Numerical Methods for Resonance Calculations

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Outline

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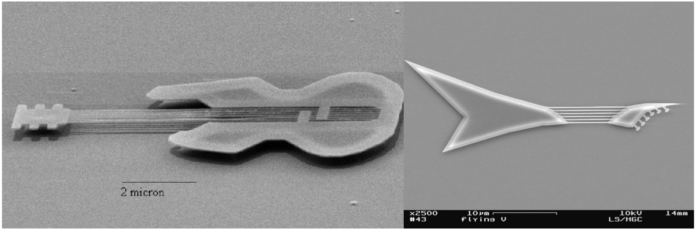
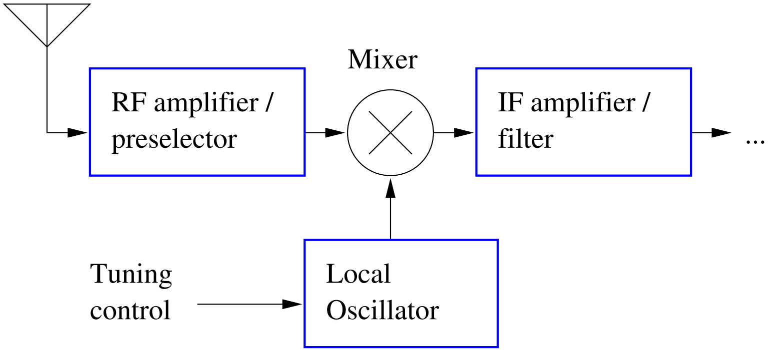
Resonant RF MEMS



Microguitars from Cornell University (1997 and 2003)

- MHz-GHz mechanical resonators
- Favorite application: radio on chip
- Close second: really high-pitch guitars

The Mechanical Cell Phone

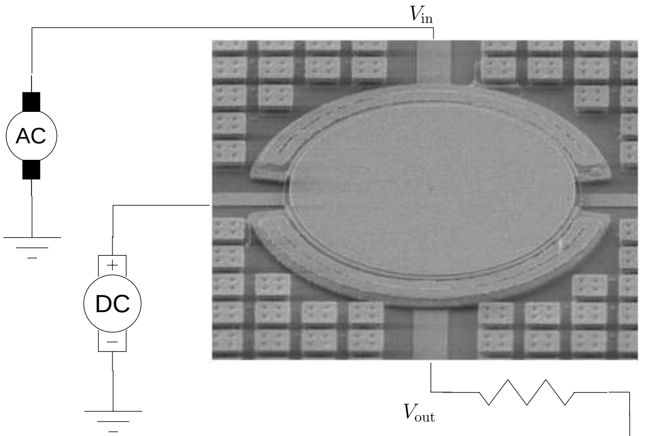


- Your cell phone has many moving parts!
- What if we replace them with integrated MEMS?

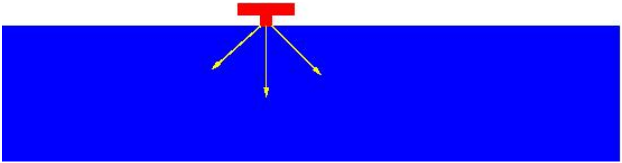
Ultimate Success

"Calling Dick Tracy!"

Disk Resonator



Damping Mechanisms



Possible loss mechanisms:

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

This is a resonance computation!

Outline

Simple 1D Problem

Consider 1D Schrödinger:

$$\left(-\frac{d^2}{dx^2} + V(x)\right)\psi = E\psi.$$

How do we:

1. Quickly compute resonances (nice enough V)?
2. Make sure the computations are correct?

Simple 1D Problem

Consider 1D Schrödinger:

$$\left(-\frac{d^2}{dx^2} + V(x)\right)\psi = E\psi.$$

If $\operatorname{supp}(V) \subset [a, b]$, write

$$\left(-\frac{d^2}{dx^2} + V(x) - k^2\right)\psi = 0, x \in (a, b)$$
$$\left(\frac{d}{dx} - ik\right)\psi = 0, x = b$$
$$\left(\frac{d}{dx} + ik\right)\psi = 0, x = a$$

$\operatorname{Im} k \geq 0$ for eigenvalues, $\operatorname{Im} k < 0$ for resonances.

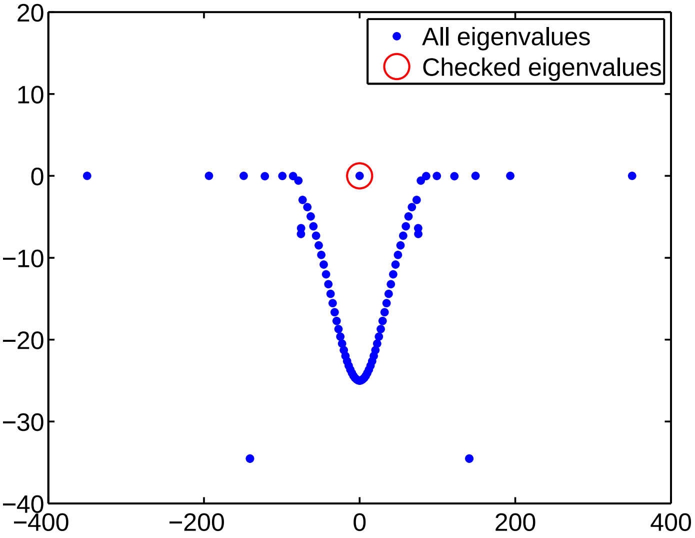
Pseudospectral Discretization

Sample ψ at Chebyshev nodes and approximate $d\psi/dx$ by differentiating the interpolant:

$$\left(-D^2 + V(x) - k^2\right)\psi = 0, x \in (a, b)$$
$$(D - ik)\psi = 0, x = b$$
$$(D + ik)\psi = 0, x = a$$

Now linearize (introduce auxiliary variable $\phi = k\psi$) to get an ordinary generalized eigenvalue problem.

Is it that easy?



Backward Error Analysis

If $\hat{\psi}$ is a numerical solution, there is some $\hat{V}$ s.t.

$$\left(-\frac{d^2}{dx^2} + \hat{V}(x) - k^2\right)\hat{\psi} = 0, x \in (a, b)$$

First-order sensitivity to changes in $\hat{V}$ is

$$\begin{aligned} \delta k &= \frac{\int_a^b \hat{\psi}(\delta V)\hat{\psi}}{2k\int_a^b \hat{\psi}^2 + i(\hat{\psi}^2(a) + \hat{\psi}^2(b))} \\ &= \frac{\int_a^b \hat{\psi}(H_V - k^2)\hat{\psi}}{2k\int_a^b \hat{\psi}^2 + i(\hat{\psi}^2(a) + \hat{\psi}^2(b))}. \end{aligned}$$

Compute $\hat{V}$ by evaluating residual for approximate $\hat{\psi}$ on a fine mesh.

Backward Error Analysis

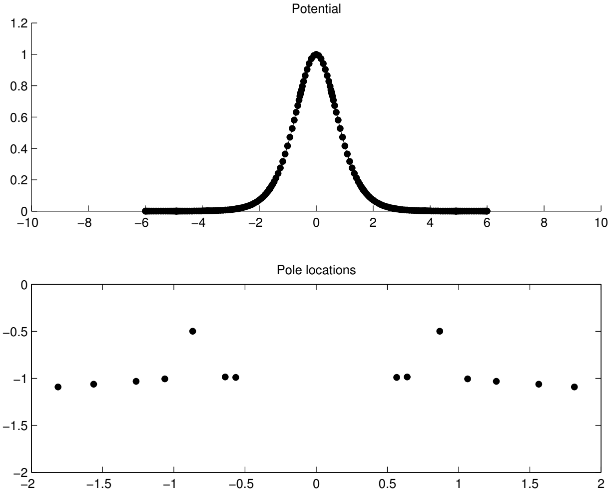
First-order sensitivity to changes in $\hat{V}$ is

$$\delta k = \frac{\int_a^b \hat{\psi}(\delta V)\hat{\psi}}{2k\int_a^b \hat{\psi}^2 + i(\hat{\psi}^2(a) + \hat{\psi}^2(b))}.$$

Now think about perturbing from a truncated potential to a non-compactly supported potential. Above bound says this is okay as long as $|V|/\exp(2\,\mathrm{Im}(k)|x|) \to 0$ as $|x| \to \infty$.

Backward Error Analysis

Example: truncate Eckart potential $\cosh^{-2}(x)$



More General Picture

Consider Schrödinger with compactly supported V in R^d.
On resolvent set,

$$
\begin{aligned}
(H_V - E)\psi &= f \text{ on } \Omega \\
\frac{\partial \psi}{\partial n} - B(E)\psi &= 0 \text{ on } \Gamma
\end{aligned}
$$

where $B(E)$ is the Dirichlet-to-Neumann map on $\partial\Omega$
Admits a variational formulation:

$$
\begin{aligned}
I(\psi) = & \frac{1}{2}\int_\Omega \left((\nabla\psi)^T(\nabla\psi) + \psi(V-E)\psi\right) d\Omega + \\
& \frac{1}{2}\int_\Gamma \psi B(E)\psi \, d\Gamma - \int_\Omega \psi f \, d\Omega.
\end{aligned}
$$

Rayleigh Quotient Analogue

Now define a residual for an approximate eigenpair:

$$r(\psi, E) = \int_\Omega \left((\nabla\psi)^T (\nabla\psi) + \psi(V - E)\psi \right) + \int_\Gamma \psi B(E)\psi.$$

Take variations and use symmetry of B:

$$\begin{aligned}
\delta r(\psi, E) &= 2\int_\Omega \delta\psi \left[(-\Delta + V - E)\psi\right] + \\
&\quad 2\int_\Gamma \delta\psi \left[\frac{\partial\psi}{\partial n} - B(E)\psi\right] + \\
&\quad \delta E \left[\int_\Omega \psi^2 - \int_\Gamma \psi B'(E)\psi\right]
\end{aligned}$$

Rayleigh Quotient Analogue

We now implicitly define a differentiable function $\tilde{E}(\psi)$ in the neighborhood of an eigenpair (ψ, E_*), with $r(\psi, E(\psi)) = 0$ and $E(\psi) = E_*$. Such a function should exist if

$$\int_\Omega \psi^2 - \int_\Gamma \psi B'(E) \psi \neq 0$$

Stationary precisely when (ψ, E) an eigenpair.

Sensitivity

Now assume δV a compactly-supported perturbation, and look at effect of δV on Rayleigh quotient analogue. Gives that isolated eigenvalues change like

$$\delta E = \frac{\int_\Omega \delta V \psi^2}{\int_\Omega \psi^2 - \int_\Gamma \psi B'(E)\psi}$$

Can also write in terms of a residual for ψ as a solution for the potential $V + \delta V$:

$$\delta E = \frac{\int_\Omega \psi(-\Delta + (V + \delta V) - E)\psi}{\int_\Omega \psi^2 - \int_\Gamma \psi B'(E)\psi}.$$

Some Computational Issues

In general, using the domain equation + DtN map to find resonances is problematic because:

1. The DtN map is nonlocal, expensive to work with computationally.
2. The Green's function (and hence the DtN map) for an elastic half space problem is hard to write down.
3. Nonlinear eigenvalue problems are trickier than linear problems to solve.

Outline

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:

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

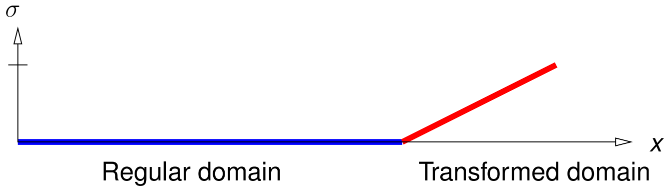
- Fourier transform:

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

- Solution:

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

Model with Perfectly Matched Layer

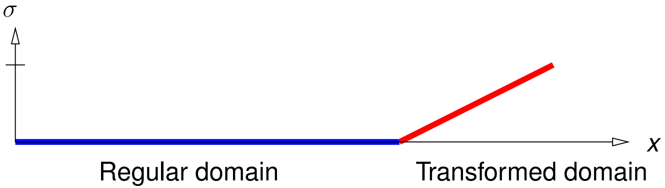


$$\frac{d\tilde{x}}{dx} = \lambda(x) \text{ where } \lambda(s) = 1 - i\sigma(s)$$

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

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

Model with Perfectly Matched Layer



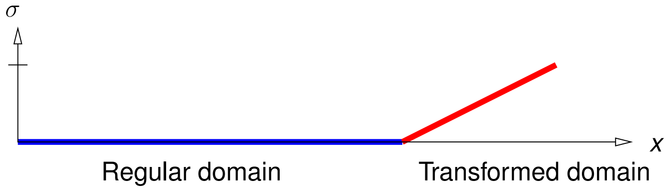
$$\frac{d\tilde{x}}{dx} = \lambda(x) \text{ where } \lambda(s) = 1 - i\sigma(s),$$

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

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

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

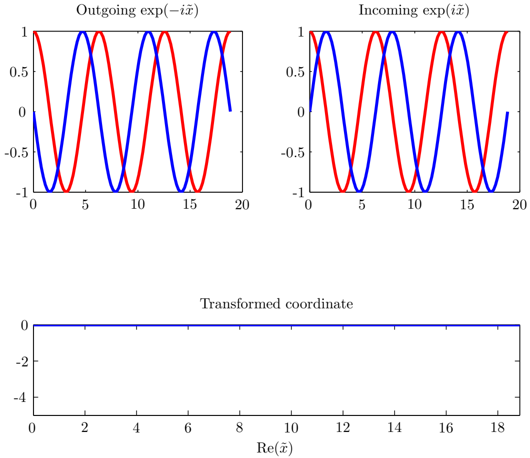
Model with Perfectly Matched Layer



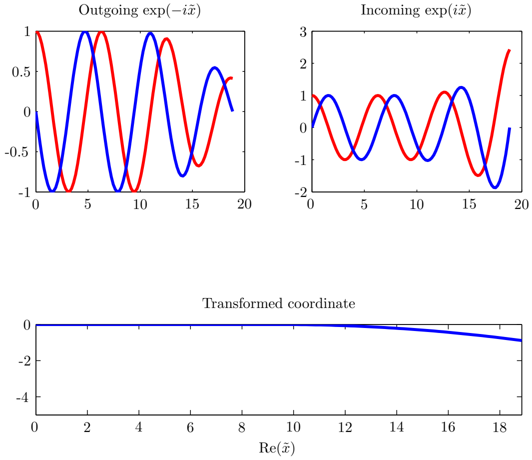
If solution clamped at $x = L$ then

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

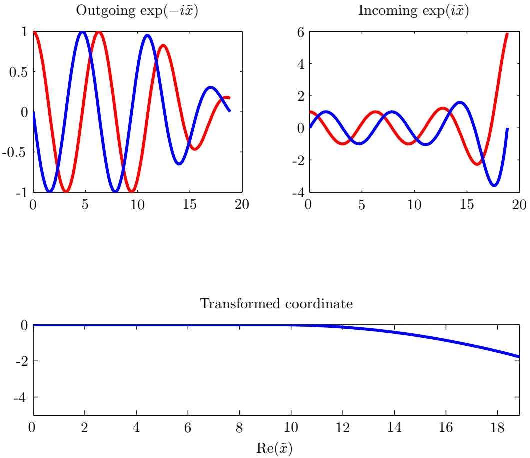
Model Problem Illustrated



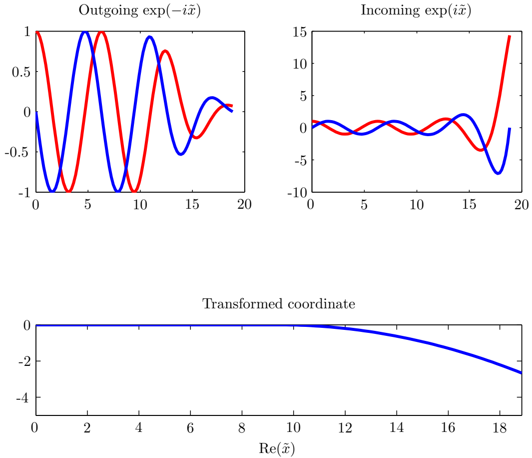
Model Problem Illustrated



Model Problem Illustrated



Model Problem Illustrated



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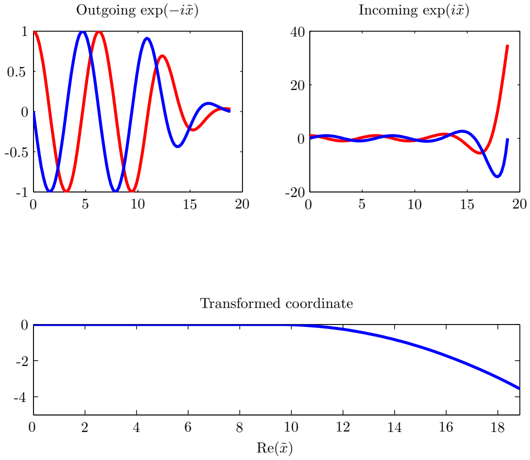
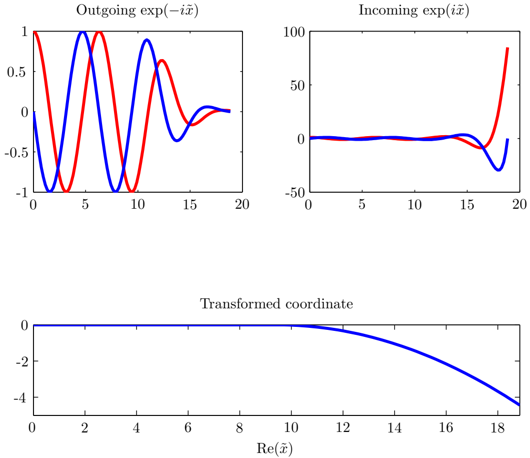
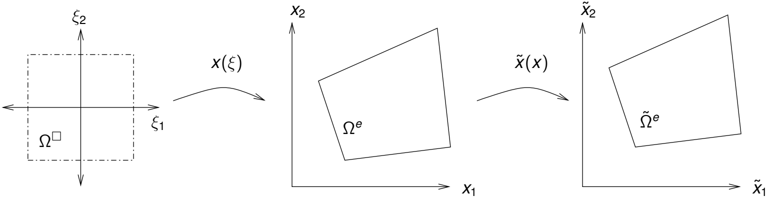


Model Problem Illustrated



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*

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):

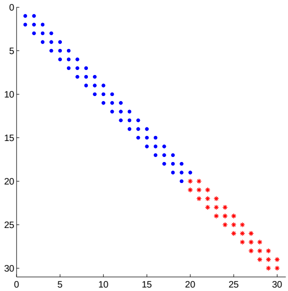
$$\theta(v) = \frac{v^T K v}{v^T M v}$$

- First-order accurate eigenvectors $\implies$ Second-order accurate eigenvalues.
- Key: relation between left and right eigenvectors.

Relation to the DtN approach

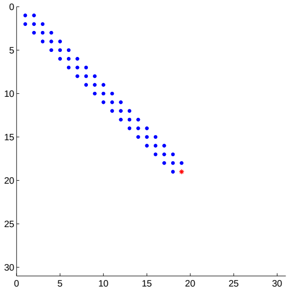
PML provides a *local rational approximation* to the DtN conditions. Suppose regions 1, 2, and 3 are the ordinary domain, the boundary, and the PML. Eliminating the variables from region 3 in $(K - \lambda M)\psi = 0$ yields something like the DtN version of the eigenvalue / resonance problem.

DtN approximation in PML



- Start with $(K - \omega^2 M)u = e_1$
- Schur complement to eliminate PML unknowns
- Compare last coefficient with exact (discrete) BC

DtN approximation in PML



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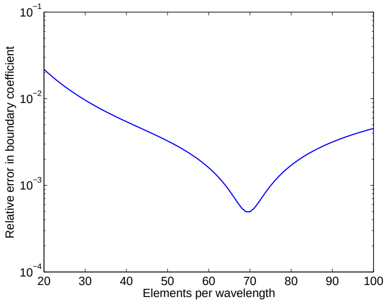
DtN approximation in PML



- Start with $(K - \omega^2 M)u = e_1$
- Schur complement to eliminate PML unknowns
- Compare last coefficient with exact (discrete) BC

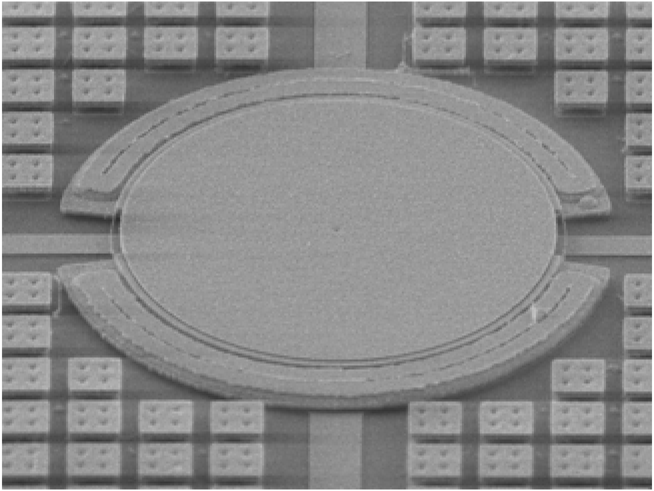
Outline

Conclusions

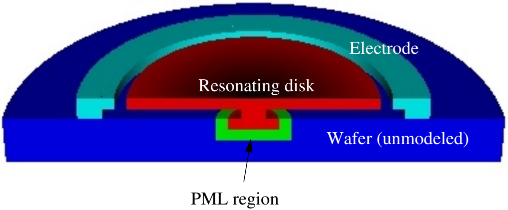
1. Can compute resonances via nonlinear eigenvalue problems
2. Can also use PMLs / complex scaling
3. Want error estimates along with computations; nonlinear variational approach is a useful.

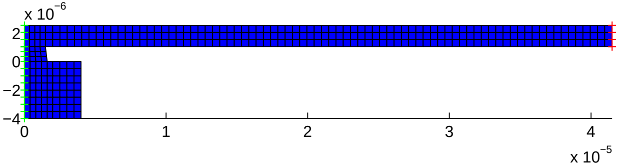
See also:
`http://www.cims.nyu.edu/~dbindel/matscat/`

Disk Resonator Simulations



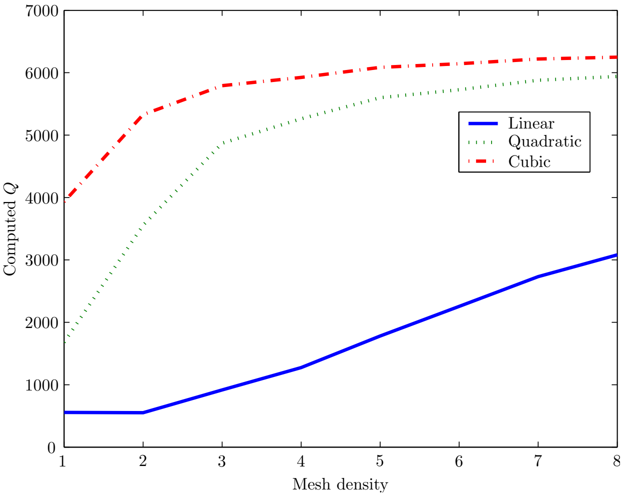
Disk Resonator Mesh





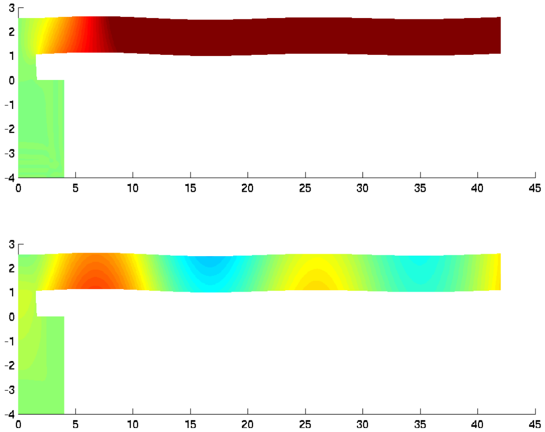
- Axisymmetric model with bicubic mesh
- About 10K nodal points in converged calculation

Mesh Convergence

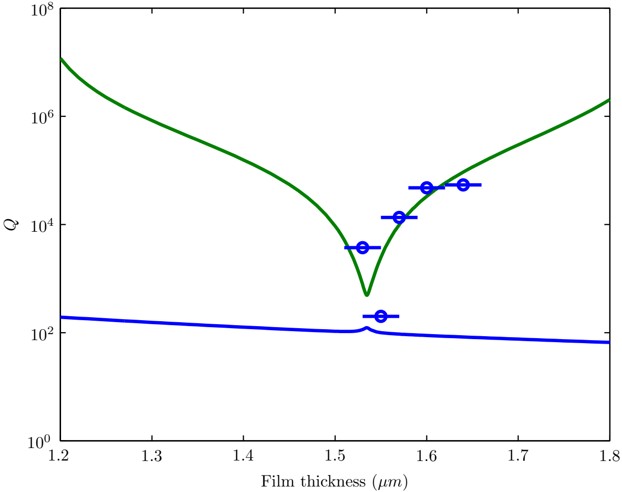


Cubic elements converge with reasonable mesh density

Response of the Disk Resonator

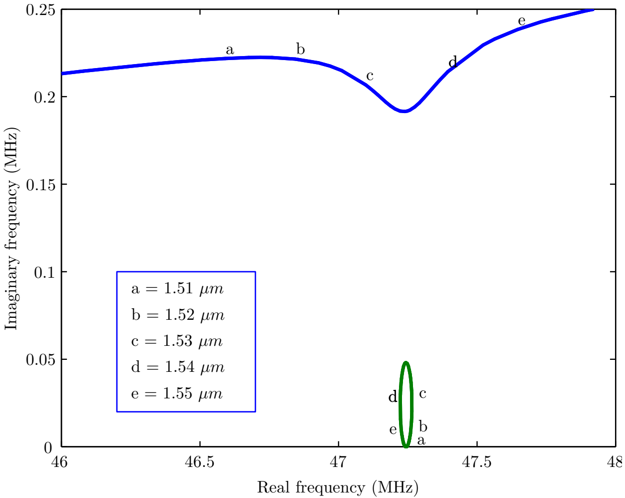


Variation in Quality of Resonance



Simulation and lab measurements vs. disk thickness

Explanation of Q Variation



Interaction of two nearby eigenmodes