Resonance Computations

D. Bindel

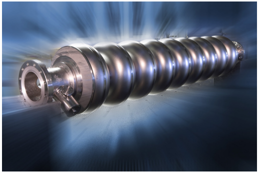
Courant Institute of Mathematical Sciences
New York University

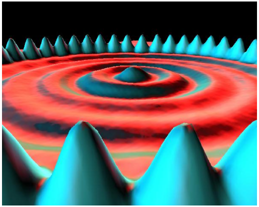
DOE visit, 2 Feb 2009

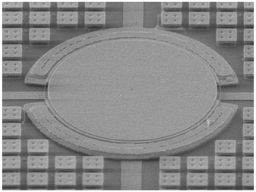
Radiation and Resonance

- Care about resonance in many places
  - Electromagnetic design
  - Meta-stable quantum states
  - Electromechanical devices
- May want
  - No resonance (e.g. waveguides)
  - High quality resonance (e.g. resonator)
- Questions:
  - How do we compute resonances?
  - Why believe our computations?

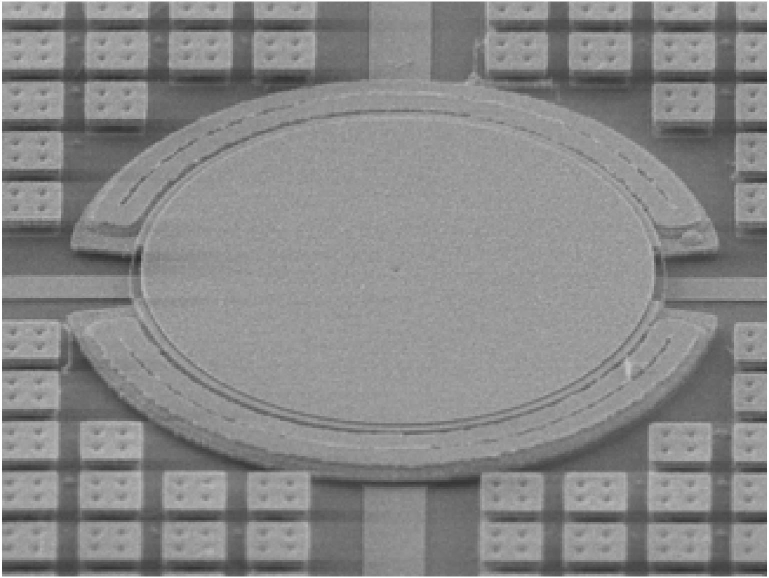
Images from ILC image bank, Almaden STM gallery, Sunil Bhave.



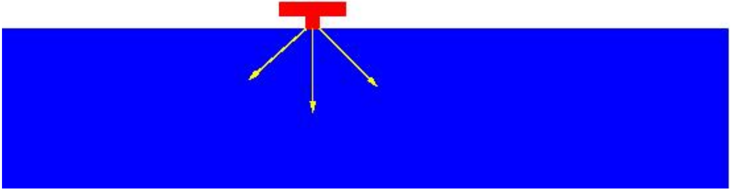




Example: MEMS Disk Resonator



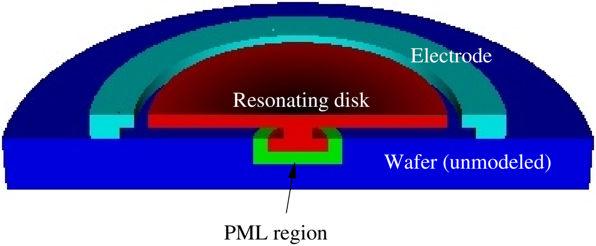
Damping in Disk Resonator



Possible loss mechanisms:

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

MEMS Disk Resonator Model



To compute, we:

- Ignore packaging, other devices, some physics
- Idealize geometry
- Approximate substrate as unbounded
- Model unbounded domain with PML
- Discretize with finite elements

Computational approach

1. Write PDE + DtN map to get *nonlinear eigenvalue problem*

$$A(k)\psi = 0$$

2. Approximate far field, discretize to get approximate NEP

$$\widehat{A}(k)\hat{\psi} = 0$$

3. Approximate $A(k)$ near k_0 by a *linearized* eigenproblem

$$(K - k^2 M)\phi = 0$$

4. Project onto a low-dimensional subspace and solve

$$W^*(K - k^2 M)V\,\widehat{\phi} = 0$$

Example: 1D Schrödinger

$$\left(-\frac{d^2}{dx^2} + V(x)\right)\psi = E\psi, \qquad \operatorname{supp}(V) \subset [a, b].$$

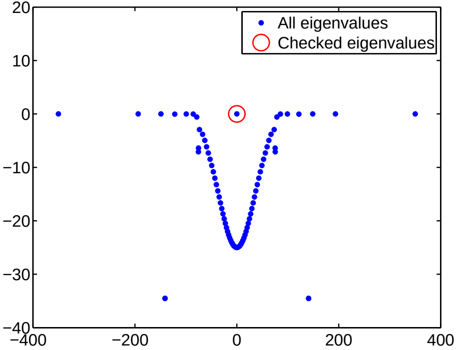
1. Replace with bounded domain problem, nonlinear in E:

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

   $E = k^2$, $\operatorname{Im} k \geq 0$ for eigenvalues, $\operatorname{Im} k < 0$ for resonances.

2. Discretize, linearize, and solve via standard methods.

Example: 1D Schrödinger error assessment



Evaluate error in resonant pair (k, ψ) by backward error analysis:

1. Satisfies exact modified equation with potential $V + \delta V$.
2. Error estimate from linearizing about *numerical* problem

Error and sensitivity analysis

Given nonlinear $\hat{A}(k) \approx A(k)$ in some part of $\mathbb{C}$:

1. First-order analysis gives estimates of difference between nonlinear eigenvalues (as above).
2. Compute *nonlinear spectral inclusion regions* (like pseudospectra, Gershgorin disks) to show A and $\hat{A}$ have *same number* of nonlinear eigenvalues in some set.

Latter result is useful for showing all resonances in a region have been computed (or that a region is resonance-free).

Current work

Theoretical:

1. Backward error analysis framework for error estimates
2. Error bounds via nonlinear spectral inclusion regions

Computational:

1. `HiQLab` – calculates resonances in MEMS using PML. Convergence analysis, experimental verification, only limited analysis of error from BC.
2. `MatScat` – calculates resonances for 1D Schrödinger. Error estimates via backward error analysis for exact BC.
3. 2D model problem – calculate resonances on quantum corral. Error estimates via backward error analysis for approx BC.