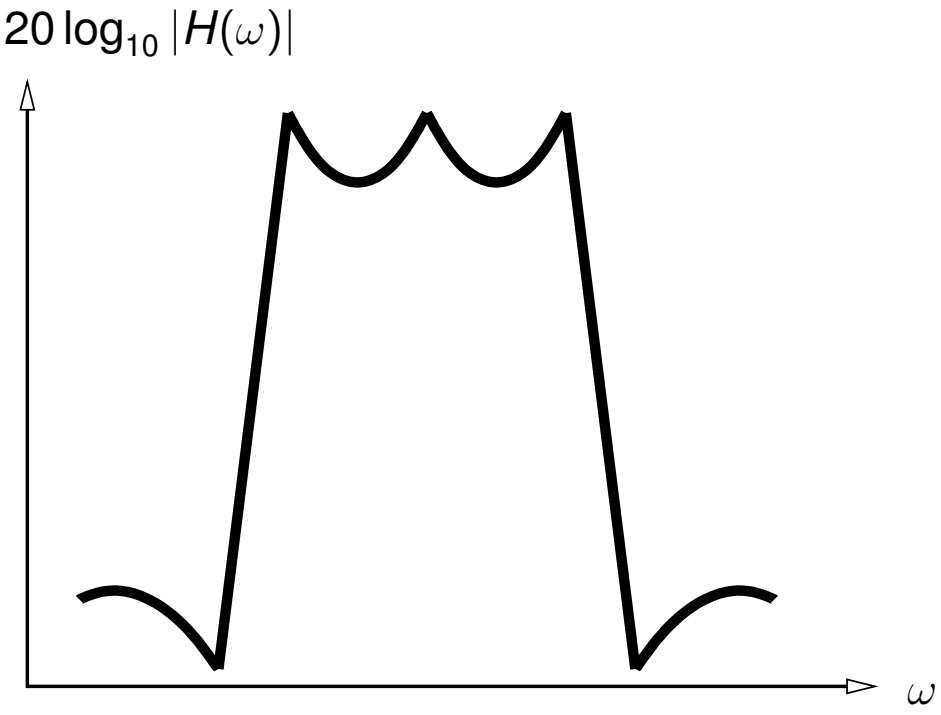
$$\begin{aligned} -\omega^2 M\hat{u} + i\omega C\hat{u} + K\hat{u} &= b\hat{\phi}(\omega) \\ \hat{y}(\omega) &= p^T \hat{u} \end{aligned}$$

Transfer function:

$$\begin{aligned} H(\omega) &= p^T(-\omega^2 M + i\omega C + K)^{-1} b \\ \hat{y}(\omega) &= H(\omega)\hat{\phi}(\omega) \end{aligned}$$

# Narrowband Filter Needs

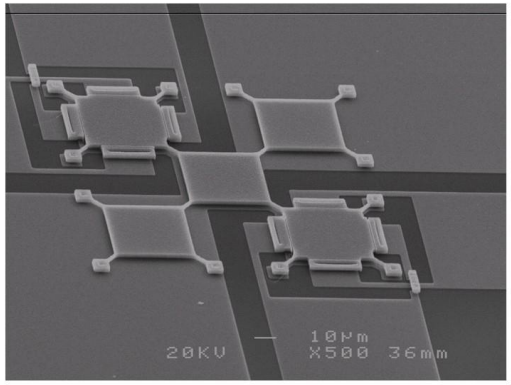


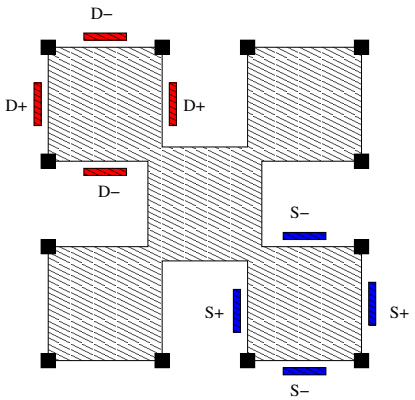


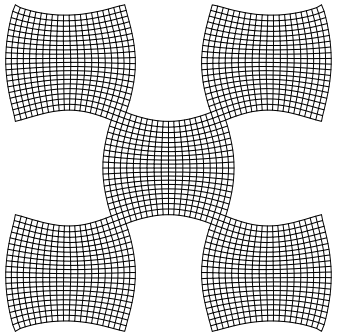

- Want “sharp” poles for narrowband filters
- $\Longrightarrow$ Want to minimize damping

# Checkerboard Resonator





- Anchored at outside corners
- Excited at northwest corner
- Sensed at southeast corner
- Surfaces move only a few nanometers

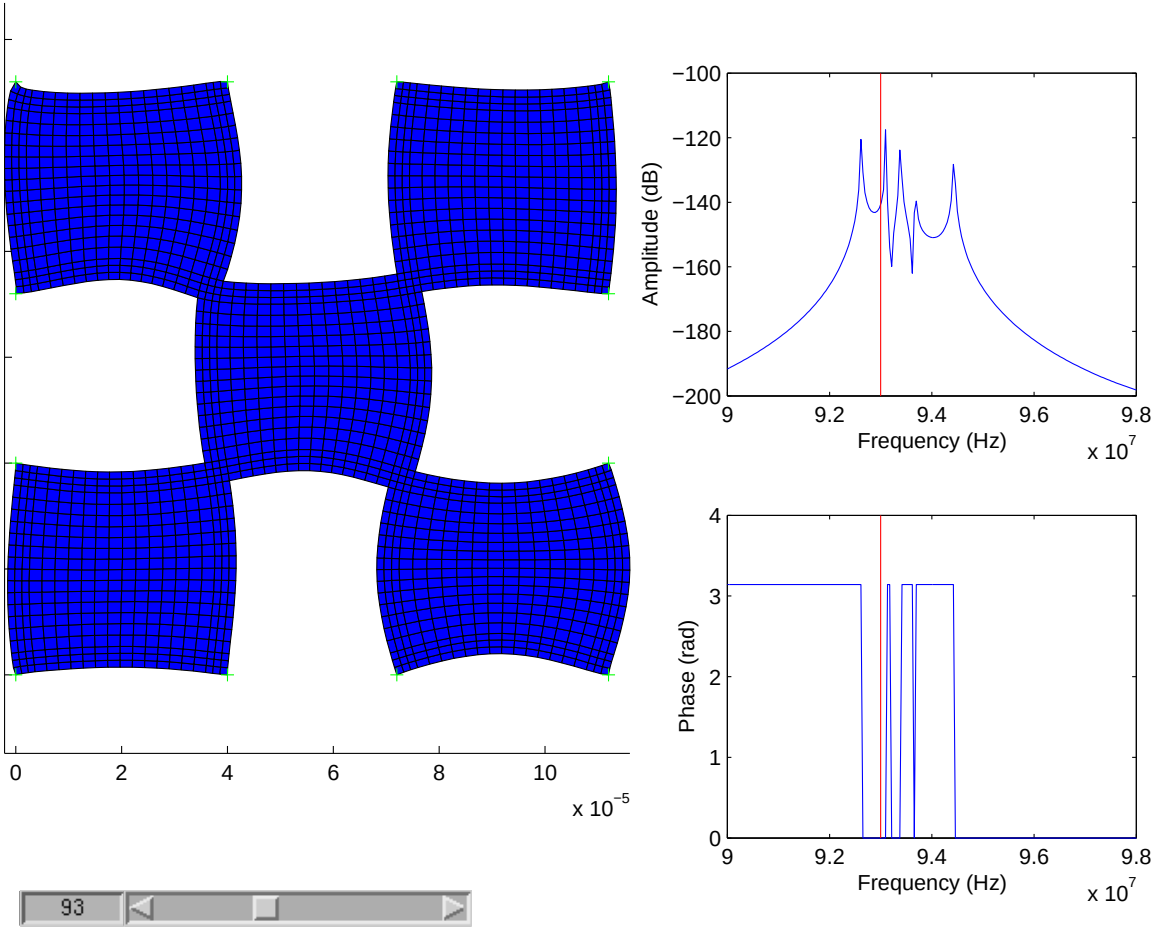
# Checkerboard Model Reduction



- Finite element model: $N = 2154$
  - Expensive to solve for every $H(\omega)$ evaluation!
- Build a reduced-order model to approximate behavior
  - Reduced system of 80 to 100 vectors
  - Evaluate $H(\omega)$ in milliseconds instead of seconds
  - Without damping: standard Arnoldi projection
  - With damping: Second-Order ARnoldi (SOAR)

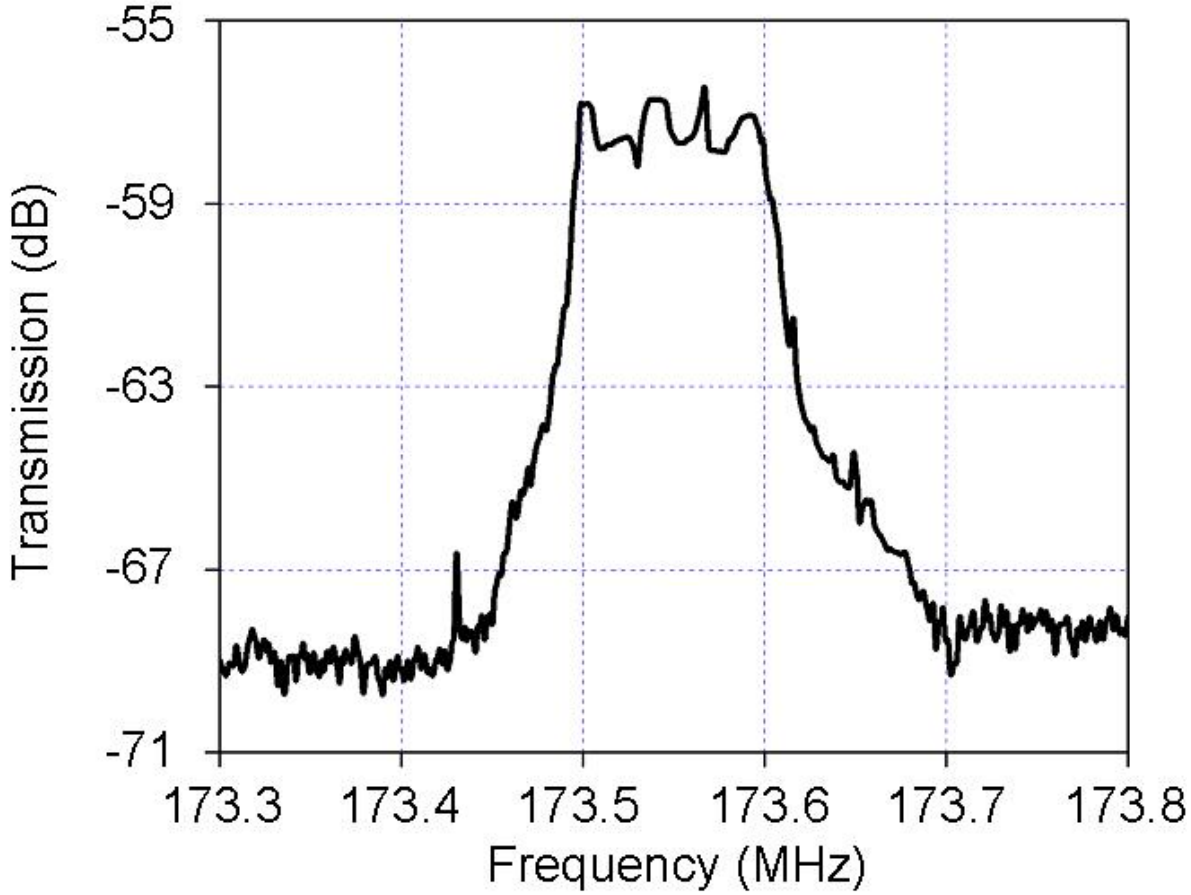
# Checkerboard Simulation





# Checkerboard Measurement






S. Bhave, MEMS 05

# 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 $\omega \in \mathbb{C}$:

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

# Enter HiQLab

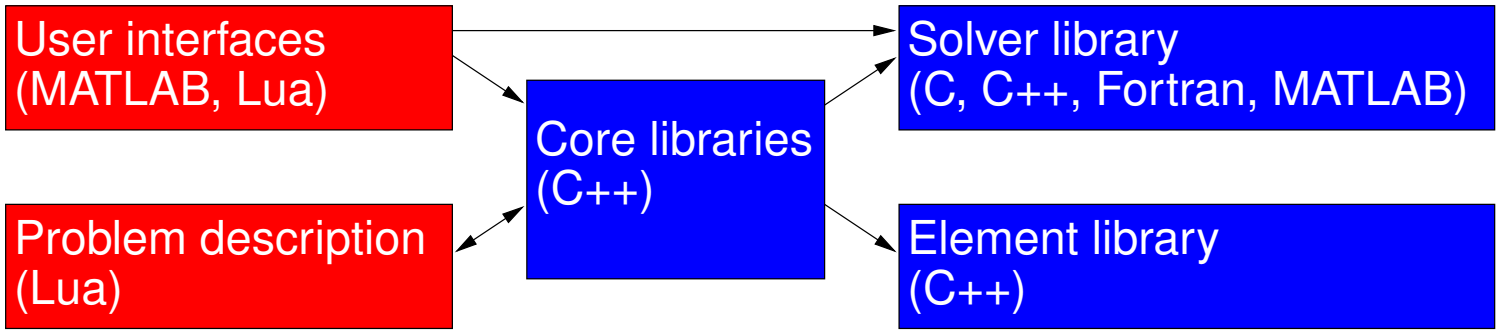




- Existing codes do not compute quality factors
- ... and awkward to prototype new solvers
- ... and awkward to programmatically define meshes
- So I wrote a new finite element code: HiQLab

# HiQLab Structure






- Full scripting language for mesh input
- Callbacks for boundary conditions, material properties
- MATLAB interface for quick algorithm prototyping
- Cross-language bindings are automatically generated

# Contributions





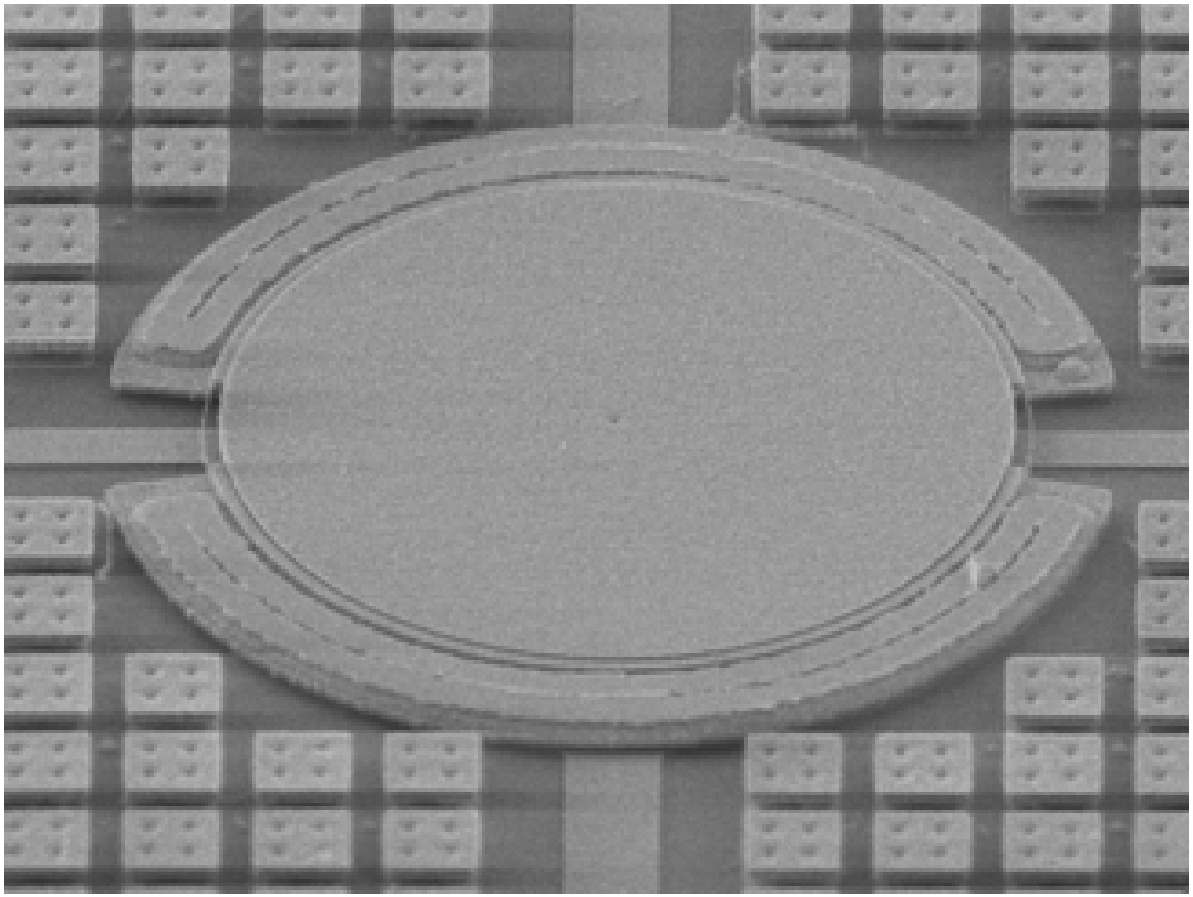
- Built predictive model used to design checkerboard
- Used model reduction to get thousand-fold speedup – fast enough for interactive use
- Wrote FEAPMEX to script parameter studies
- Wrote a new code, HiQLab, to study damping

# Outline

# Example: Disk Resonator



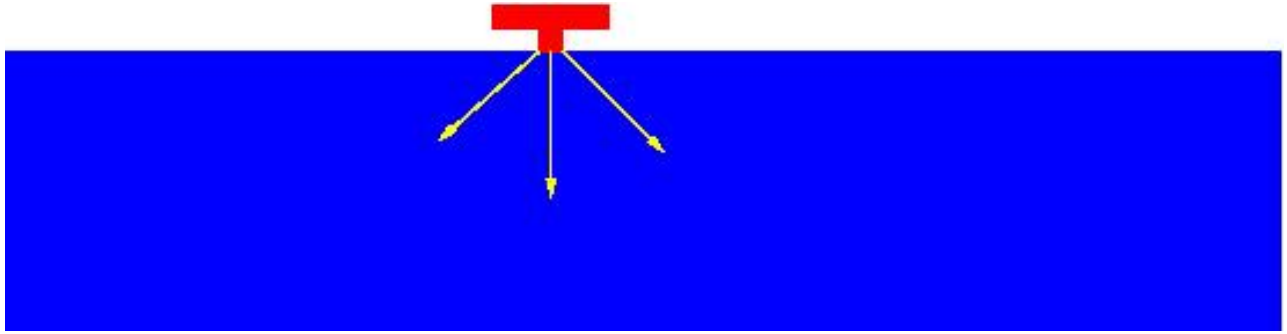




SiGe disk resonators built by E. Quévy

# Damping Mechanisms





Possible loss mechanisms:

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

Model substrate as semi-infinite with a

Perfectly Matched Layer (PML).

# 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)

# Model Problem



- Domain: $x \in [0, \infty)$
- Governing eq:

$$\frac{\partial^2 u}{\partial x^2} - \frac{1}{c^2}\frac{\partial^2 u}{\partial t^2} = 0$$

- Fourier transform:

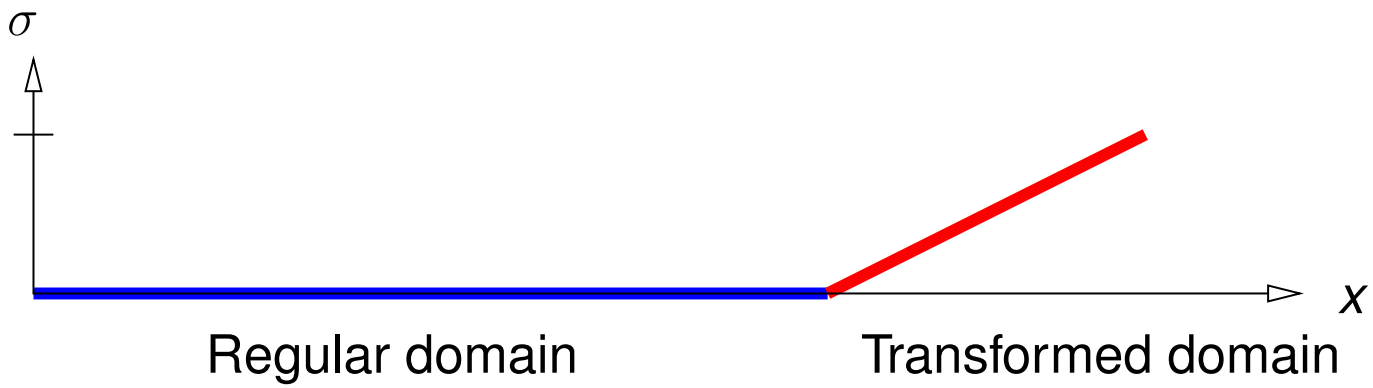
$$\frac{d^2 \hat{u}}{dx^2} + k^2 \hat{u} = 0$$

- Solution:

$$\hat{u} = c_{\text{out}} e^{-ikx} + c_{\text{in}} e^{ikx}$$

# Model with Perfectly Matched Layer





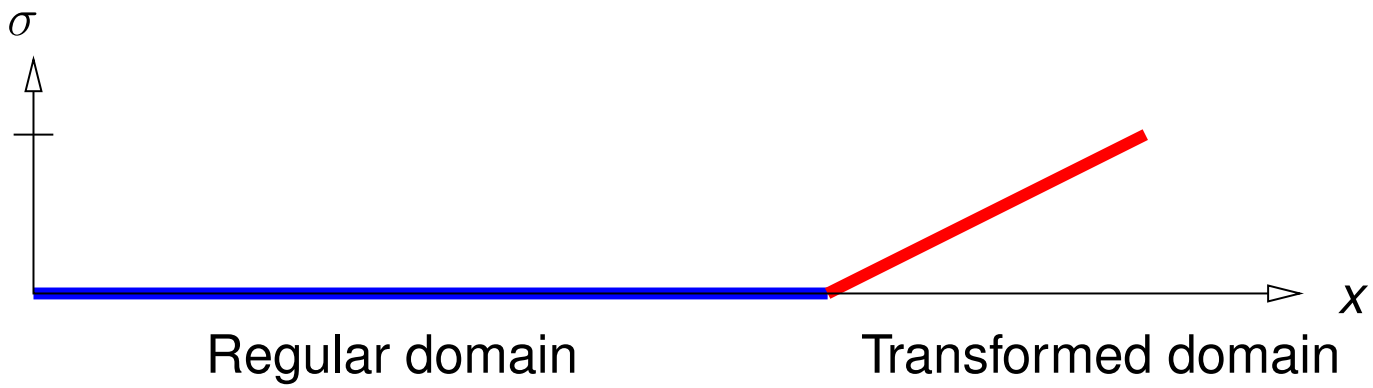

$$\frac{d\tilde{x}}{dx} = \lambda(x) \text{ where } \lambda(s) = 1 - i\sigma(s)$$

$$\frac{d^2\hat{u}}{d\tilde{x}^2} + k^2\hat{u} = 0$$

$$\hat{u} = c_{\text{out}} e^{-ik\tilde{x}} + c_{\text{in}} e^{ik\tilde{x}}$$

# Model with Perfectly Matched Layer






$$\frac{d\tilde{x}}{dx} = \lambda(x) \text{ where } \lambda(s) = 1 - i\sigma(s),$$

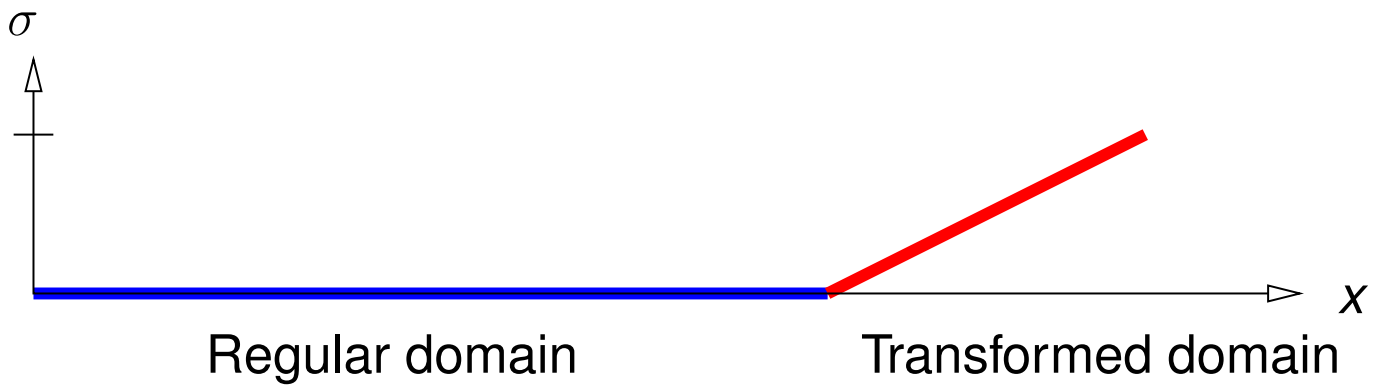
$$\frac{1}{\lambda}\frac{d}{dx}\left(\frac{1}{\lambda}\frac{d\hat{u}}{dx}\right) + k^2\hat{u} = 0$$

$$\hat{u} = c_{\text{out}}e^{-ikx-k\Sigma(x)} + c_{\text{in}}e^{ikx+k\Sigma(x)}$$

$$\Sigma(x) = \int_0^x \sigma(s)\,ds$$

# Model with Perfectly Matched Layer



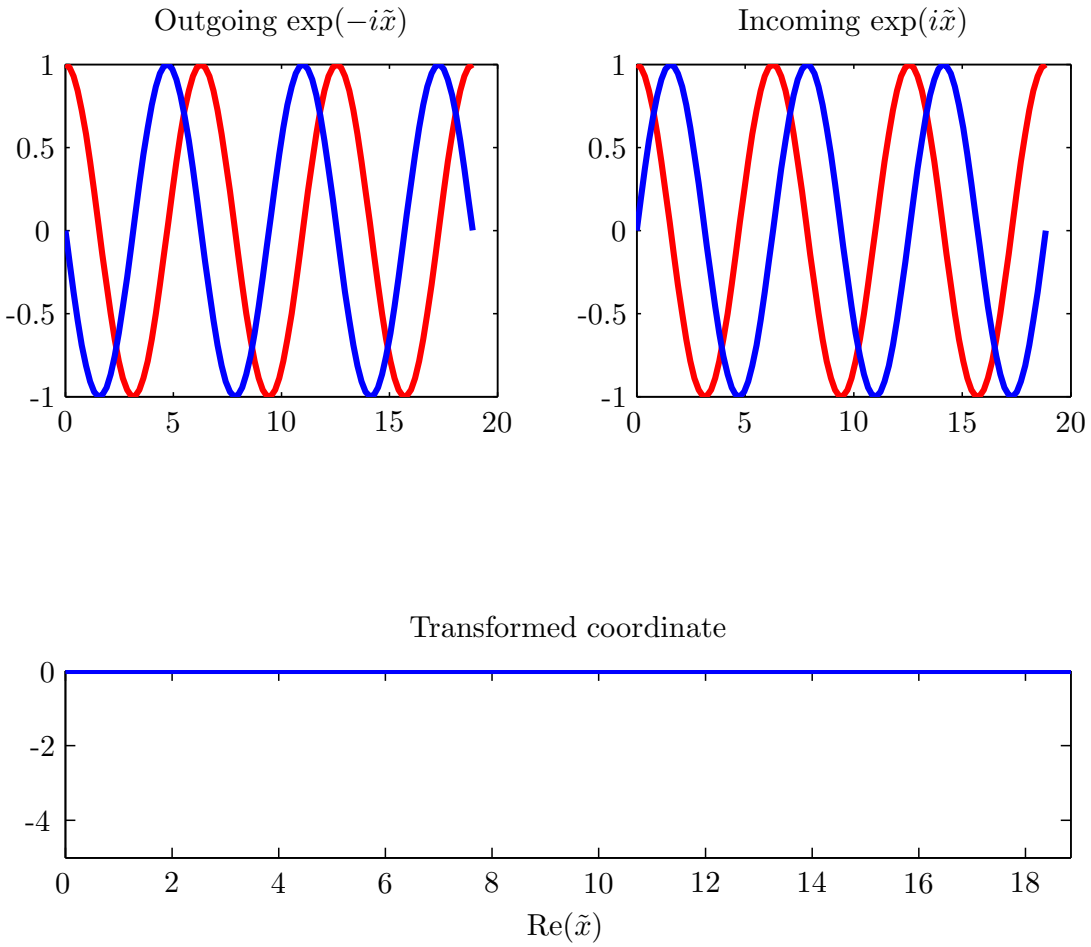



If solution clamped at $x = L$ then

$$\frac{c_{\text{in}}}{c_{\text{out}}} = O(e^{-k\gamma}) \text{ where } \gamma = \Sigma(L) = \int_0^L \sigma(s)\, ds$$

# Model Problem Illustrated





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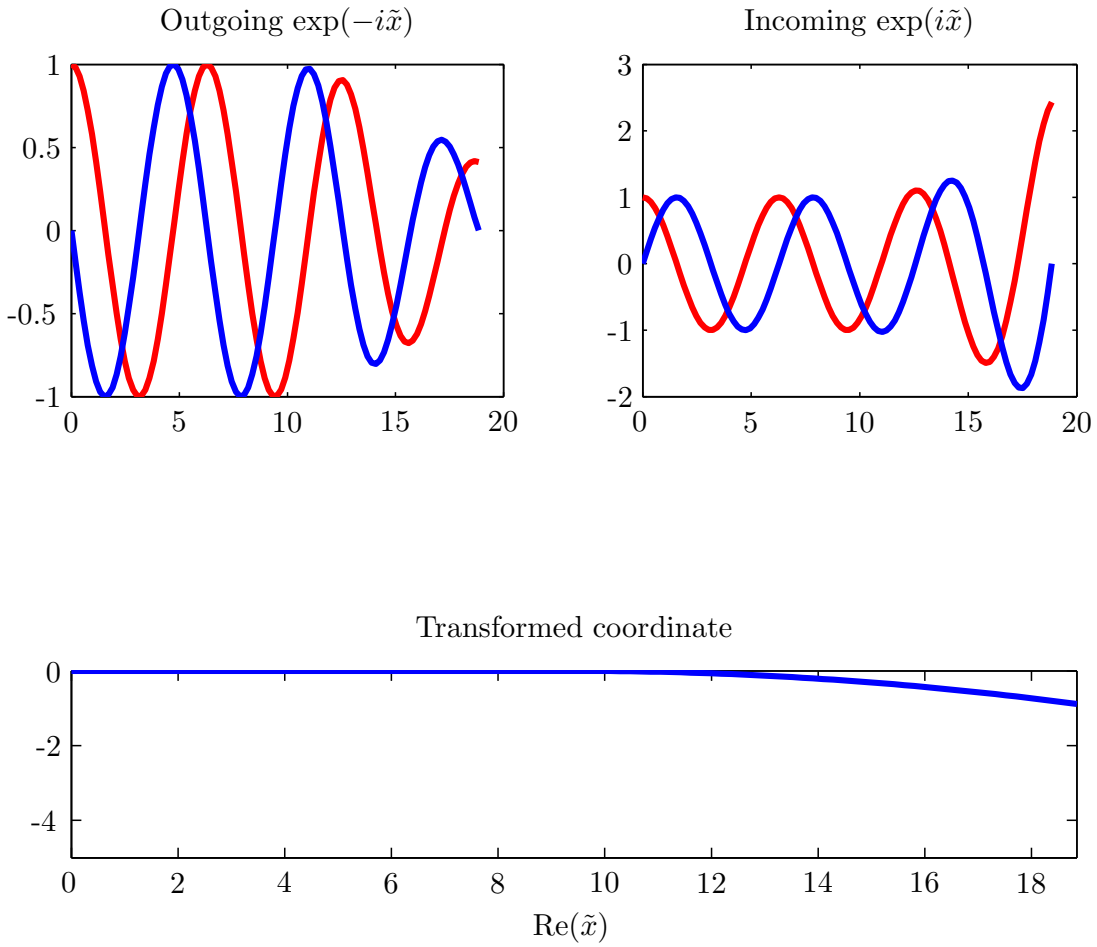

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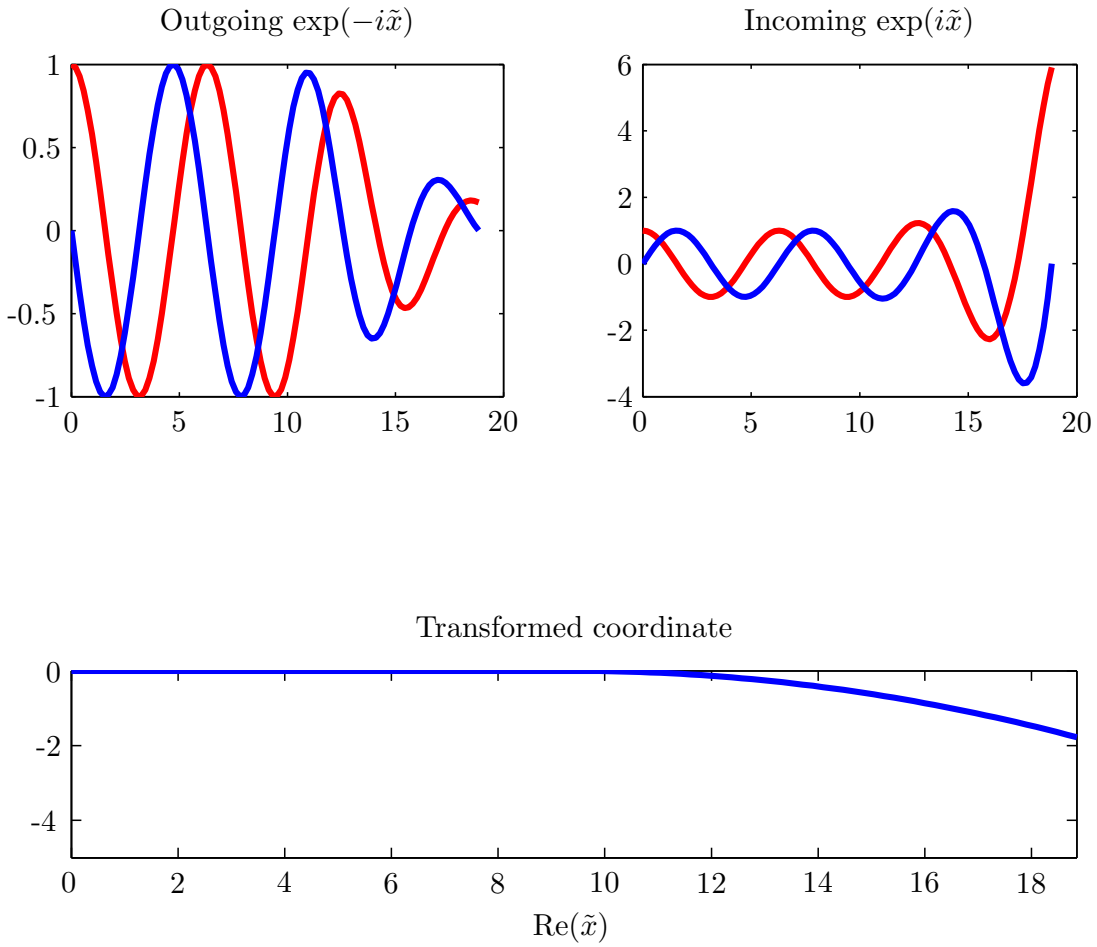

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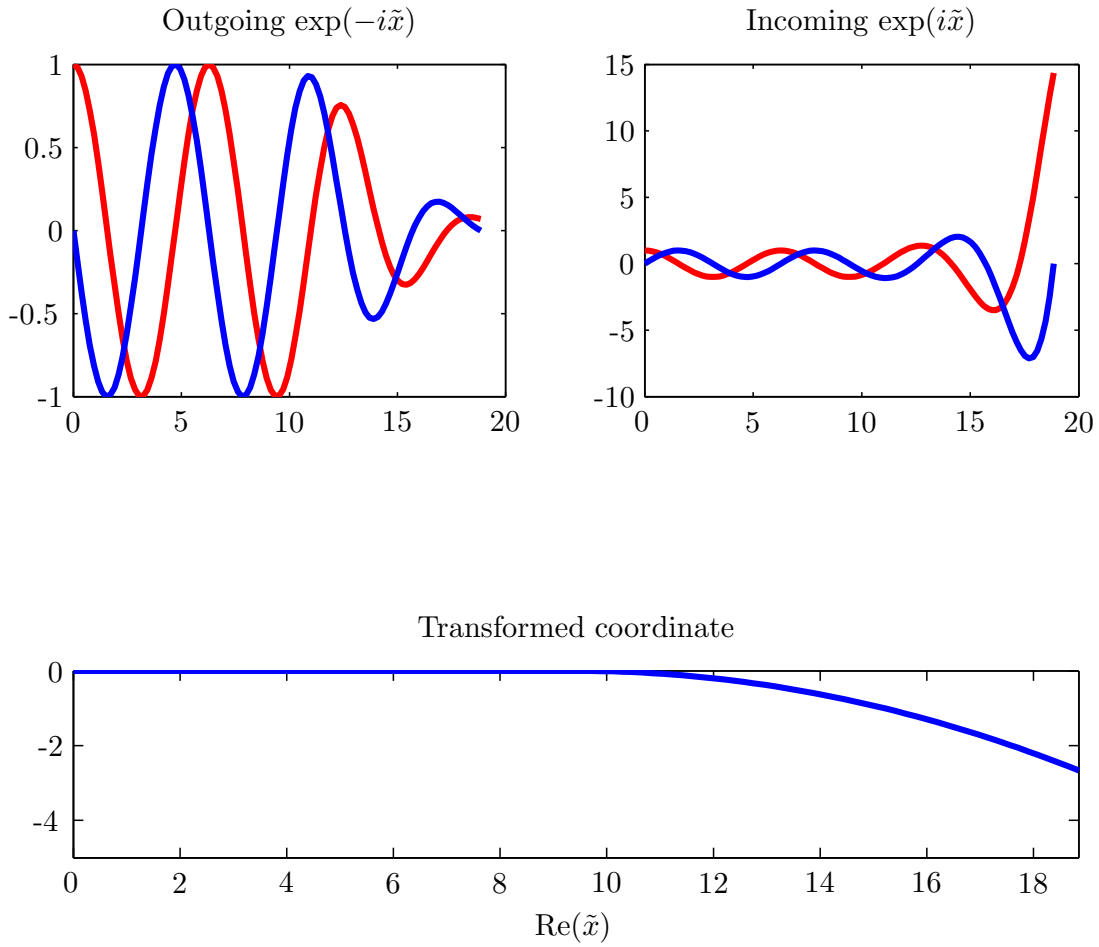

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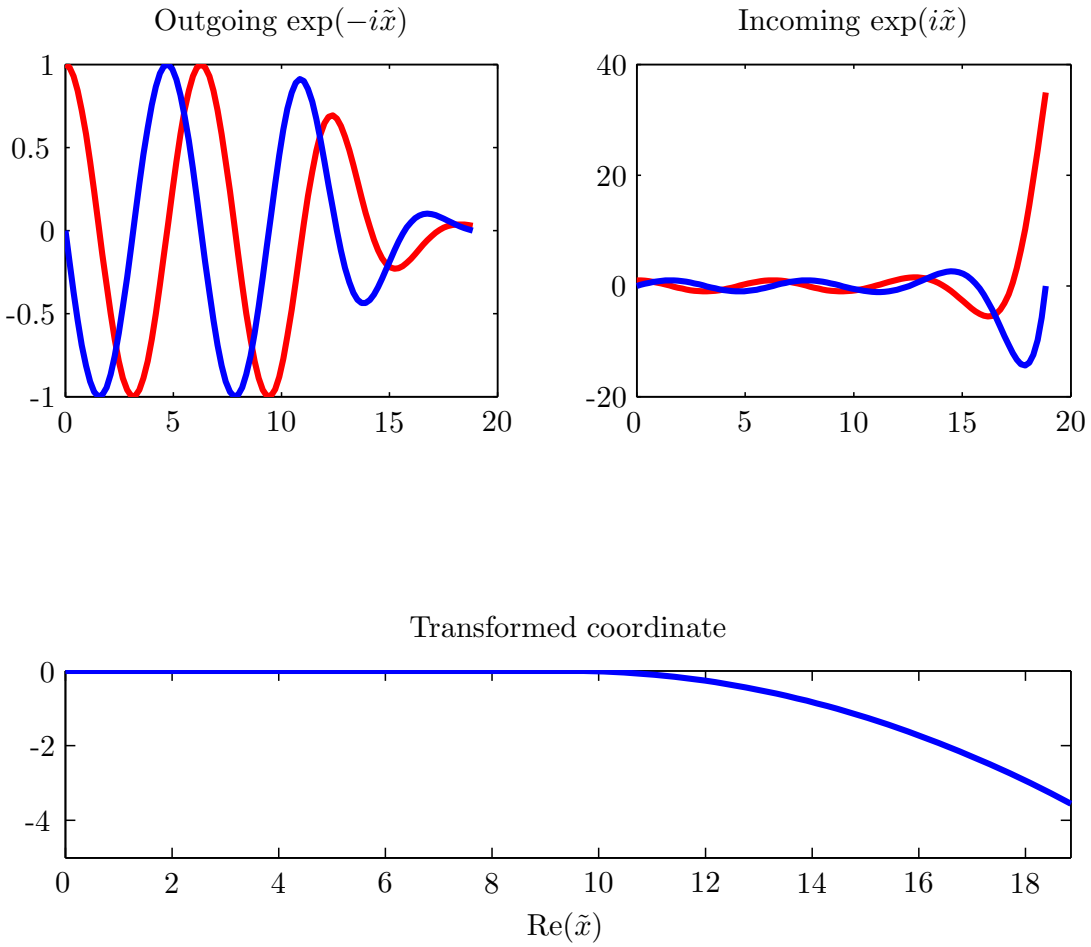

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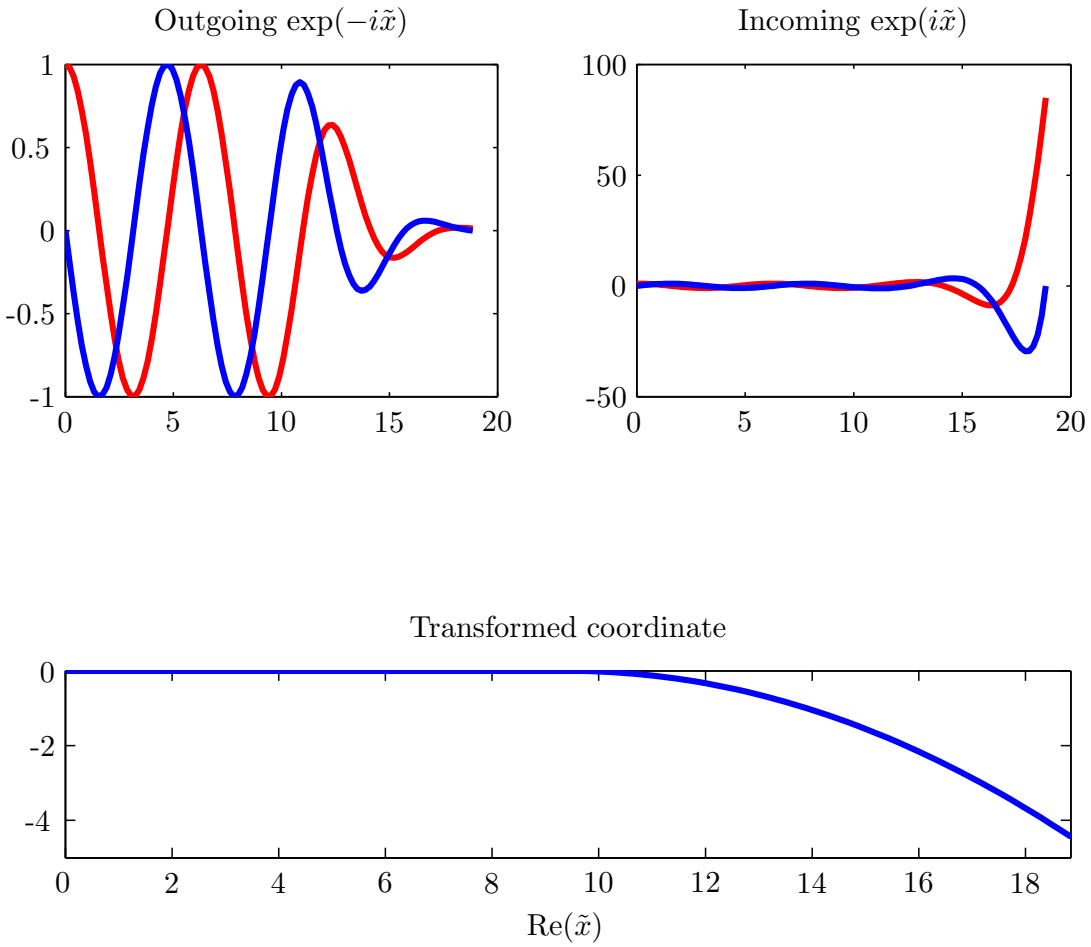
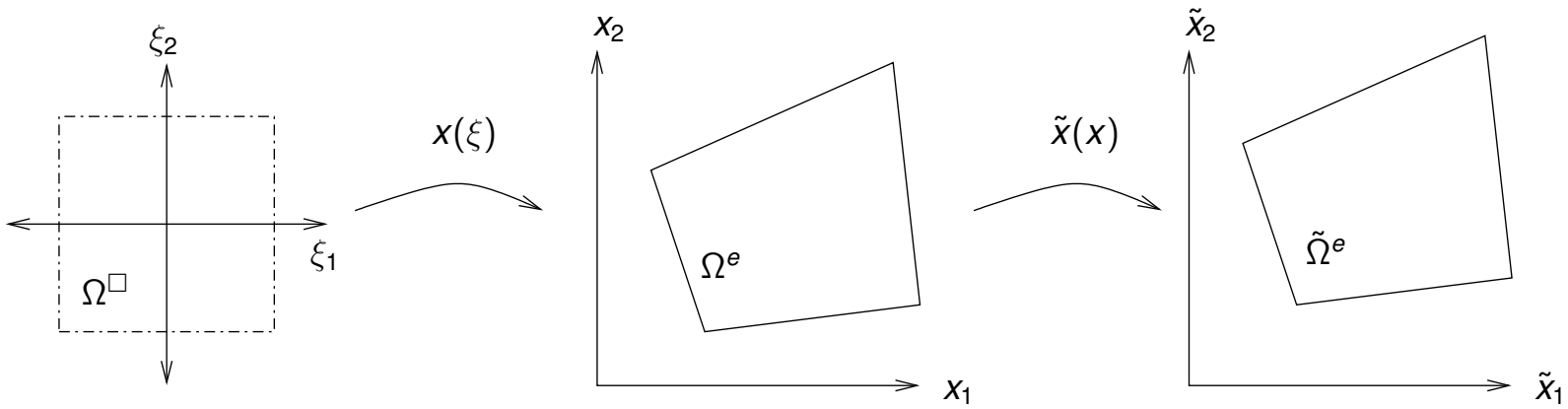


# Finite Element Implementation






- Combine PML and isoparametric mappings

$$\mathbf{k}^e = \int_{\Omega^{\square}} \tilde{\mathbf{B}}^T \mathbf{D} \tilde{\mathbf{B}} \tilde{J} \, d\Omega^{\square}$$

$$\mathbf{m}^e = \int_{\Omega^{\square}} \rho \mathbf{N}^T \mathbf{N} \tilde{J} \, d\Omega^{\square}$$

- Matrices are *complex symmetric*

# Outline

# Eigenvalues and Model Reduction



Want to know about the transfer function $H(\omega)$:

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

Can either

- Locate poles of $H$ (eigenvalues of $(K, M)$)
- Plot $H$ in a frequency range (Bode plot)

Usual tactic: subspace projection

- Build an Arnoldi basis $V$
- Compute with much smaller $V^* K V$ and $V^* M V$

Can we do better?

# 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.
- Key: relation between left and right eigenvectors.

# Accurate Model Reduction



- Build new projection basis from $V$:

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

- 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

# Contributions

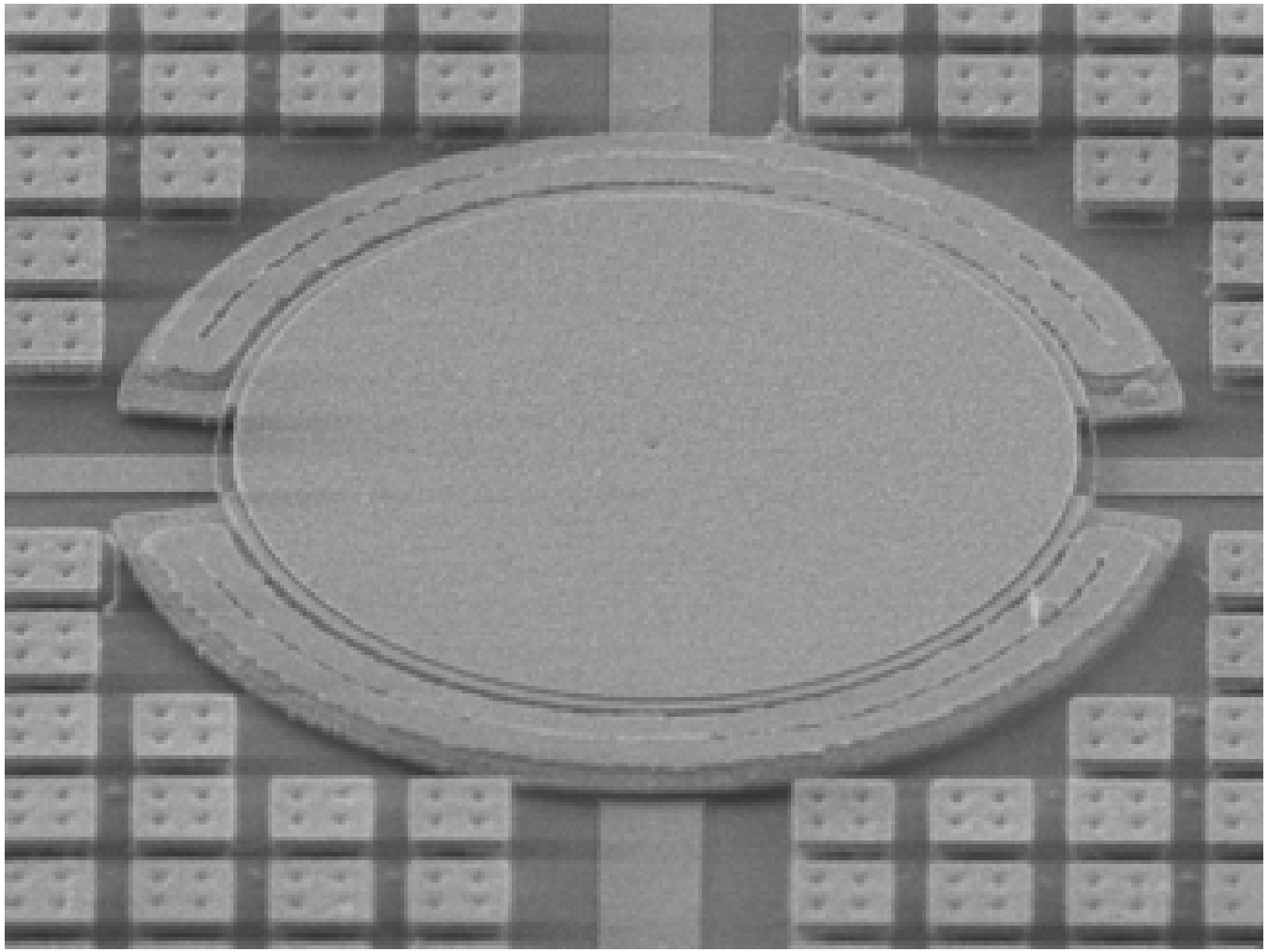


- New formulation of perfectly matched layers
  - Easy to apply PML to axisymmetric, 2D, or 3D models
  - Same formulation applies to electromagnetics, etc.
- Analysis of discretization error for perfectly matched layers
  - Results in cheap, automatic parameter optimization
- Structure-preserving model reduction for complex symmetric systems
  - Double accuracy for same work as standard method

# Outline

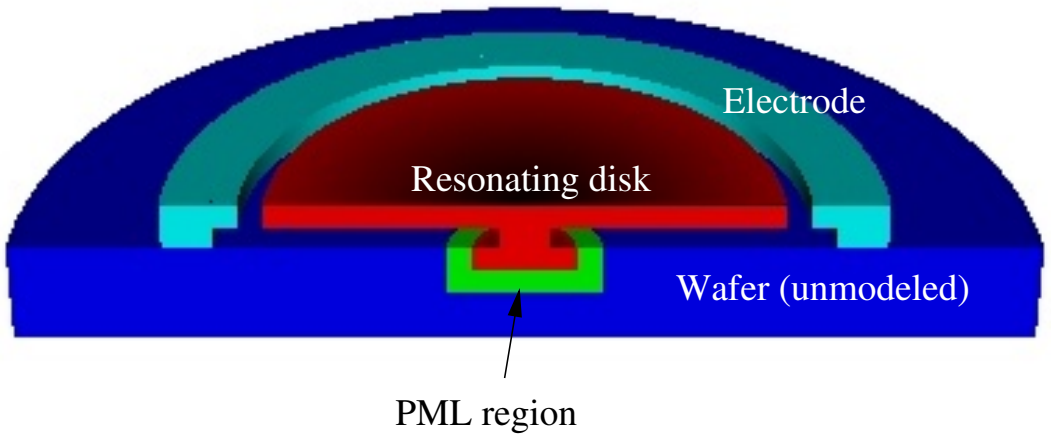
# Disk Resonator Simulations

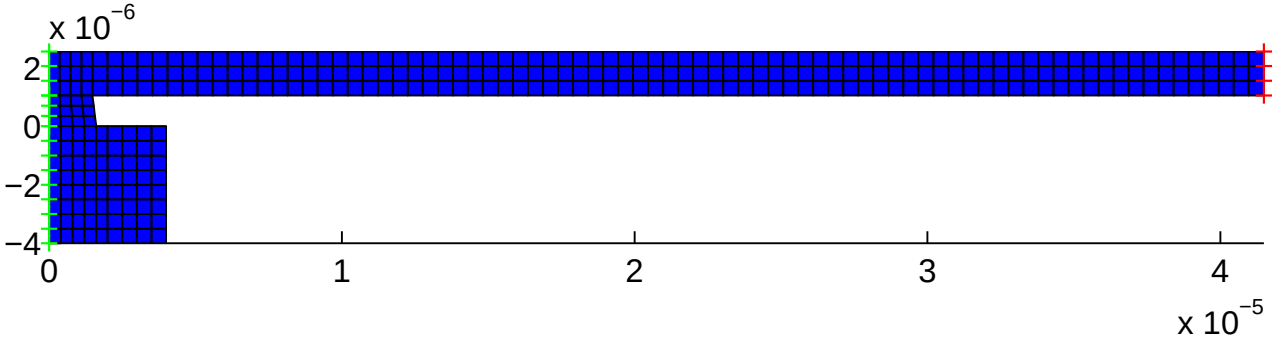




# Disk Resonator Mesh



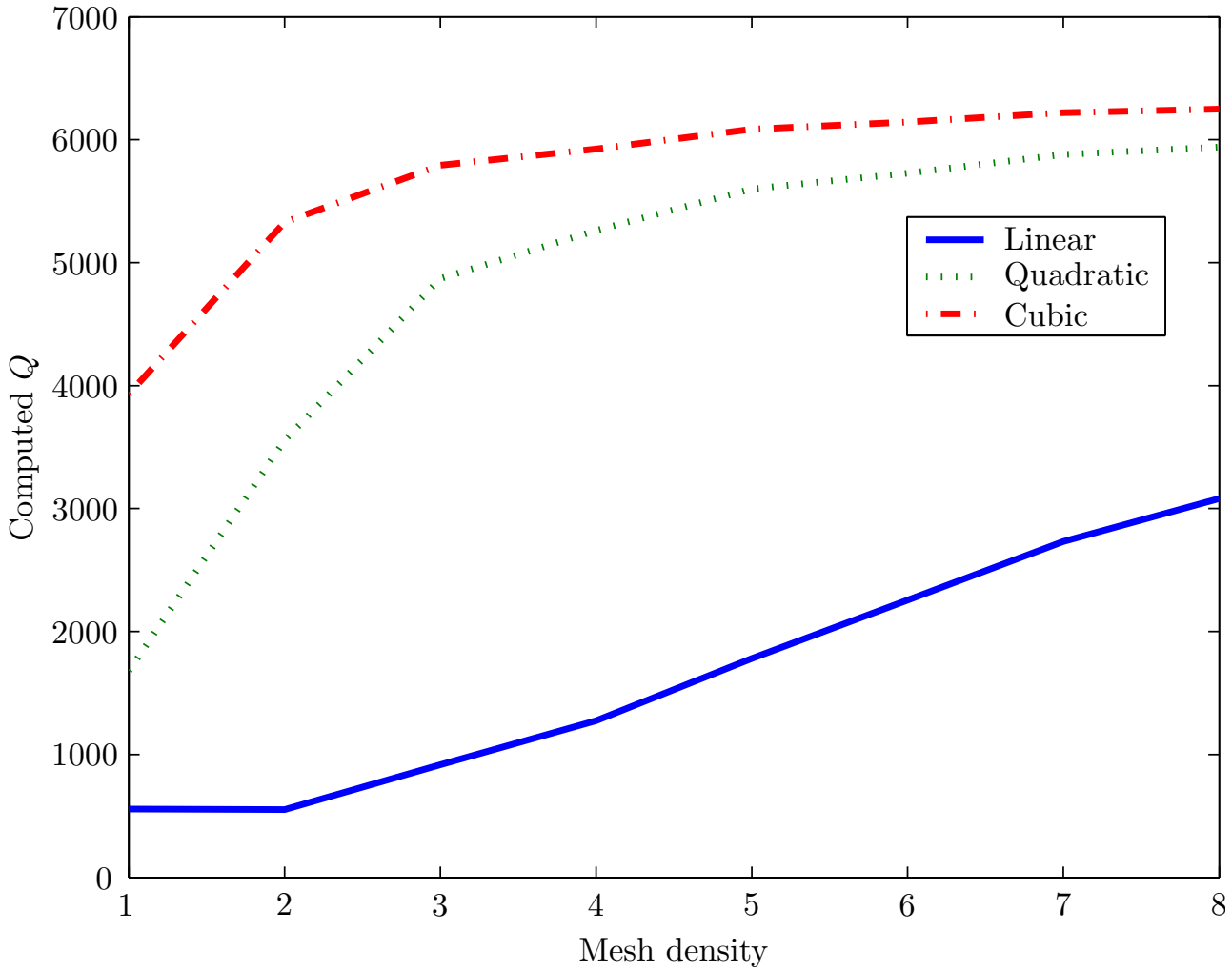



- Axisymmetric model with bicubic mesh
- About 10K nodal points in converged calculation

# Mesh Convergence

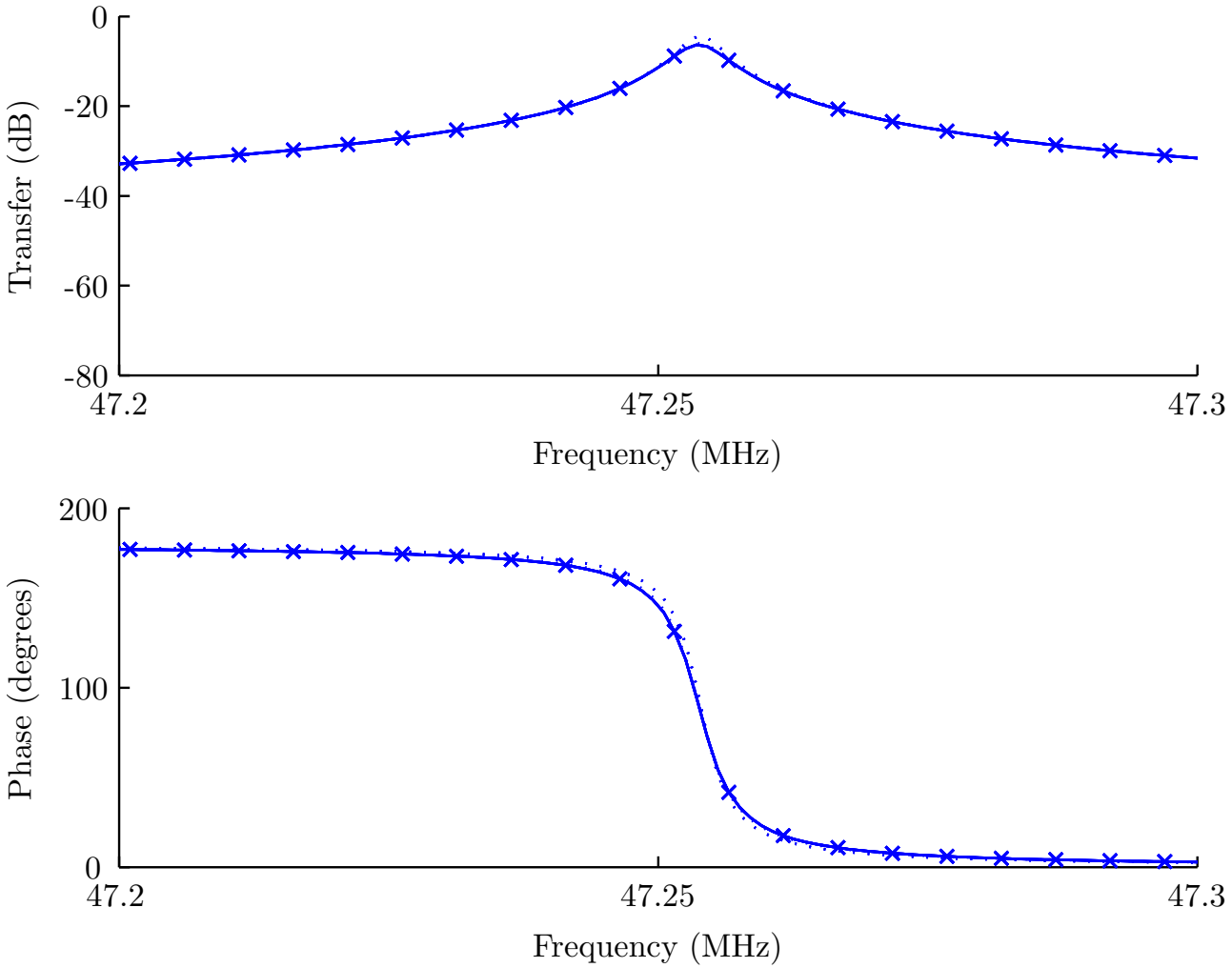





Cubic elements converge with reasonable mesh density

# Model Reduction Accuracy

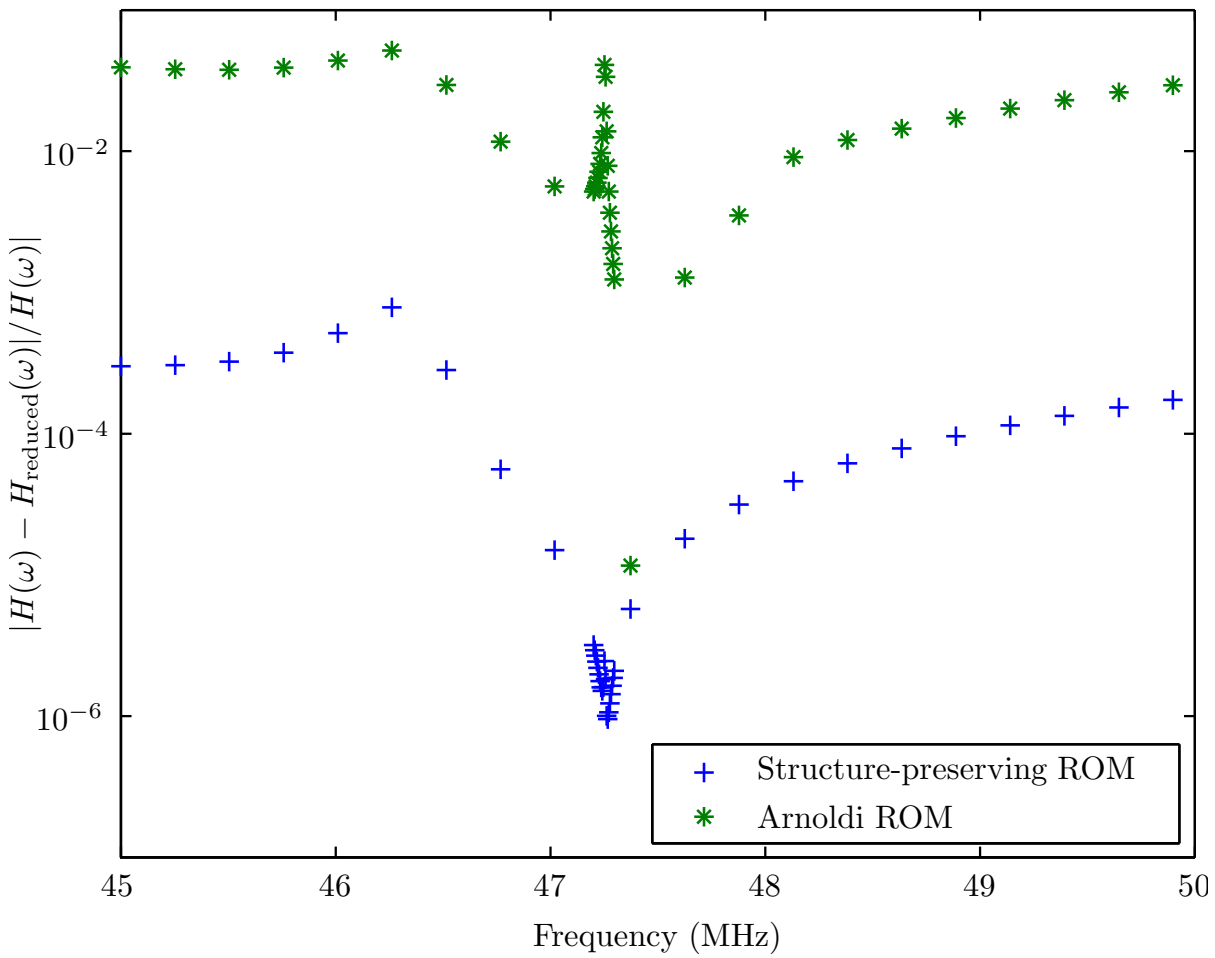





Results from ROM (solid and dotted lines) near indistinguishable from full model (crosses)

# Model Reduction Accuracy

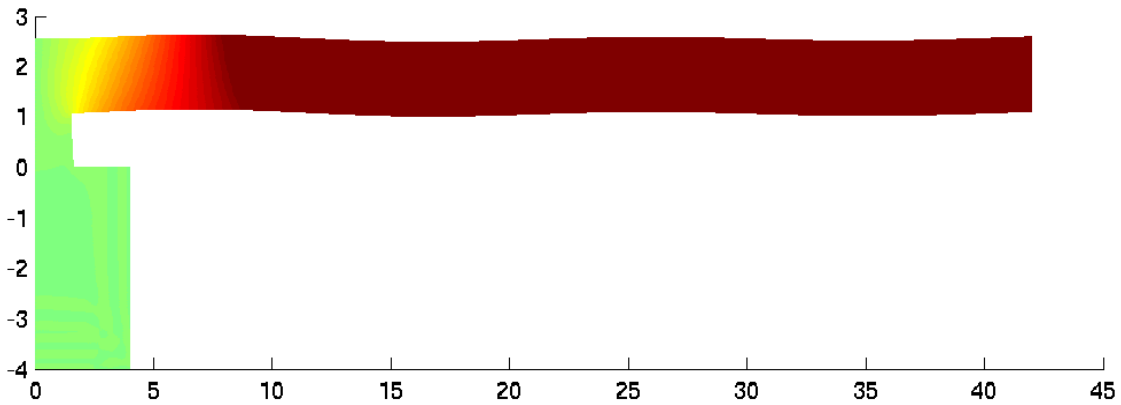


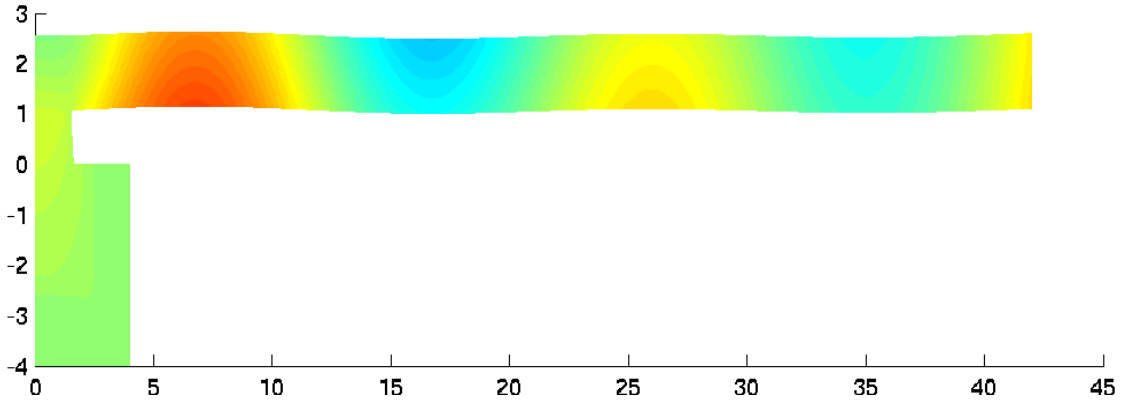



Preserve structure $\Longrightarrow$
get twice the correct digits

# Response of the Disk Resonator

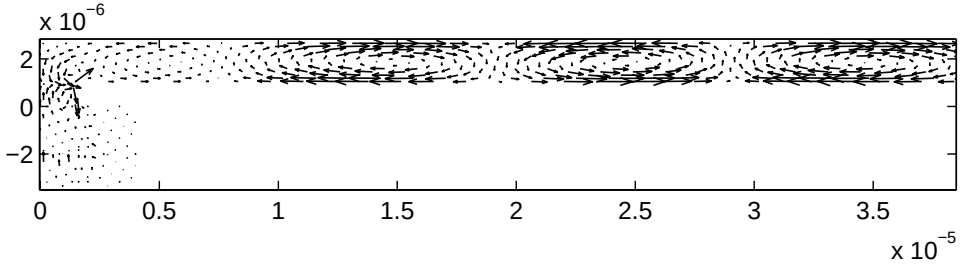


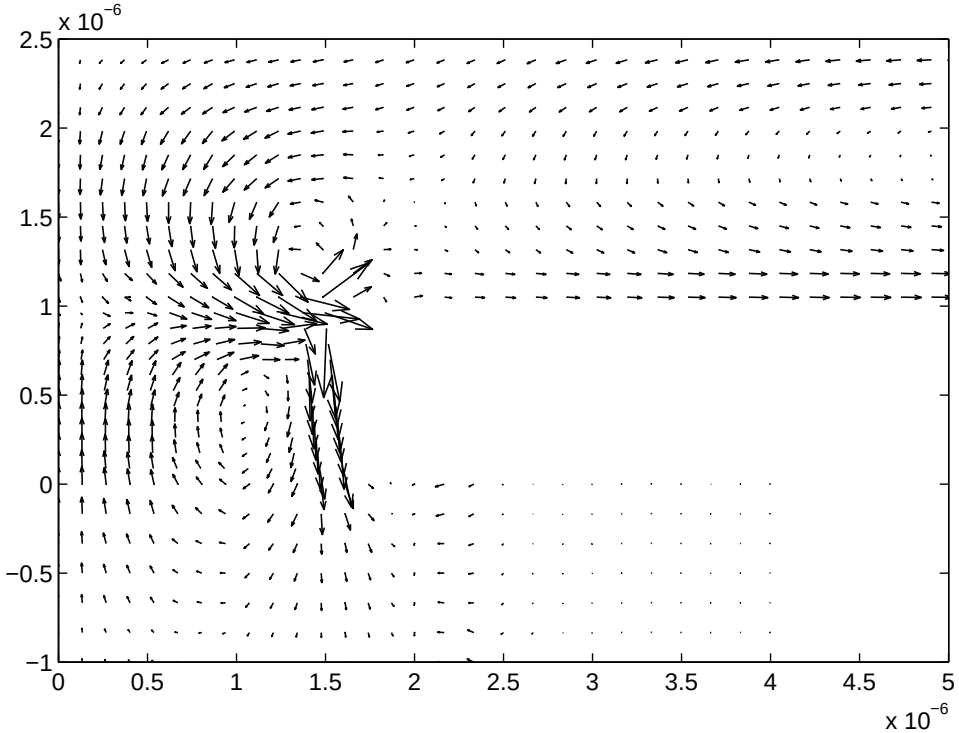


# Time-Averaged Energy Flux

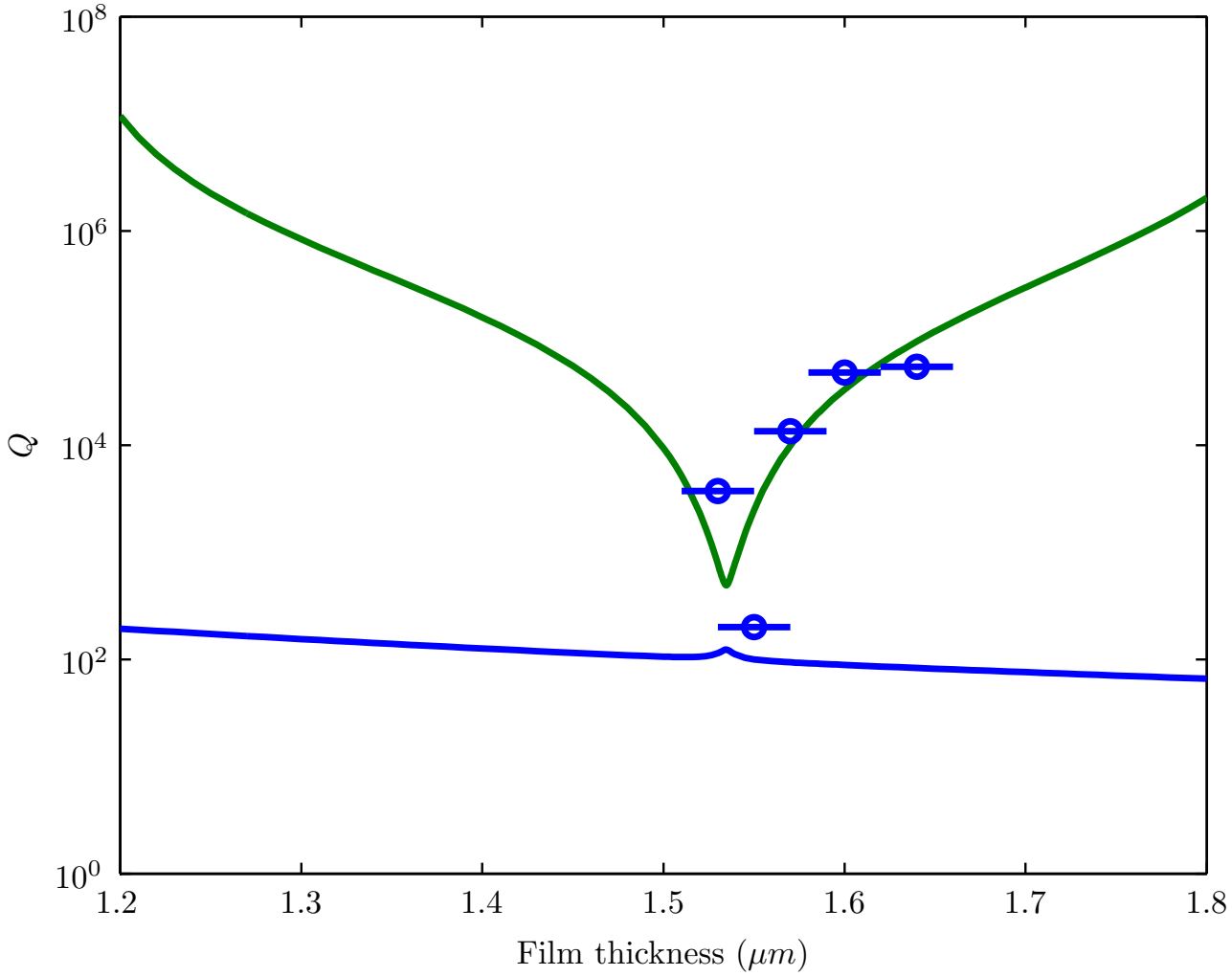




# Variation in Quality of Resonance

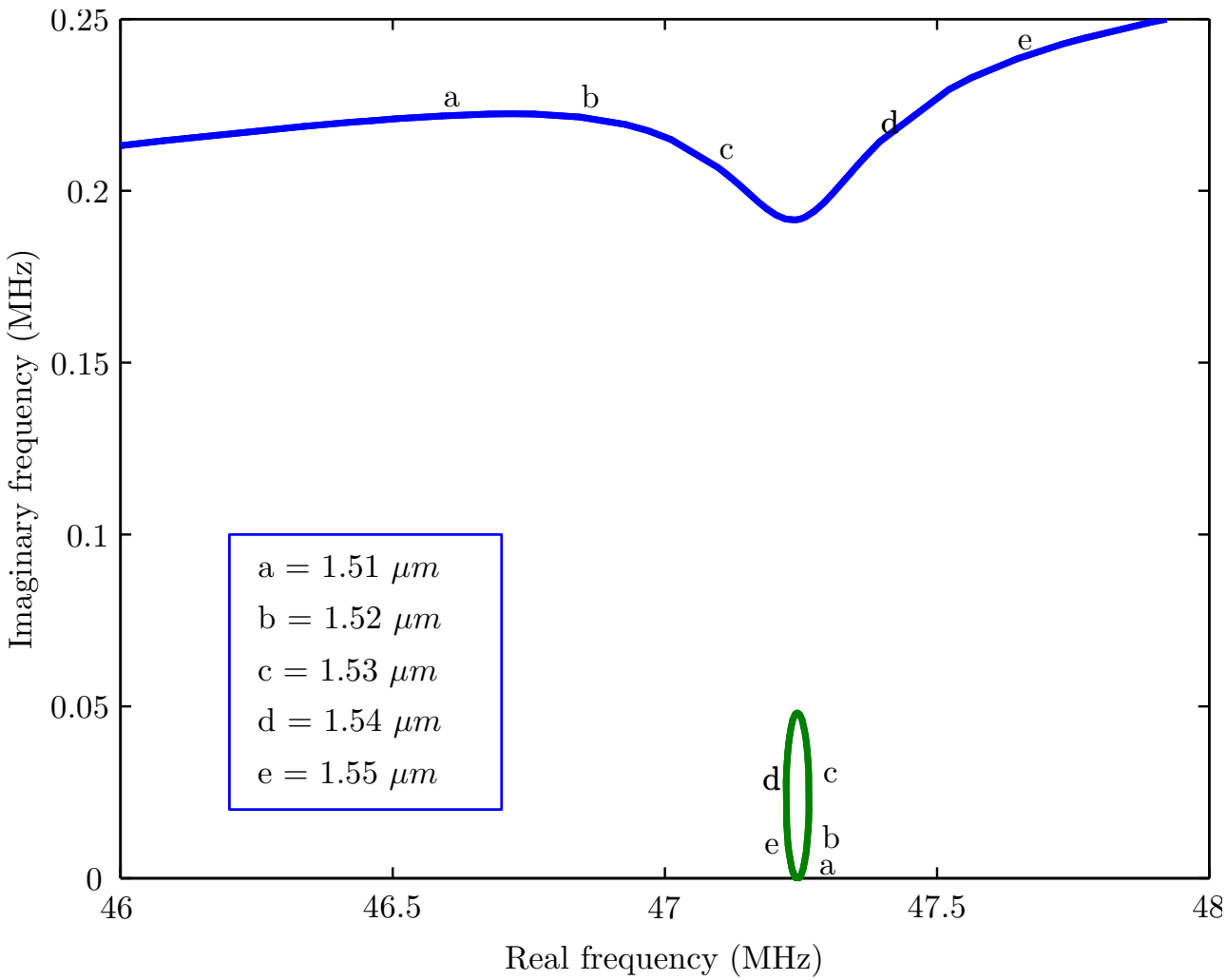





Simulation and lab measurements vs. disk thickness

# Explanation of $Q$ Variation






Interaction of two nearby eigenmodes

# Contributions



- Built disk model in HiQLab and verified against lab measurements
- Demonstrated dominance of anchor loss for this device
- Predicted geometric sensitivity of quality factor $Q$ (which was subsequently verified in the lab)
- Explained $Q$ sensitivity in terms of mode interference

# Contributions Summary (1)



- Application modeling
  - Finite element models of several devices
  - Discovery of effects of mode interference
  - Importance of anchor loss vs thermoelastic damping
- Mathematical analysis
  - Reformulation of perfectly-matched layers
  - Analysis of discretization and parameter choice in PMLs
  - Complex symmetry-preserving model reduction
  - Perturbation solution for thermoelastic damping
- Software: HiQLab, FEAPMEX, SUGAR

# Contributions Summary (2)



- HiQLab (about 33000 lines of code)
  - Collaborations at Berkeley, Cornell, Stanford, Bosch
- FEAPMEX (about 5000 lines of code)
  - 2400+ page views
  - Used for instrument models, stochastic structural analysis, ultrasonic nondestructive evaluation problems, material parameter identification problems
- SUGAR (about 18000 lines of code)
  - 2000+ downloads
  - Used in classes at Berkeley, Cornell, Johns Hopkins
  - Continued research use for design optimization

# Other Contributions



- Lowered complexity of `roots` from $O(n^3)$ to $O(n^2)$
  - Code to go into next LAPACK release
- Developed first sparse subspace continuation code
  - Going into the next Matcont release
- Developed new network tomography method
- Designed initial security model for OceanStore
- Served as IEEE 754R secretary
- Responsible for last CLAPACK version

# Future Work



- Code development
  - Structural elements and elements for different physics
  - Design and implementation of parallelized version
- Theoretical analysis
  - More damping mechanisms
  - Sensitivity analysis and variational model reduction
- Application collaborations
  - Use of nonlinear effects (quasi-static and dynamic)
  - New designs (e.g. internal dielectric drives)
  - Continued experimental comparisons

# Conclusions



- RF MEMS are a great source of problems
  - Interesting applications
  - Interesting physics (and not altogether understood)
  - Interesting numerical mathematics

`http://www.cs.berkeley.edu/~dbindel`

# Sources of Damping





- Fluid damping
  - Air is a viscous fluid ($\mathrm{Re} \ll 1$)
  - Can operate in a vacuum
  - Shown not to dominate in many RF designs
- Material losses
  - Low intrinsic losses in silicon, diamond, germanium
  - Terrible material losses in metals
- Thermoelastic damping
  - Volume changes induce temperature change
  - Diffusion of heat leads to mechanical loss
- Anchor loss
  - Elastic waves radiate from structure

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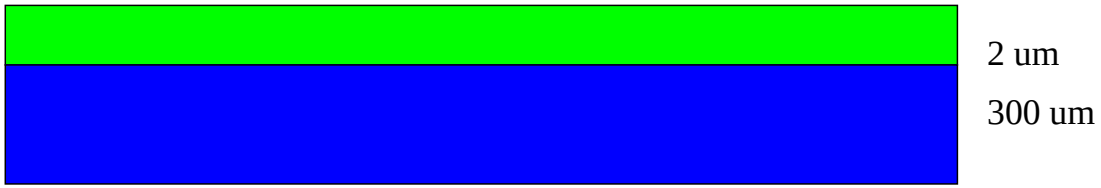
# Fabrication Outline




1. Si wafer
2. Deposit 2 microns SiO2
3. Pattern and etch SiO2 layer
4. Deposit 2 microns polycrystalline Si
5. Pattern and etch Si layer
6. Release etch remaining SiO2

# Fabrication Outline






1. Si wafer
2. Deposit 2 microns SiO2
3. Pattern and etch SiO2 layer
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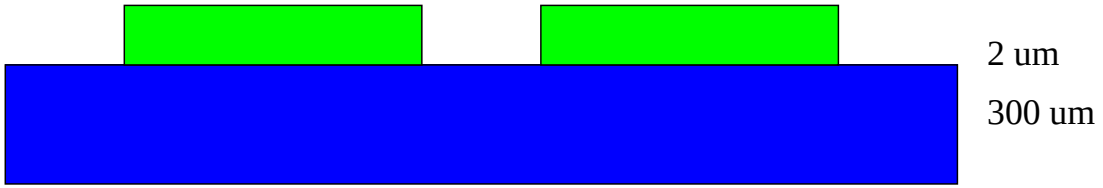
# Fabrication Outline



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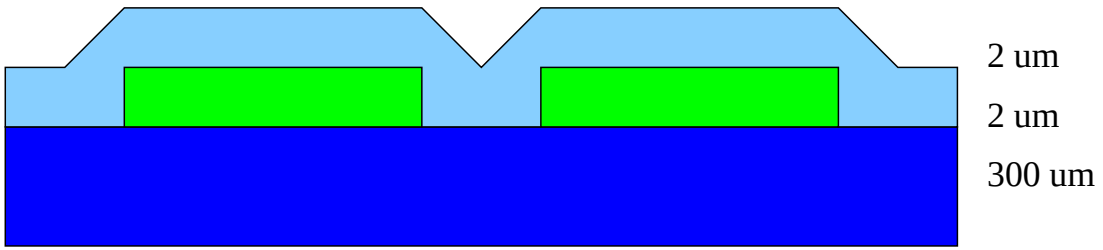


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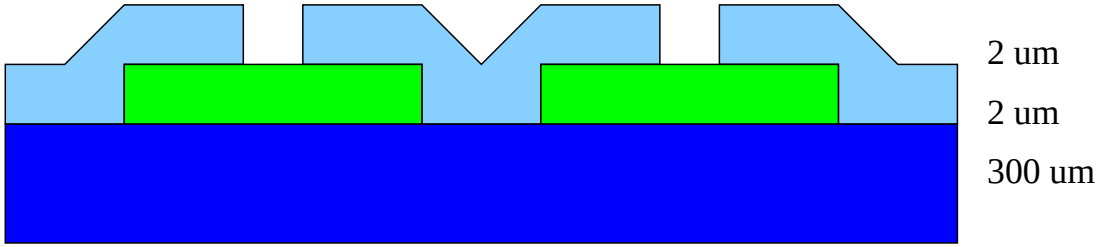


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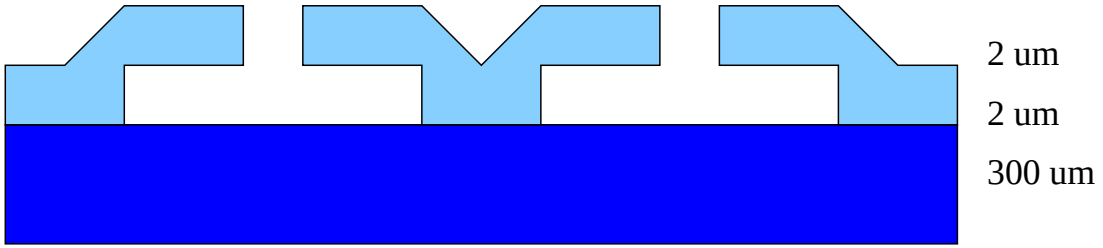


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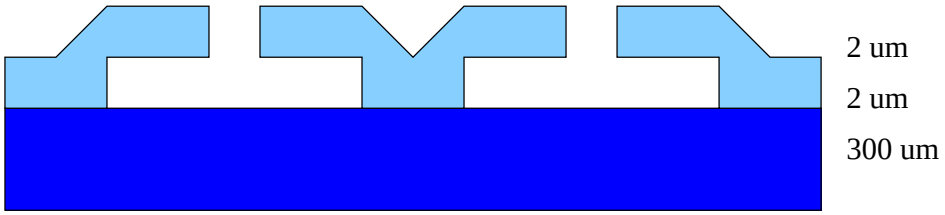
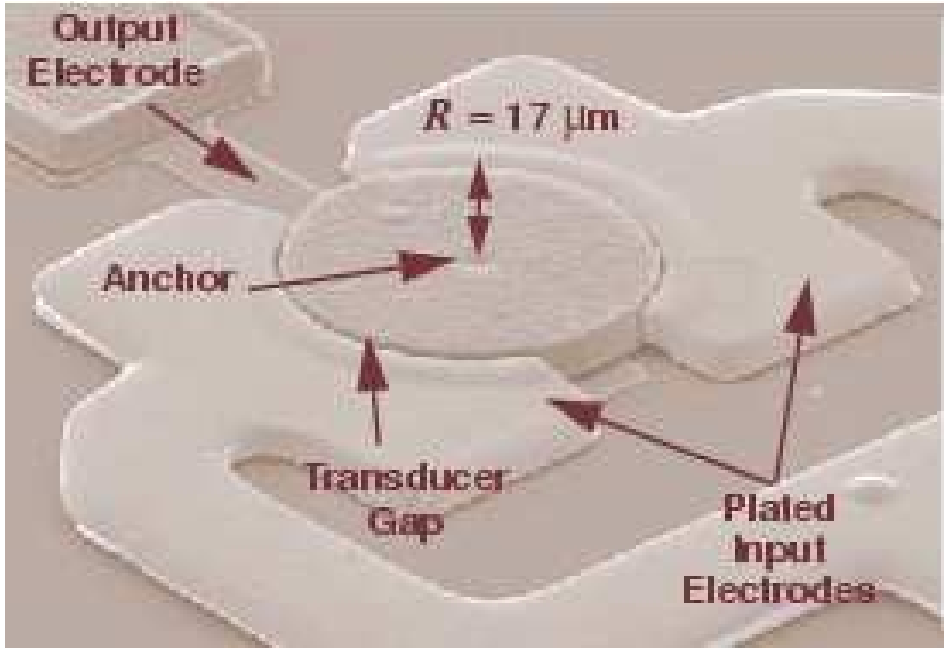
# Fabrication Result








(C. Nguyen, iMEMS 02)

# Role of simulation





HiQLab: Modeling RF MEMS

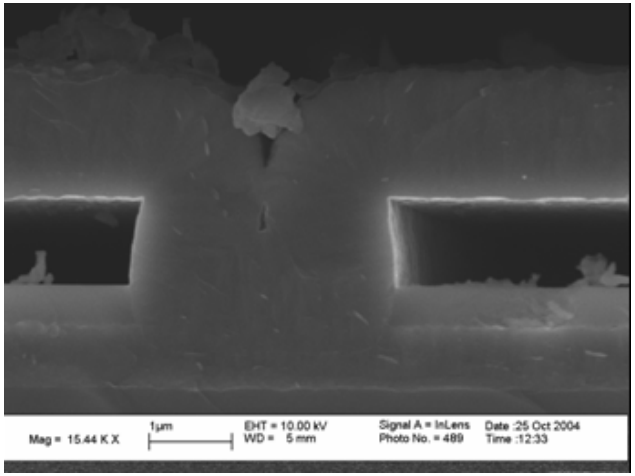
- Explore fundamental device physics
  - Particularly details of damping
- Detailed finite element modeling
- Reduced models eventually to go into SUGAR

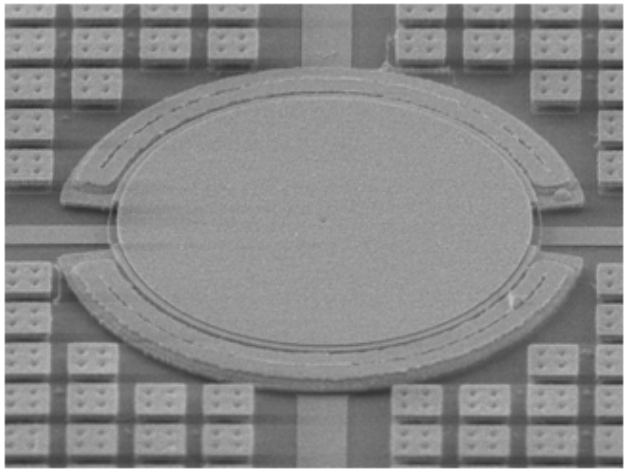
SUGAR: “Be SPICE to the MEMS world”

- Fast enough for early design stages
- Simple enough to attract users
- Support design, analysis, optimization, synthesis
- Verify models by comparison to measurement

# Why simulate?





- "Build and break" is too expensive
  - Wafer processing costs months, thousands of dollars
  - Fabrication is imprecise
  - Days or weeks to take good measurements
- Good experiments need good hypotheses
- Even when device behavior is understood, still need to understand system behavior

# From simulation to synthesis





Computer can assist at many levels:

- Fundamental physics
- Detailed device models
- System-level models and macromodels
- Metrology
- Design optimization
- Design synthesis

# Research thrusts





- Model development (e.g. new finite elements)
- Numerical algorithms (e.g. model reduction)
- Numerical software engineering (SUGAR, HiQLab)
- Metrology and comparison to measurement
- Optimization and design synthesis

# Research group

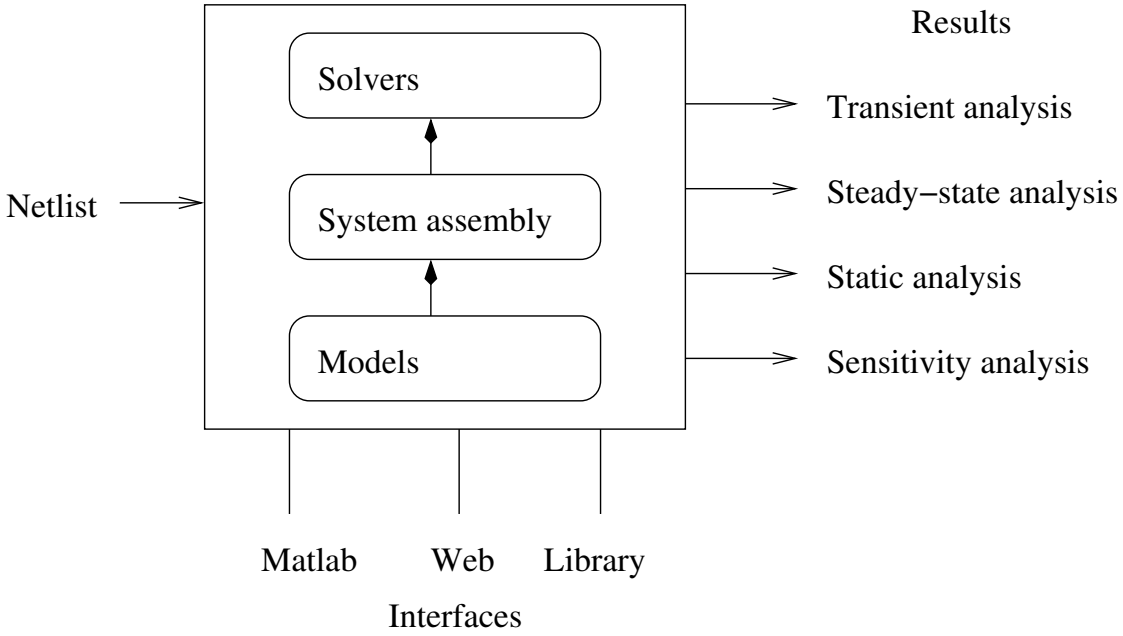
| Faculty | | Students | |
|---|---|---|---|
| A. Agogino | (ME) | D. Bindel | (CS) |
| Z. Bai | (Math,CS,UCD) | J.V. Clark | (AS&T) |
| J. Demmel | (Math,CS) | C. Cobb | (ME) |
| S. Govindjee | (CEE) | D. Garmire | (CS) |
| R. Howe | (EE,ME) | T. Koyama | (CEE) |
| K.S.J. Pister | (EE) | J. Nie | (Math) |
| C. Sequin | (CS) | H. Wei | (CEE) |
| | | Y. Zhang | (CEE) |

# SUGAR



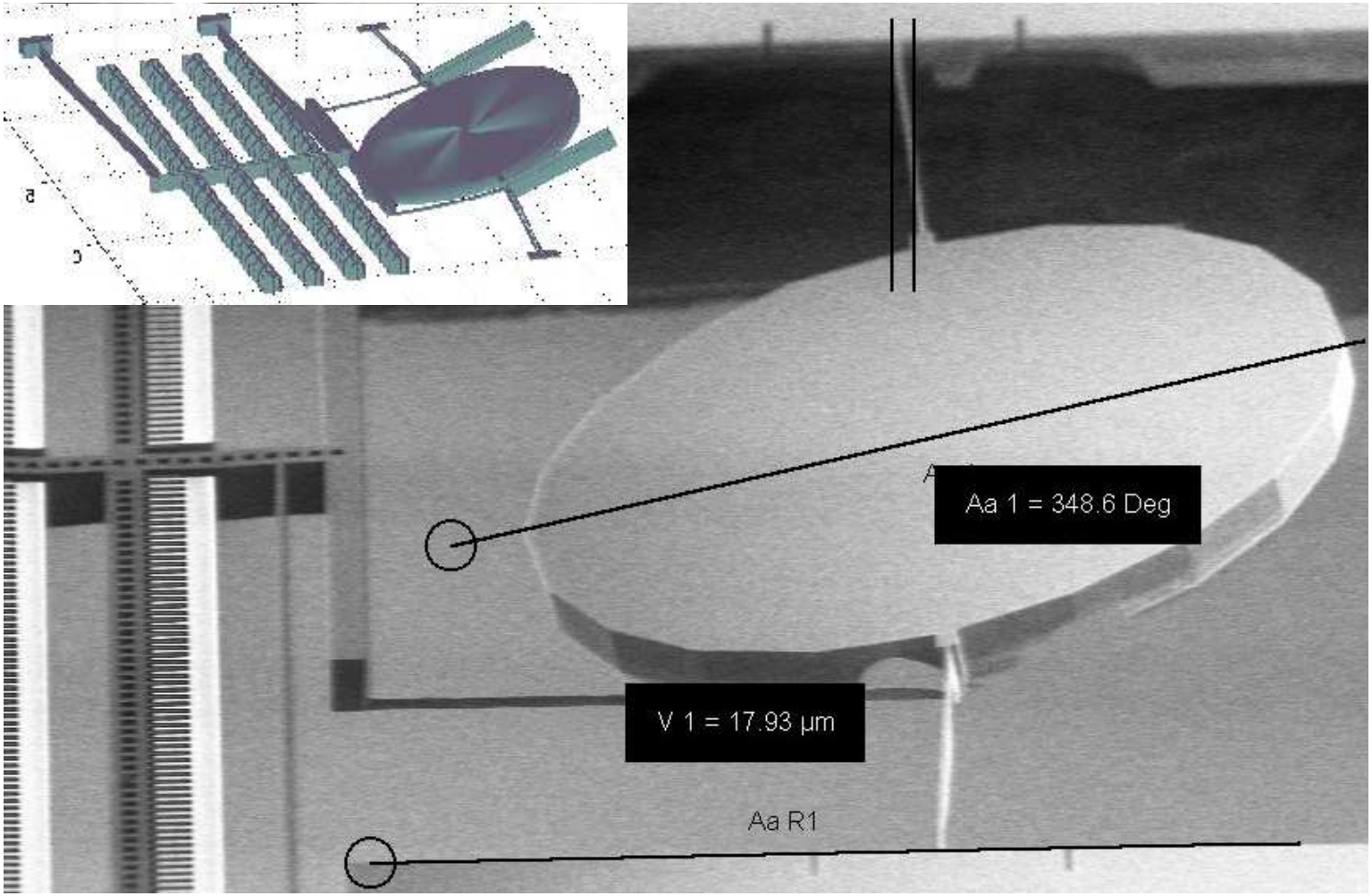
Goal: "Be SPICE to the MEMS world"

- Fast enough for early design stages
- Simple enough to attract users
- Support design, analysis, optimization, synthesis
- Verify models by comparison to measurement



# SUGAR: Analysis of a micromirror

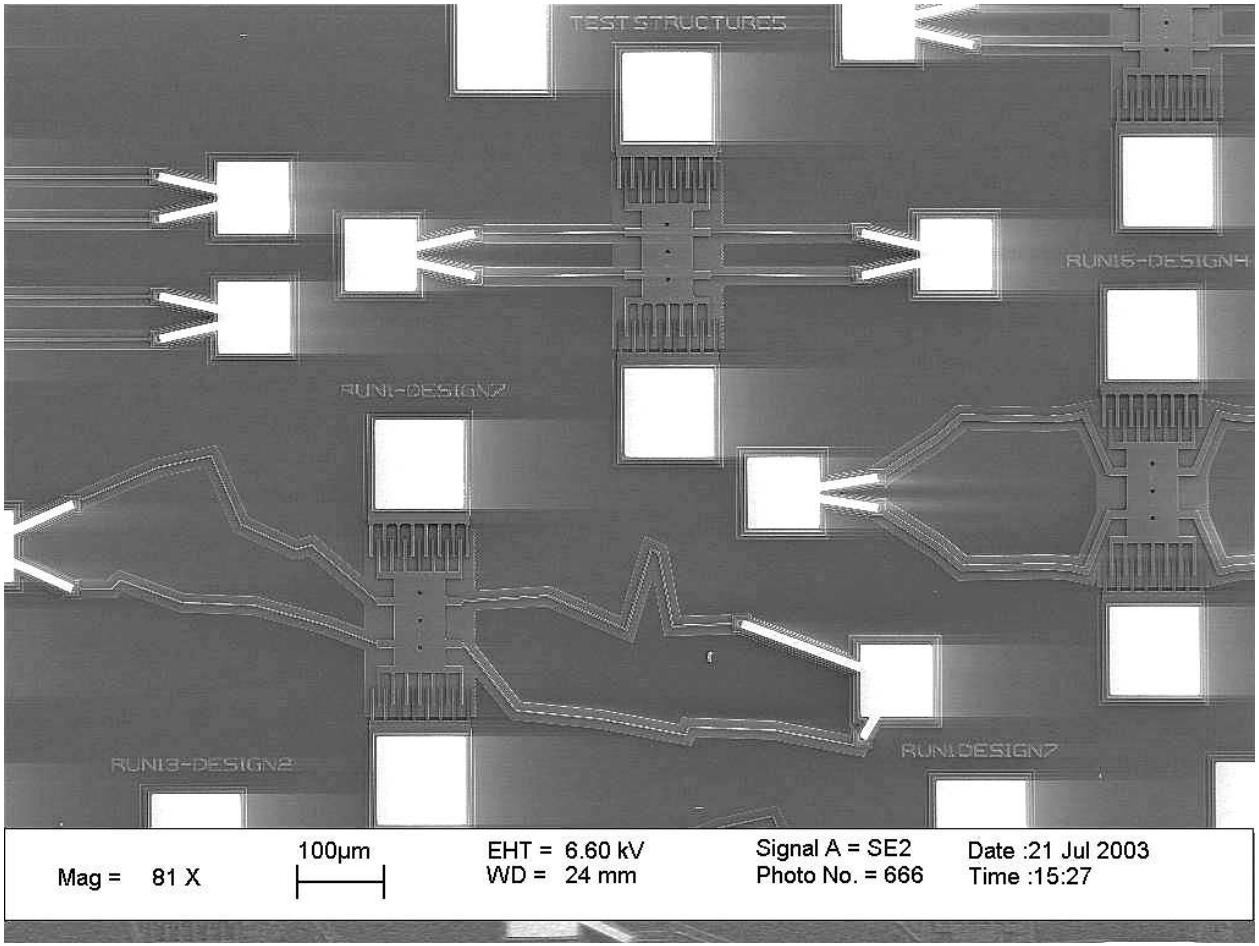


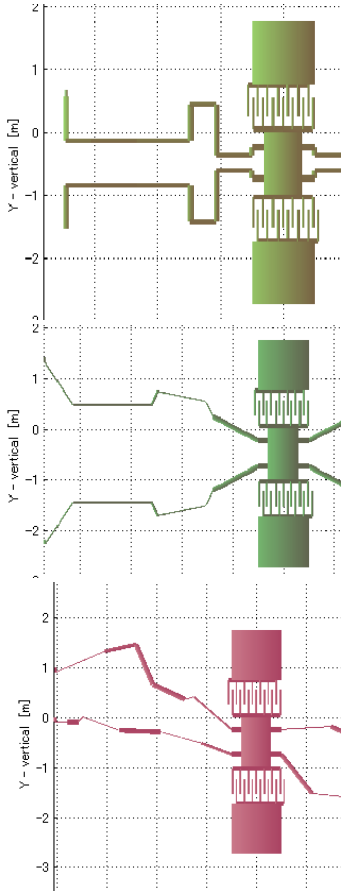



(Mirror design by M. Last)

# SUGAR: Design synthesis

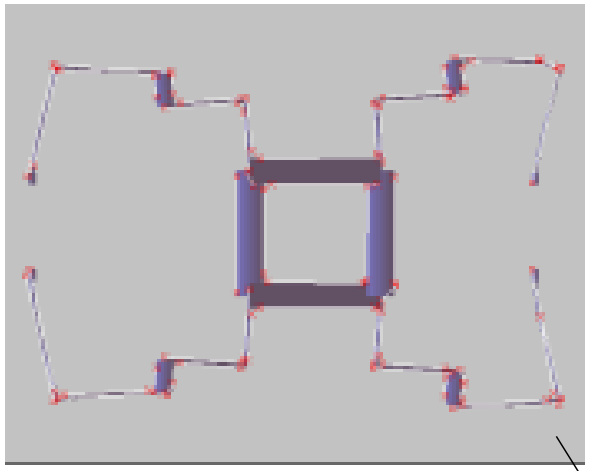


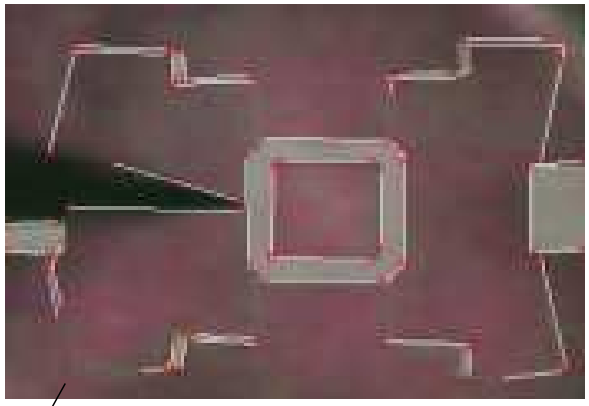


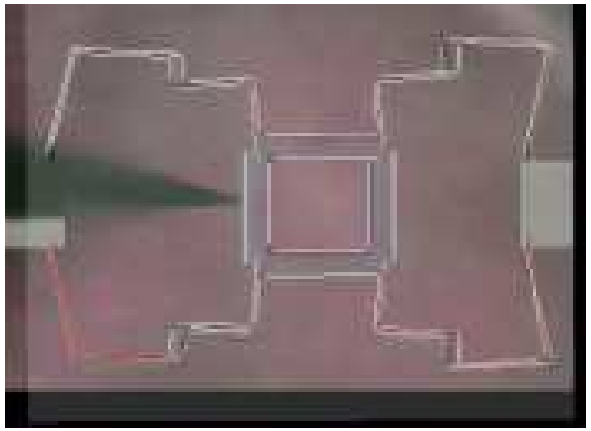



# SUGAR: Comparison to measurement









# Elastic PMLs





$$\int_\Omega \epsilon(w) : \mathsf{C} : \epsilon(u)\, d\Omega - \omega^2 \int_\Omega \rho w \cdot u\, d\Omega = \int_\Gamma w \cdot t_n d\Gamma$$

$$\epsilon(u) = \left(\frac{\partial u}{\partial x}\right)^s$$

- Start from standard weak form
- Introduce transformed $\tilde{x}$ with $\frac{\partial \tilde{x}}{\partial x} = \Lambda$
- Map back to reference system ($J_\Lambda = \det(\Lambda)$)
- All terms are symmetric in $w$ and $u$

# Elastic PMLs





$$\int_{\tilde{\Omega}} \tilde{\epsilon}(w) : \mathsf{C} : \tilde{\epsilon}(u)\, d\tilde{\Omega} - \omega^2 \int_{\tilde{\Omega}} \rho w \cdot u\, d\tilde{\Omega} = \int_{\Gamma} w \cdot t_n d\Gamma$$

$$\tilde{\epsilon}(u) = \left(\frac{\partial u}{\partial \tilde{x}}\right)^s = \left(\frac{\partial u}{\partial x}\Lambda^{-1}\right)^s$$

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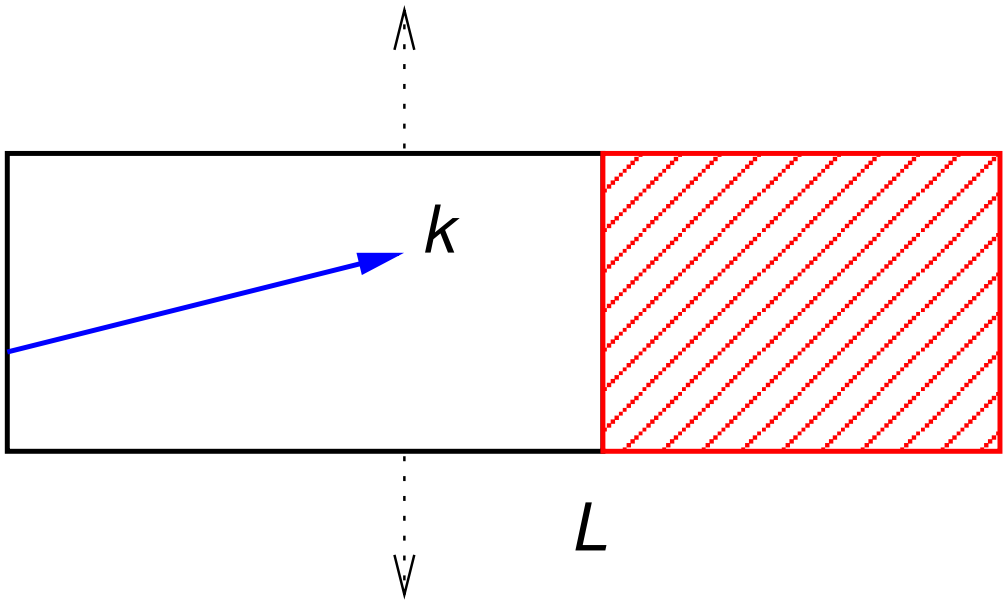
# Continuum 2D model problem



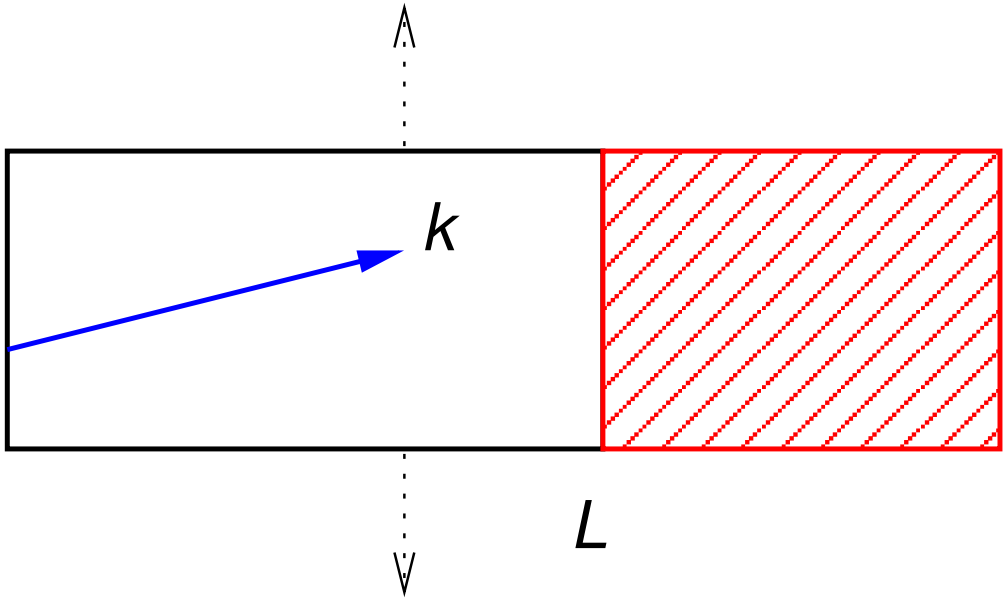



$$\lambda(x) = \begin{cases} 1 - i\beta|x - L|^p, & x > L \\ 1 & x \leq L. \end{cases}$$

$$\frac{1}{\lambda}\frac{\partial}{\partial x}\left(\frac{1}{\lambda}\frac{\partial u}{\partial x}\right) + \frac{\partial^2 u}{\partial y^2} + k^2 u = 0$$

# Continuum 2D model problem



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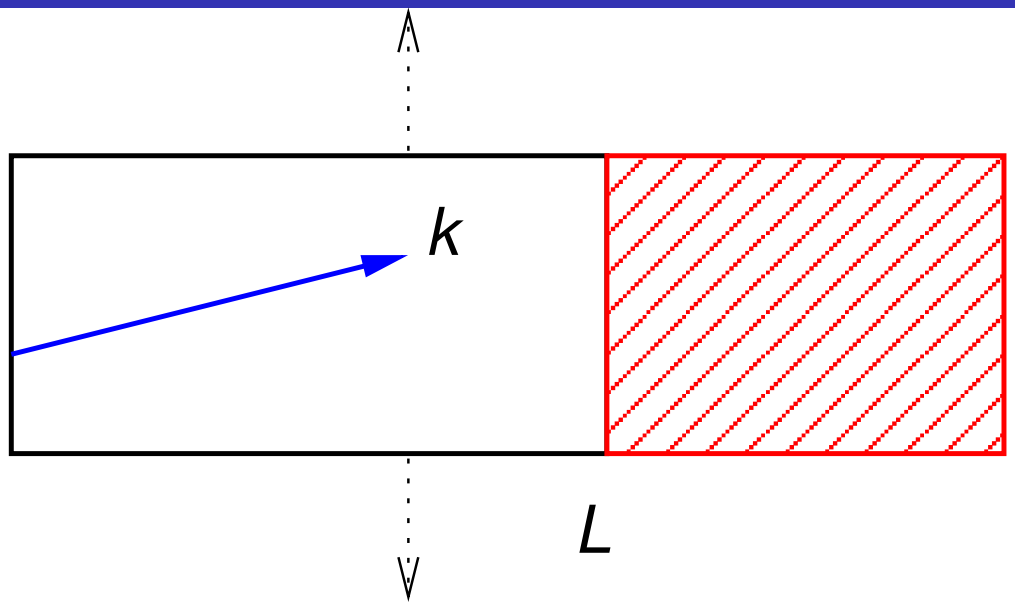
$$\frac{1}{\lambda}\frac{\partial}{\partial x}\left(\frac{1}{\lambda}\frac{\partial u}{\partial x}\right) - k_y^2 u + k^2 u = 0$$

# Continuum 2D model problem





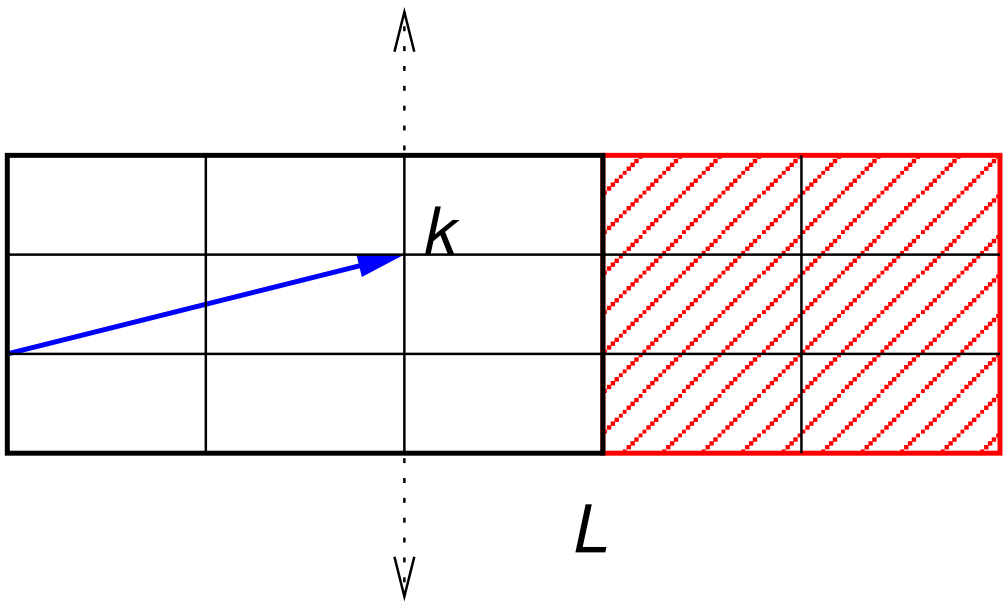

$$\lambda(x) = \begin{cases} 1 - i\beta|x - L|^p, & x > L \\ 1 & x \leq L. \end{cases}$$

$$\frac{1}{\lambda}\frac{\partial}{\partial x}\left(\frac{1}{\lambda}\frac{\partial u}{\partial x}\right) + k_x^2 u = 0$$

1D problem, reflection of $O(e^{-k_x \gamma})$

# Discrete 2D model problem

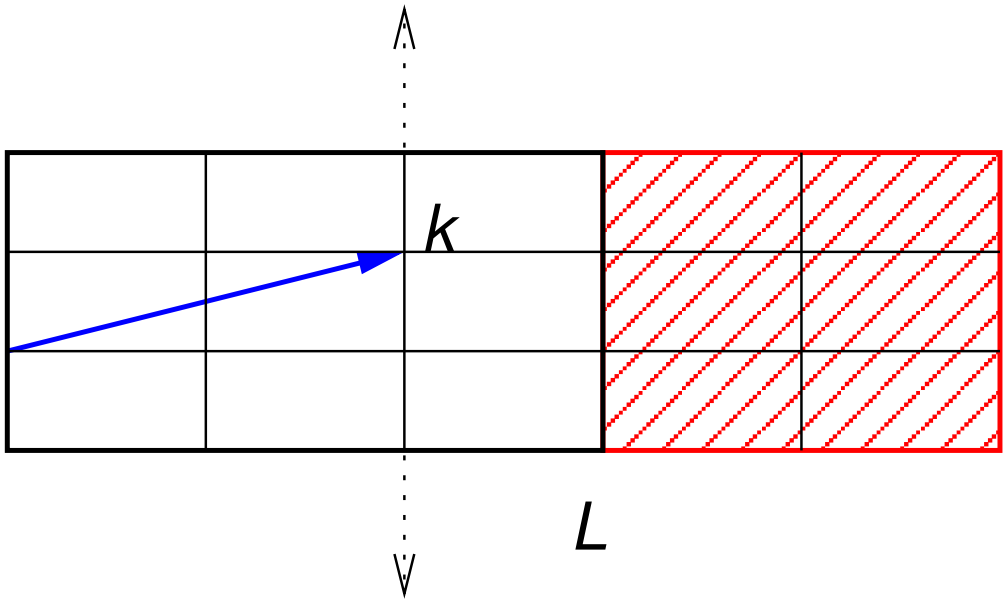





- Discrete Fourier transform in $y$
- Solve numerically in $x$
- Project solution onto infinite space traveling modes
- Extension of Collino and Monk (1998)

# Nondimensionalization



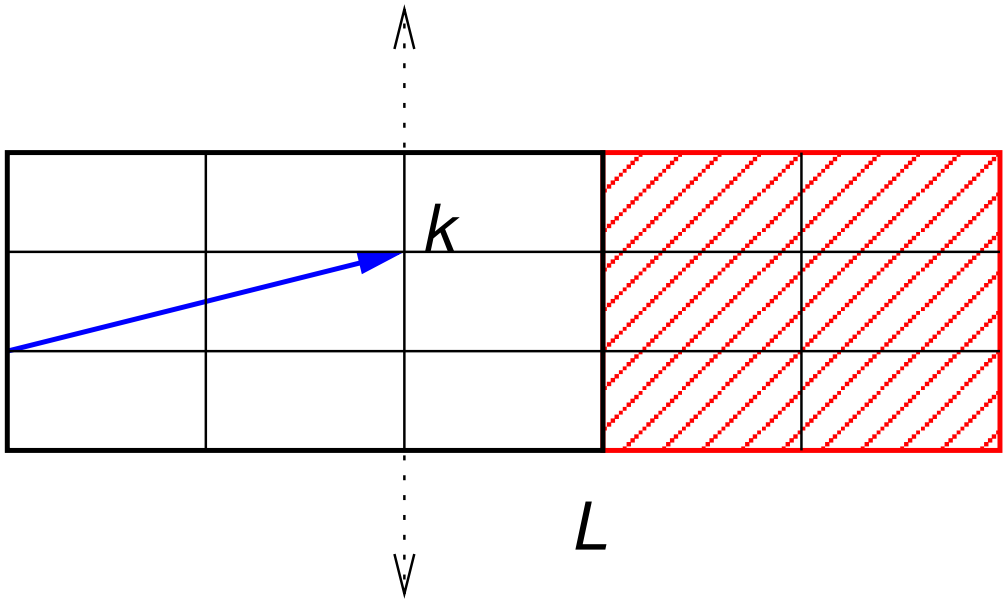



$$\lambda(x) = \begin{cases} 1 - i\beta|x - L|^p, & x > L \\ 1 & x \leq L. \end{cases}$$

| | |
|---|---|
| Rate of stretching: | $\beta h^p$ |
| Elements per wave: | $(k_x h)^{-1}$ and $(k_y h)^{-1}$ |
| Elements through the PML: | $N$ |

# Nondimensionalization



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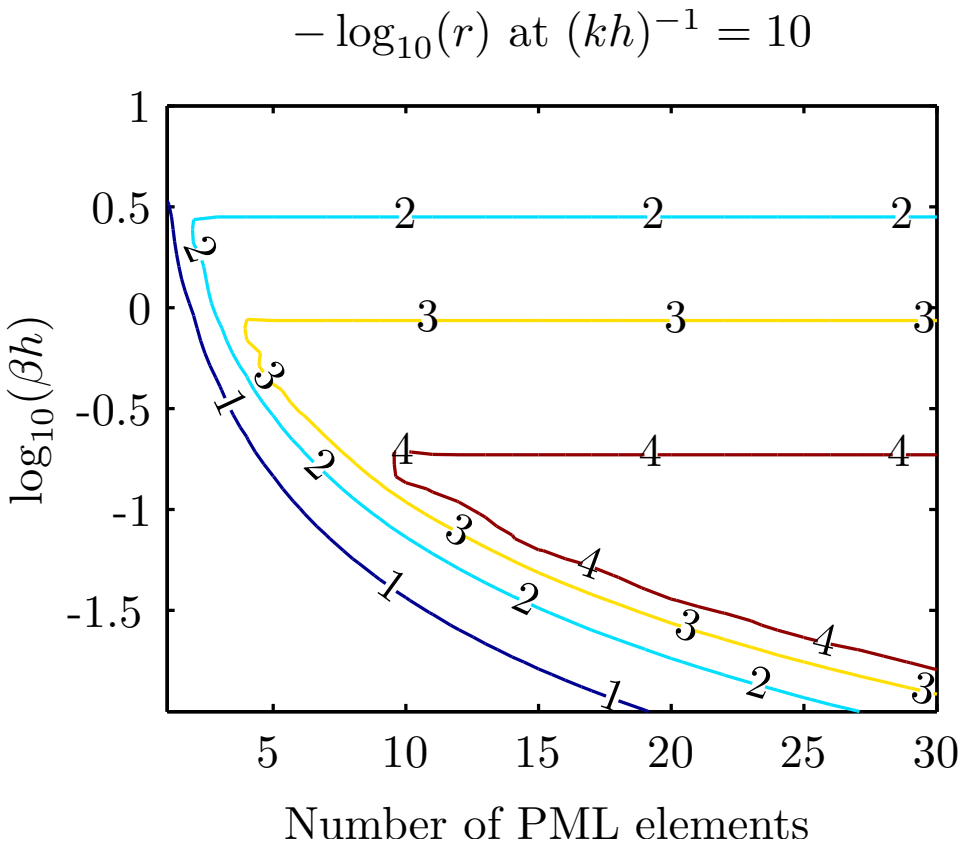
# Discrete reflection behavior






Quadratic elements, $p = 1$, $(k_x h)^{-1} = 10$

# Discrete reflection decomposition



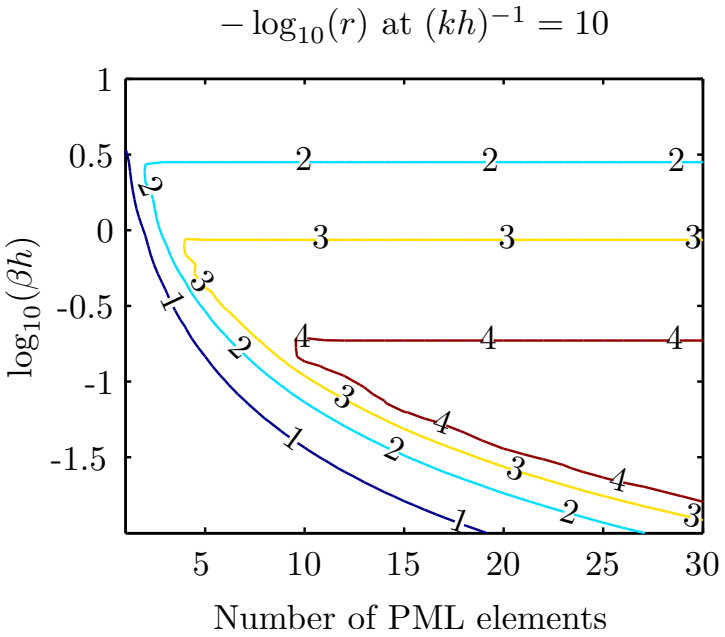


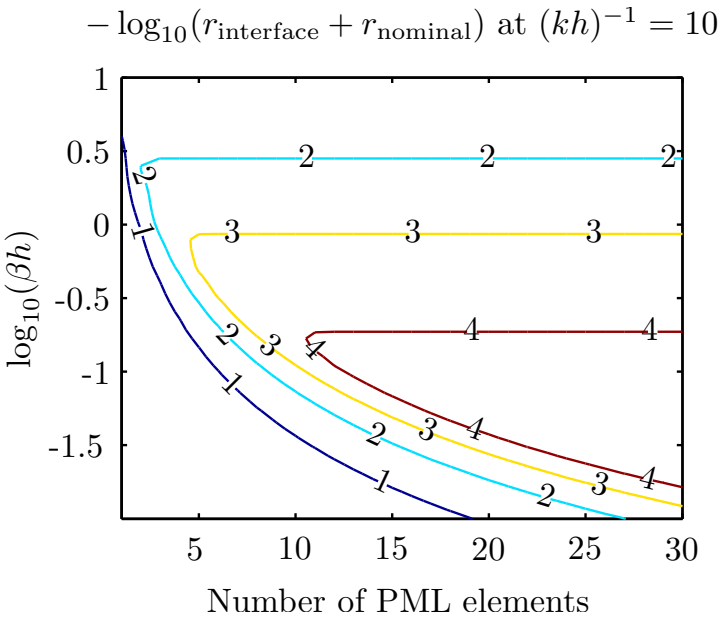
Model discrete reflection as two parts:

- Far-end reflection (clamping reflection)
  - Approximated well by continuum calculation
  - Grows as $(k_x h)^{-1}$ grows
- Interface reflection
  - Discrete effect: mesh does not resolve decay
  - Does not depend on $N$
  - Grows as $(k_x h)^{-1}$ shrinks

# Discrete reflection behavior






Quadratic elements, $p = 1$, $(k_x h)^{-1} = 10$

- Model does well at predicting actual reflection
- Similar picture for other wavelengths, element types, stretch functions

# Choosing PML parameters





- Discrete reflection dominated by
  - Interface reflection when $k_x$ large
  - Far-end reflection when $k_x$ small
- Heuristic for PML parameter choice
  - Choose an acceptable reflection level
  - Choose $\beta$ based on interface reflection at $k_x^{\max}$
  - Choose length based on far-end reflection at $k_x^{\min}$

# Thermoelastic damping (TED)



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

$$\begin{aligned} \sigma &= C\epsilon - \beta\theta 1 \\ \rho u_{tt} &= \nabla \cdot \sigma \\ \rho c_v \theta_t &= \nabla \cdot (\kappa \nabla \theta) - \beta T_0 \operatorname{tr}(\epsilon_t) \end{aligned}$$

- Volumetric strain rate drives energy transfer from mechanical to thermal domain
  - Irreversible 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

# Nondimensionalization



$$
\begin{aligned}
\sigma &= \hat{C}\epsilon - \xi\theta 1 \\
u_{tt} &= \nabla \cdot \sigma \\
\theta_t &= \eta\nabla^2\theta - \mathrm{tr}(\epsilon_t)
\end{aligned}
$$

$$
\xi := \left(\frac{\beta}{\rho c}\right)^2 \frac{T_0}{c_v} \text{ and } \eta := \frac{\kappa}{\rho c_v c L}
$$

$$
\begin{aligned}
\text{Length} &\sim L \\
\text{Time} &\sim L/c, \text{ where } c = \sqrt{E/\rho} \\
\text{Temperature} &\sim T_0 \frac{\beta}{\rho c_v}
\end{aligned}
$$

# Scaling analysis



$$
\begin{aligned}
\sigma &= \hat{C}\epsilon - \xi\theta 1 \\
u_{tt} &= \nabla \cdot \sigma \\
\theta_t &= \eta\nabla^2\theta - \mathrm{tr}(\epsilon_t)
\end{aligned}
$$

$$
\xi := \left(\frac{\beta}{\rho c}\right)^2 \frac{T_0}{c_v} \text{ and } \eta := \frac{\kappa}{\rho c_v c L}
$$

- Micron-scale poly-Si devices: $\xi$ and $\eta$ are $\sim 10^{-4}$.
- Small $\eta$ leads to thermal boundary layers
- Linearize about $\xi = 0$

# Discrete mode equations



$$
\begin{aligned}
\sigma &= \hat{C}\epsilon - \xi\theta 1 \\
u_{tt} &= \nabla \cdot \sigma \\
\theta_t &= \eta\nabla^2\theta - \mathrm{tr}(\epsilon_t)
\end{aligned}
$$

$$
\begin{aligned}
\sigma &= \hat{C}\epsilon - \xi\theta 1 \\
-\omega^2 u &= \nabla \cdot \sigma \\
i\omega\theta &= \eta\nabla^2\theta - i\omega\,\mathrm{tr}(\epsilon)
\end{aligned}
$$

$$
\begin{aligned}
-\omega^2 M_{uu}u + K_{uu}u + K_{ut}\theta &= 0 \\
i\omega D_{tt}\theta + K_{tt}\theta + i\omega D_{tu}u &= 0
\end{aligned}
$$

# Perturbation computation



$$\begin{aligned} -\omega^2 M_{uu} u + K_{uu} u + K_{ut}\theta &= 0 \\ i\omega D_{tt}\theta + K_{tt}\theta + i\omega D_{tu} u &= 0 \end{aligned}$$

Approximate $\omega$ by perturbation about $K_{ut} = 0$:

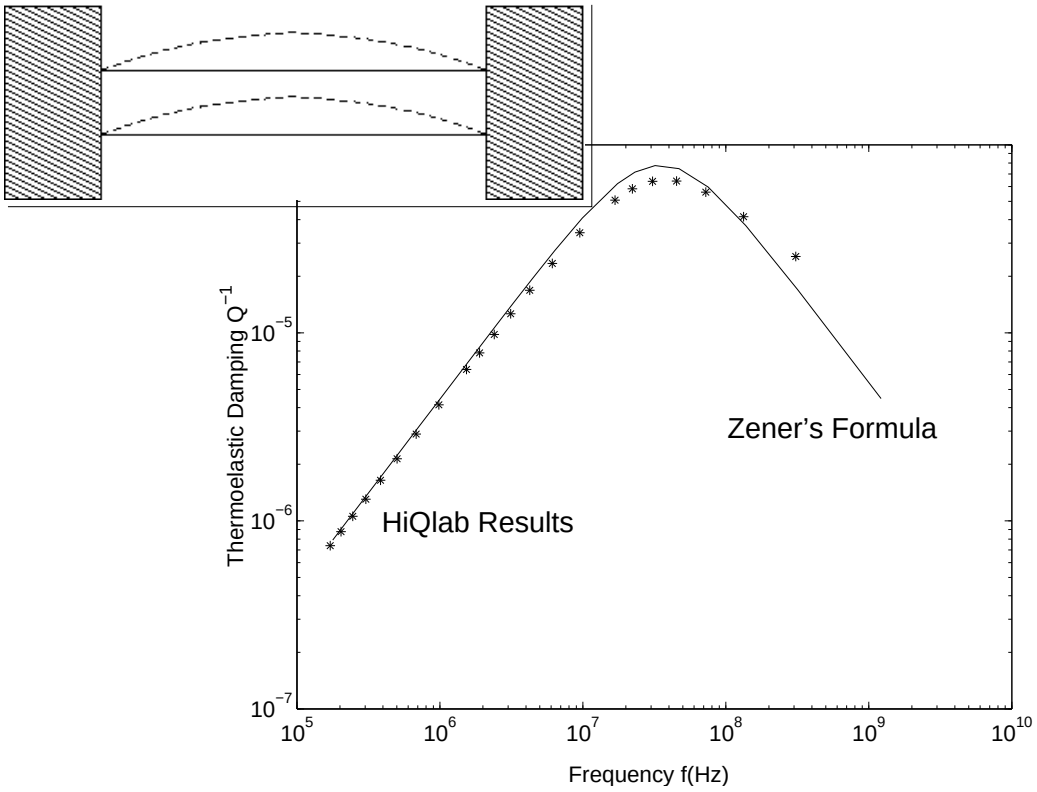
$$\begin{aligned} -\omega_0^2 M_{uu} u_0 + K_{uu} u_0 &= 0 \\ i\omega_0 D_{tt}\theta_0 + K_{tt}\theta_0 + i\omega_0 D_{tu} u_0 &= 0 \end{aligned}$$

Choose $v : v^T u_0 \neq 0$ and compute

$$\begin{bmatrix} (-\omega_0^2 M_{uu} + K_{uu}) & -2\omega_0 M_{uu} u_0 \\ v^T & 0 \end{bmatrix} \begin{bmatrix} \delta u \\ \delta\omega \end{bmatrix} = \begin{bmatrix} -K_{ut}\theta_0 \\ 0 \end{bmatrix}$$

# Comparison to Zener's model

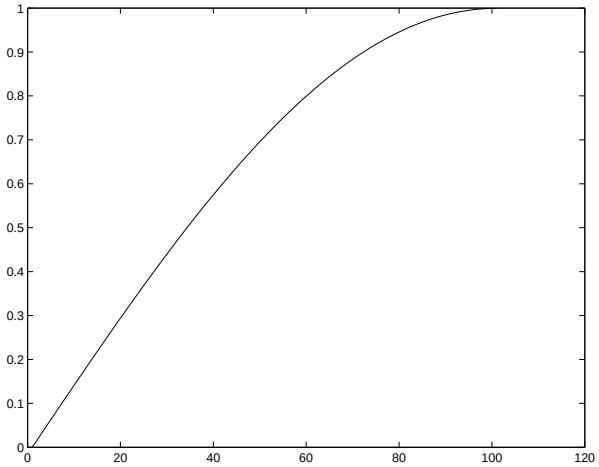


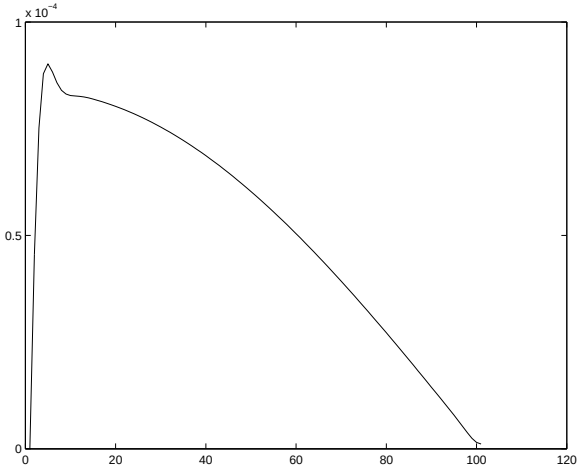



- Comparison of fully coupled simulation to Zener approximation over a range of frequencies
- Real and imaginary parts after first-order correction agree to about three digits with Arnoldi

# Thermoelastic boundary layer



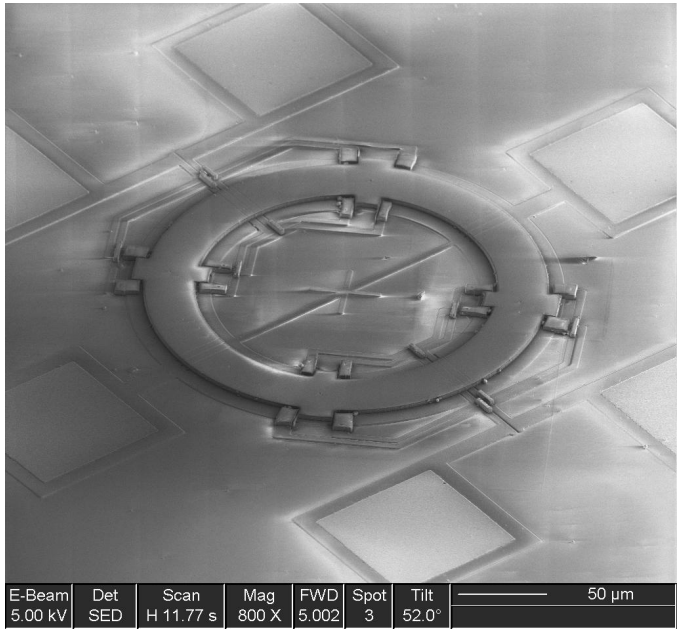


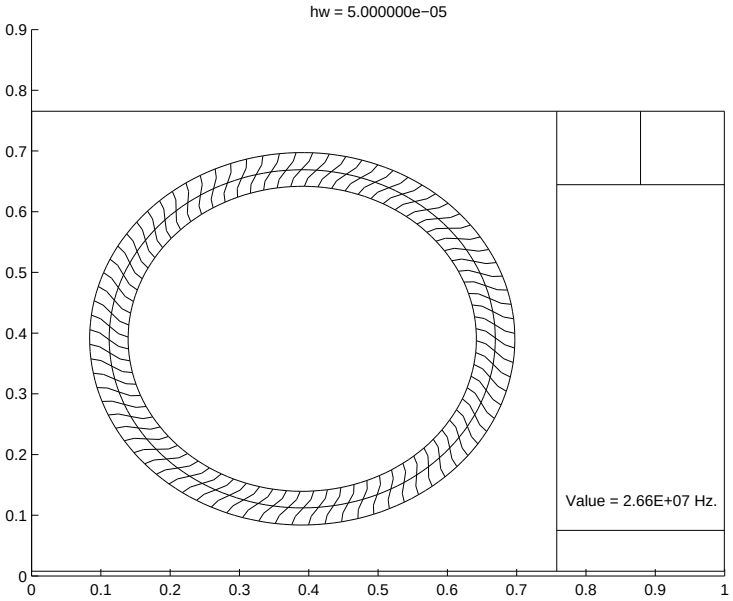




- One-dimensional test problem (longitudinal mode in a bar)
- Fixed temperature and displacement at left
- Free at right

# Shear ring resonator






- Ring is driven in a shearing motion
- Can couple ring to other resonators
- How do we track the desired mode?

# Mode tracking



Find a continuous solution to

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

- $K$ and $M$ are symmetric and $M > 0$
- Eigenvectors are $M$-orthogonal
- Perturbation theory gives good shifts
- Look if $u(s+h)$ and $u(s)$ are on the same path by looking at $u(s+h)^T M(s+h) u(s)$
- Many more subtleties in the nonsymmetric case
  - Focus of the *CIS algorithm*

# Mode tracking in a shear resonator