

Computer Aided Design of Micro-Electro-Mechanical Systems

From Energy Losses to Dick Tracy Watches

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MIT, 3 Nov 2008

The Computational Science Picture

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Resonant
MEMS and
models

HiQLab

Anchor losses
and disk
resonators

Thermoelastic
losses and
beam
resonators

Conclusion

Backup slides

- Application modeling
 - Disk resonator
 - Beam resonator
 - Shear ring resonator, checkerboard, ...
- Mathematical analysis
 - Physical modeling and finite element technology
 - Structured eigenproblems and reduced-order models
 - Parameter-dependent eigenproblems
- Software engineering
 - HiQLab
 - SUGAR
 - FEAPMEX / MATFEAP

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What are MEMS?

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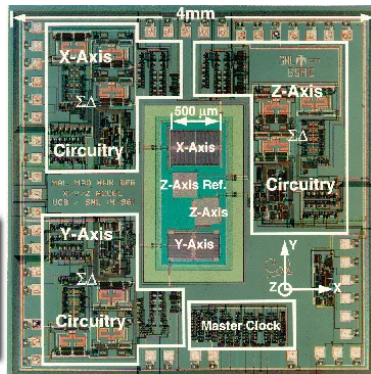
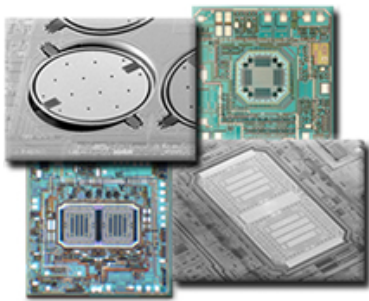
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MEMS Basics

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- 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

Resonant RF MEMS

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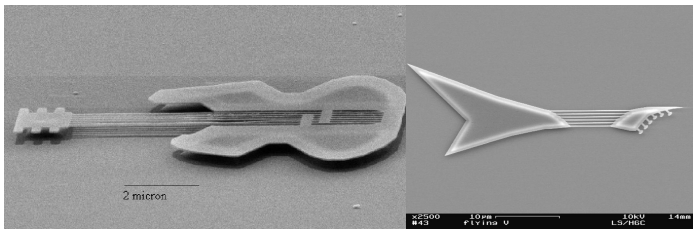
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Microguitars from Cornell University (1997 and 2003)

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

The Mechanical Cell Phone

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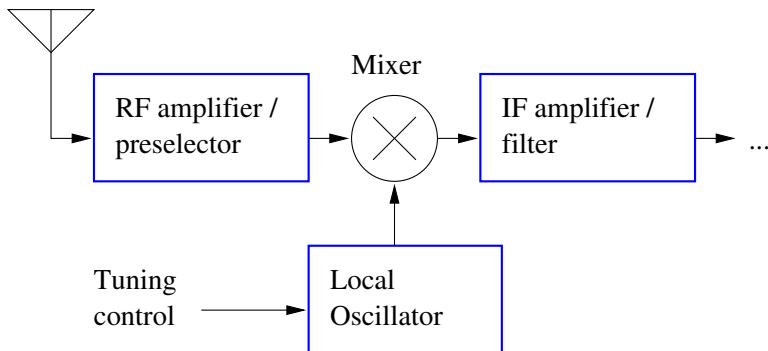
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- Your cell phone has many moving parts!
- What if we replace them with integrated MEMS?

Ultimate Success

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“Calling Dick Tracy!”



Disk Resonator

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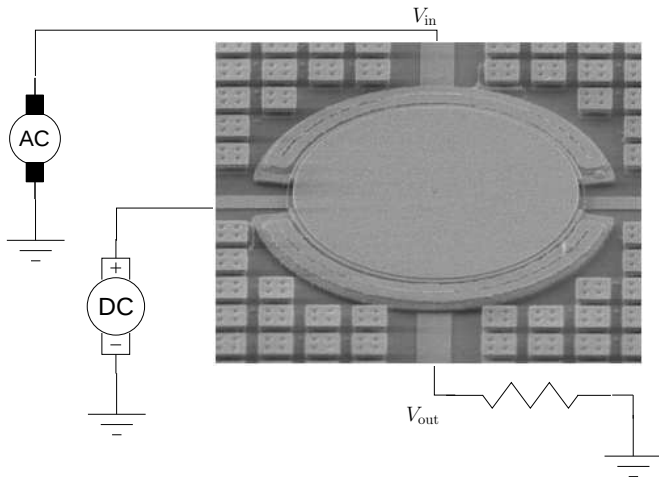
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Disk Resonator

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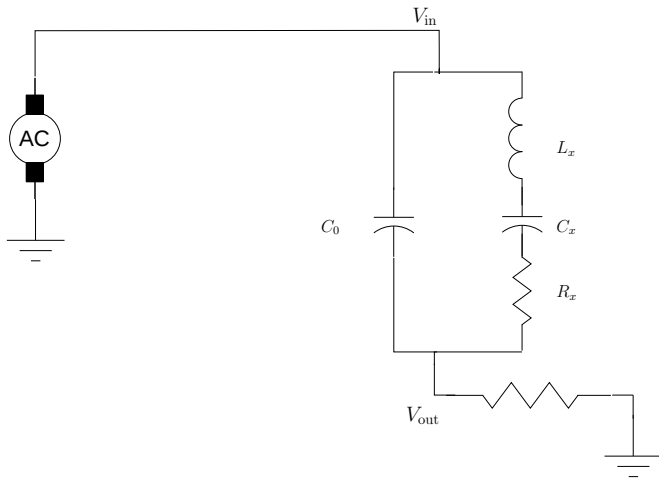
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Electromechanical Model

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Assume time-harmonic steady state, no external forces:

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

Eliminate the mechanical terms:

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

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

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

Damping and Q

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Designers want high *quality of resonance* (Q)

- Dimensionless damping in a one-dof system

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

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

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

To understand Q , we need damping models!

The Designer's Dream

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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.

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Enter HiQLab

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- 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

Heritage of HiQLab

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SUGAR: SPICE for the MEMS world

- System-level simulation using modified nodal analysis
- Flexible device description language
- C core with MATLAB interfaces and numerical routines

FEAPMEX: MATLAB + a finite element code

- MATLAB interfaces for steering, testing solvers, running parameter studies
- Time-tested finite element architecture
- But old F77, brittle in places

Other Ingredients

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“Lesser artists borrow. Great artists steal.”
– Picasso, Dali, Stravinsky?

- Lua: www.lua.org
 - Evolved from simulator data languages (DEL and SOL)
 - Pascal-like syntax fits on one page; complete language description is 21 pages
 - Fast, freely available, widely used in game design
- MATLAB: www.mathworks.com
 - “The Language of Technical Computing”
 - OCTAVE also works well
- Standard numerical libraries: ARPACK, UMFPACK
- MATEXPR, MWRAP, and other utilities

HiQLab Structure

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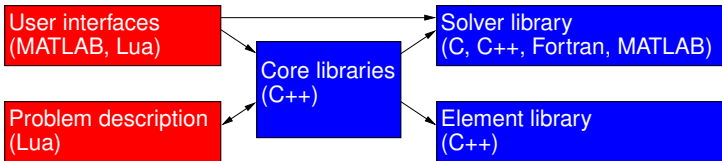
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- Standard finite element structures + some new ideas
- Full scripting language for mesh input
- Callbacks for boundary conditions, material properties
- MATLAB interface for quick algorithm prototyping
- Cross-language bindings are automatically generated

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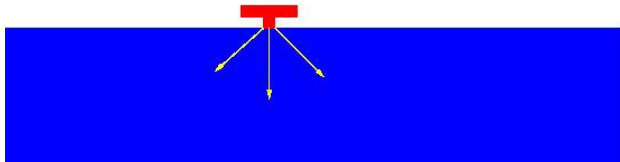
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Damping Mechanisms

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Possible loss mechanisms:

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

Model substrate as semi-infinite with a

Perfectly Matched Layer (PML).

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Perfectly Matched Layers

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- Complex coordinate transformation
- Generates a “perfectly matched” absorbing layer
- Idea works with general linear wave equations
 - Electromagnetics (Bereng r, 1994)
 - Quantum mechanics – *exterior complex scaling* (Simon, 1979)
 - Elasticity in standard finite element framework (Basu and Chopra, 2003)

Model Problem

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- 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

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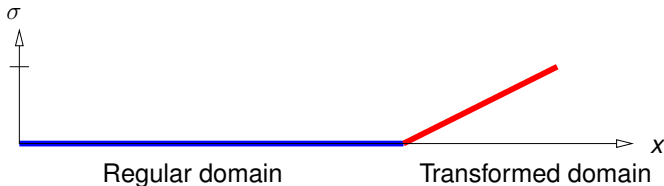
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$$\frac{d\tilde{x}}{dx} = \lambda(x) \text{ where } \lambda(s) = 1 - i\sigma(s)$$

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

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

Model with Perfectly Matched Layer

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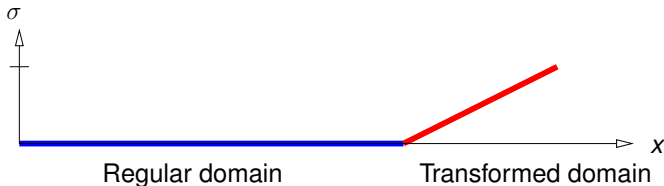
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$$\frac{d\tilde{x}}{dx} = \lambda(x) \text{ where } \lambda(s) = 1 - i\sigma(s),$$

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

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

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

Model with Perfectly Matched Layer

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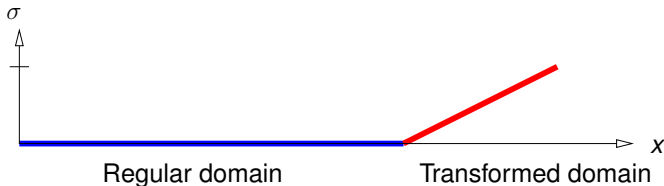
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If solution clamped at $x = L$ then

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

Model Problem Illustrated

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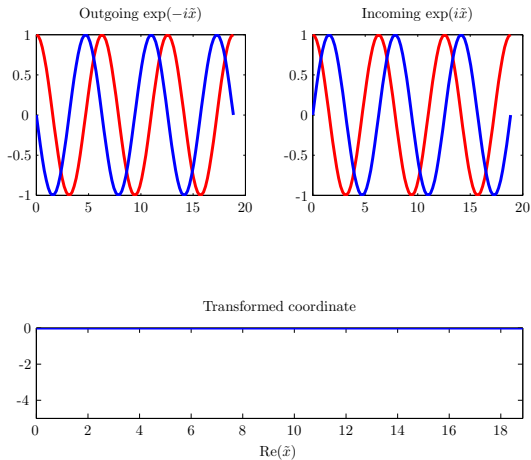
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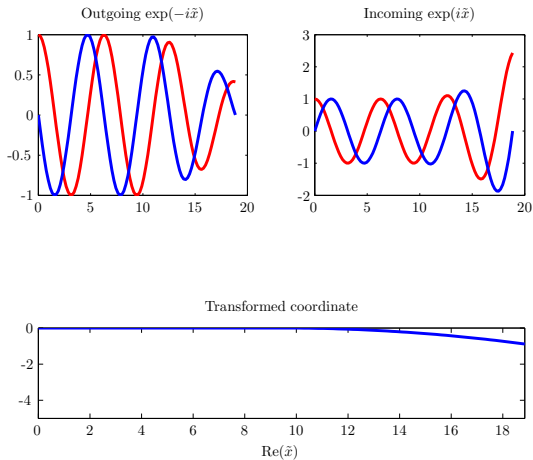
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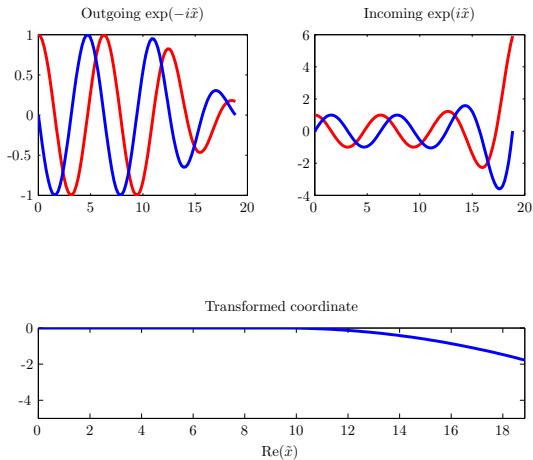
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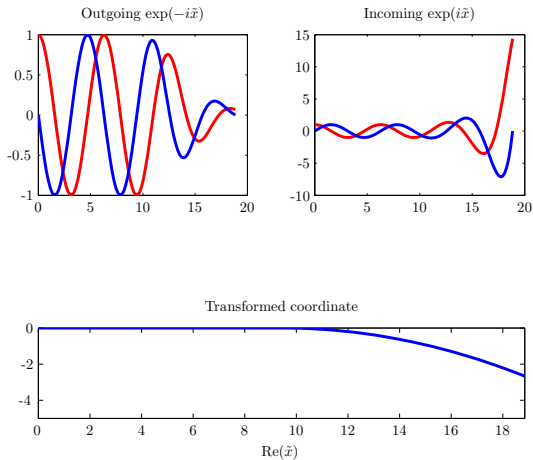
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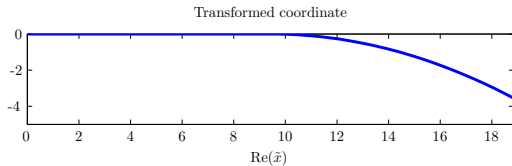
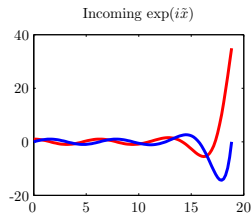
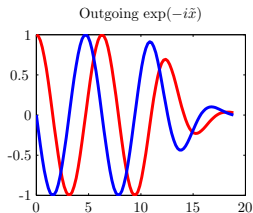
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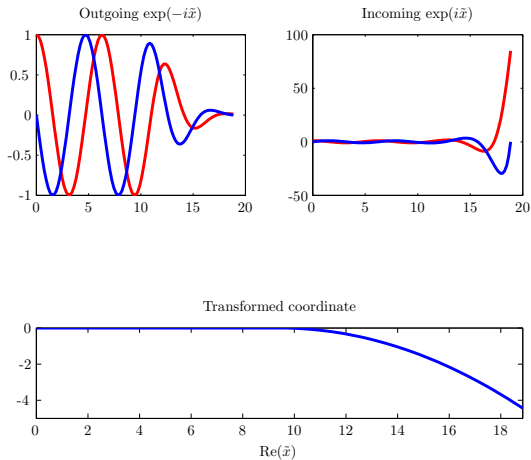
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Finite Element Implementation

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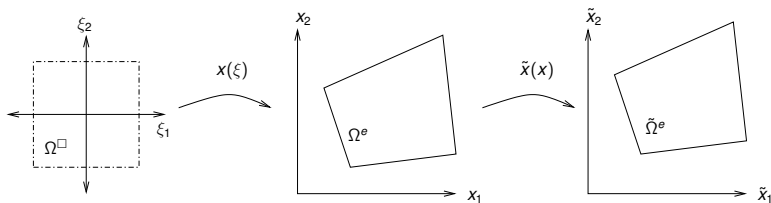
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- Combine PML and isoparametric mappings

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

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

- Matrices are *complex symmetric*

Eigenvalues and Model Reduction

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

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

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 for a Krylov subspace $\mathcal{K}_n$
- Compute with much smaller $V^* K V$ and $V^* M V$

Can we do better?

Variational Principles

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- 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

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- Build new projection basis from V :

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

- $\text{span}(W)$ 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

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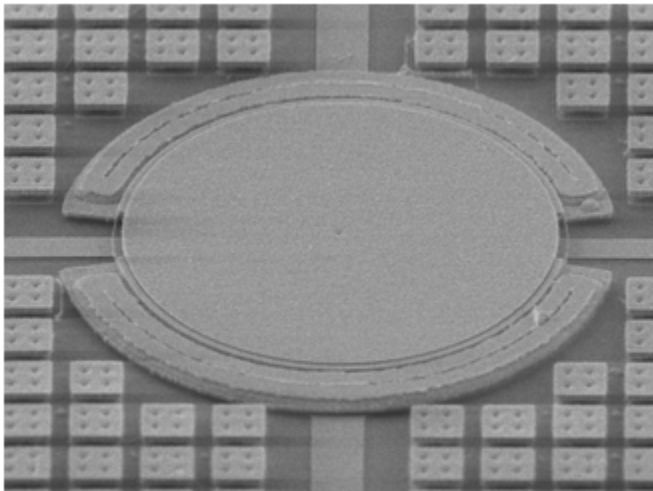
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Disk Resonator Mesh

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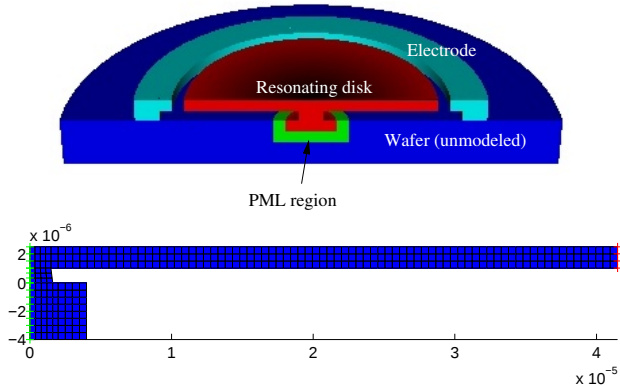
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- Axisymmetric model with bicubic mesh
- About 10K nodal points in converged calculation

Mesh Convergence

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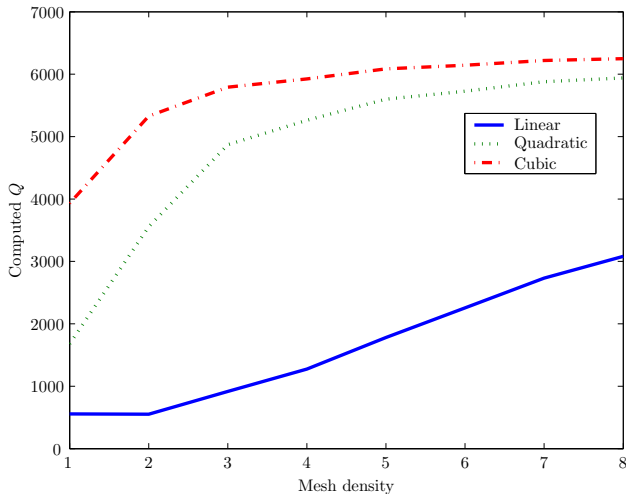
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Cubic elements converge with reasonable mesh density

Model Reduction Accuracy

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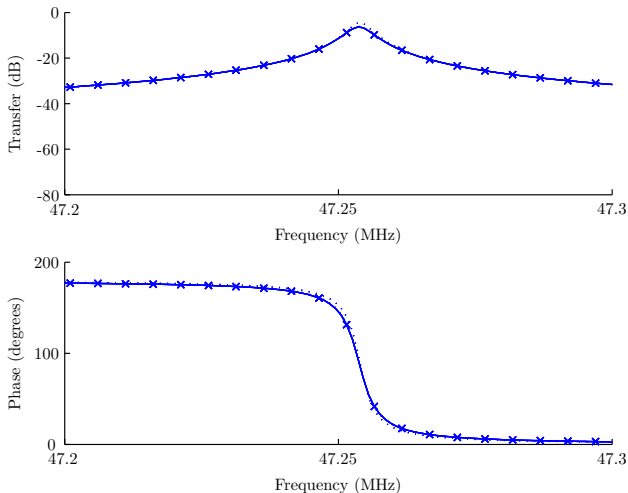
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Results from ROM (solid and dotted lines) nearly indistinguishable from full model (crosses)

Model Reduction Accuracy

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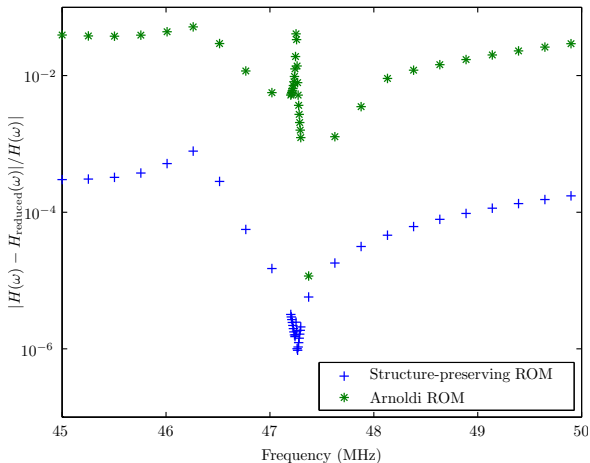
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Preserve structure $\implies$
get twice the correct digits

Response of the Disk Resonator

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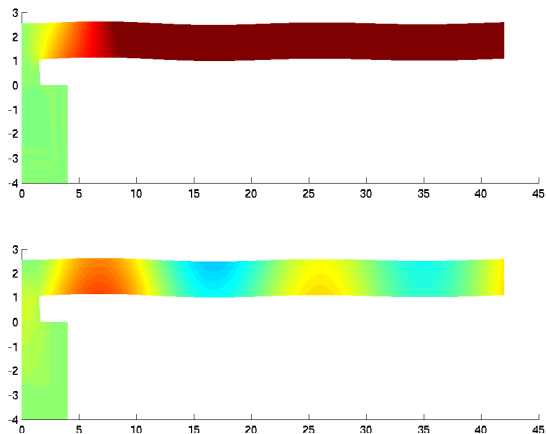
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Variation in Quality of Resonance

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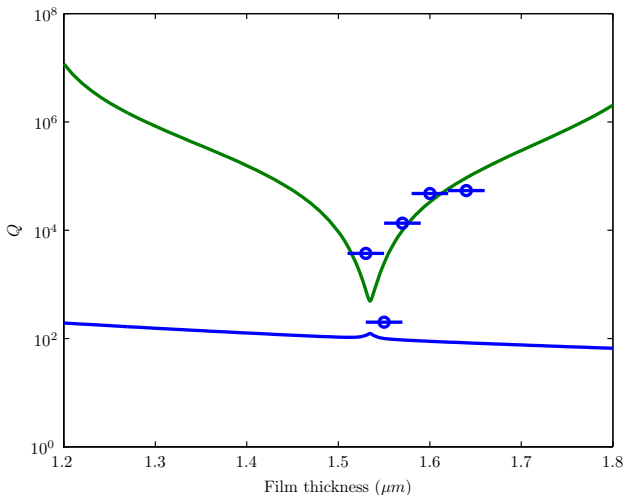
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Simulation and lab measurements vs. disk thickness

Explanation of Q Variation

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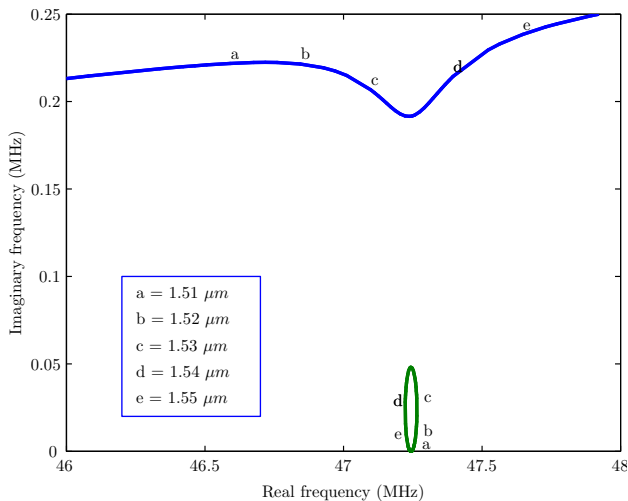
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Interaction of two nearby eigenmodes

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Thermoelastic Damping (TED)

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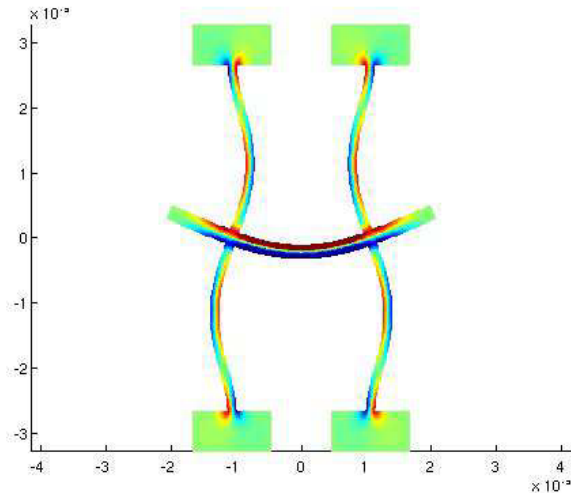
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Thermoelastic Damping (TED)

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

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

- 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

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Continuum equations:

$$\sigma = \hat{C}\epsilon - \xi\theta$$

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

$$\dot{\theta} = \eta \nabla^2 \theta - \text{tr}(\dot{\epsilon})$$

Discrete equations:

$$M_{uu}\ddot{u} + K_{uu}u = \xi K_{u\theta}\theta + f$$

$$C_{\theta\theta}\ddot{\theta} + \eta K_{\theta\theta}\theta = -C_{\theta u}\dot{u}$$

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

Perturbative Mode Calculation

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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 :

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

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Zener's Model

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- 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

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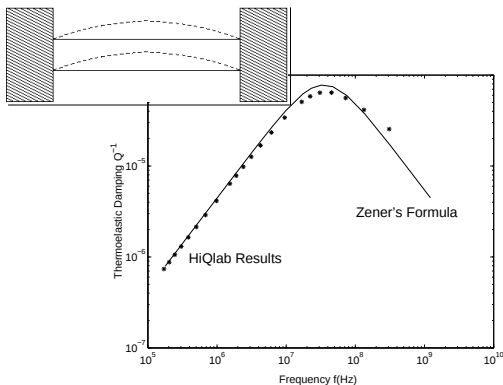
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- Comparison of fully coupled simulation to Zener approximation over a range of frequencies
- Real and imaginary parts after first-order correction agree to about three digits with Arnoldi

Outline

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- 1 Resonant MEMS and models
- 2 HiQLab
- 3 Anchor losses and disk resonators
- 4 Thermoelastic losses and beam resonators
- 5 Conclusion**

Onward!

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What about:

- Modeling more geometrically complex devices?
- Modeling general dependence on geometry?
- Modeling general dependence on operating point?
- Computing nonlinear dynamics?
- Digesting all this to help designers?

Future Work

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- 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

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Backup slides

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

<http://www.cims.nyu.edu/~dbindel>

Concluding Thoughts

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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

Checkerboard Resonator

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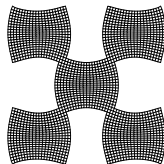
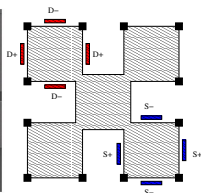
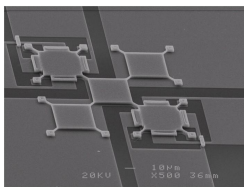
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Reflection Analysis



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

Checkerboard Model Reduction

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Reflection Analysis

- 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

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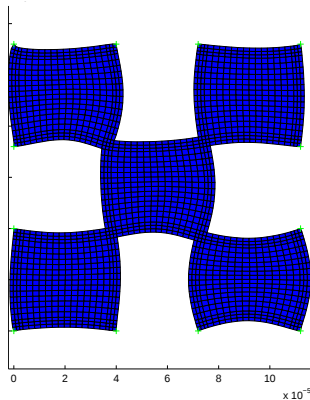
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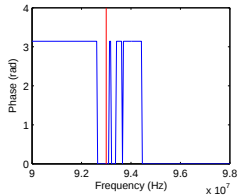
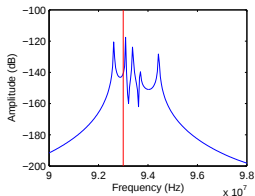
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Reflection Analysis



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Checkerboard Measurement

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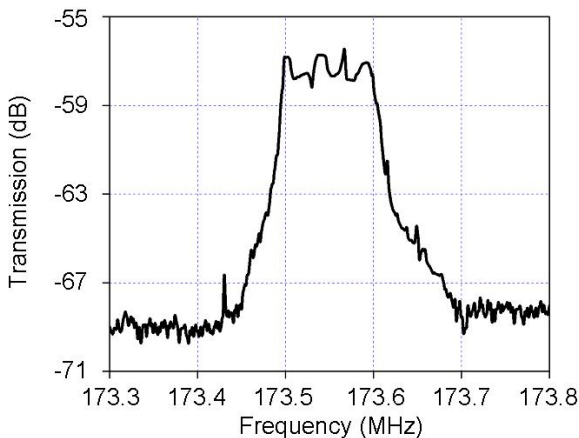
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Reflection Analysis



S. Bhawe, MEMS 05

Contributions

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Reflection Analysis

- Built predictive model used to design checkerboard
- Used model reduction to get thousand-fold speedup
– fast enough for interactive use

General Picture

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Reflection Analysis

If $w^* A = 0$ and $Av = 0$ then

$$\delta(w^* Av) = w^*(\delta A)v$$

This implies

- If $A = A(\lambda)$ and $w = w(\nu)$, have

$$w^*(\nu)A(\rho(\nu))v = 0.$$

ρ stationary when $(\rho(\nu), \nu)$ is a nonlinear eigenpair.

- If $A(\lambda, \xi)$ and w_0^* and v_0 are null vectors for $A(\lambda_0, \xi_0)$,

$$w_0^*(A_\lambda \delta \lambda + A_\xi \delta \xi)v_0 = 0.$$

Electromechanical Model

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Reflection Analysis

Kirchoff's current law and balance of linear momentum:

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

Linearize about static equilibrium (V_0, u_0) :

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

where

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

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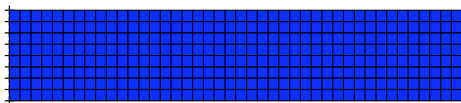
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Reflection Analysis



```
mesh = Mesh:new(2)
mat = make_material('silicon2', 'planestrain')
mesh:blocks2d( { 0, 1 }, { -w/2.0, w/2.0 },
               mat )
```

```
mesh:set_bc(function(x,y)
    if x == 0 then return 'uu', 0, 0; end
end)
```

HiQLab's Hello World

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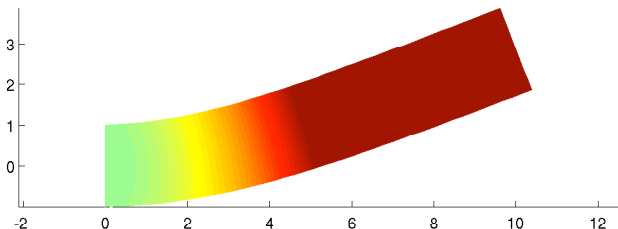
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Reflection Analysis



```
>> mesh = Mesh_load('beammesh.lua');  
>> [M,K] = Mesh_assemble_mk(mesh);  
>> [V,D] = eigs(K,M, 5, 'sm');  
>> opt.axequal = 1; opt.deform = 1;  
>> Mesh_scale_u(mesh, V(:,1), 2, 1e-6);  
>> plotfield2d(mesh, opt);
```

Continuum 2D model problem

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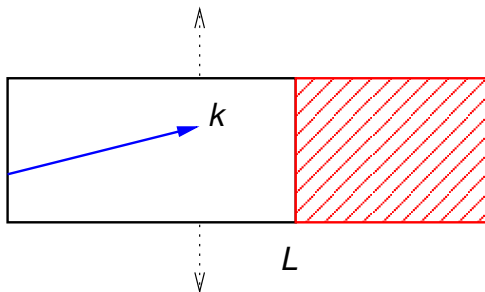
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Reflection Analysis



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

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

Continuum 2D model problem

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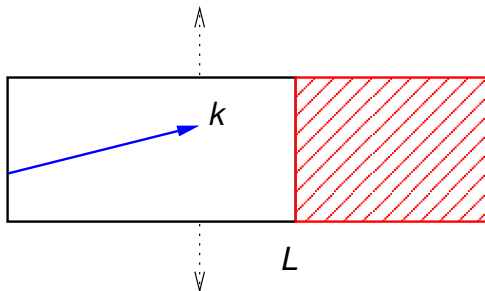
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Reflection Analysis



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

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

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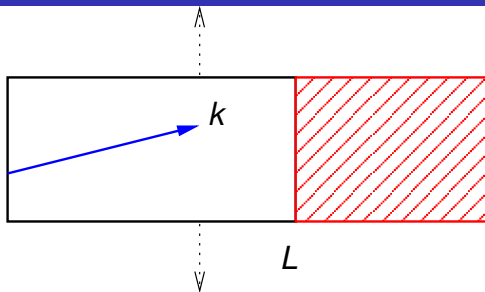
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Reflection Analysis



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

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

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

Discrete 2D model problem

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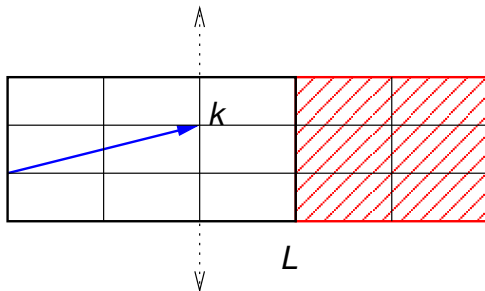
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Reflection Analysis



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

Nondimensionalization

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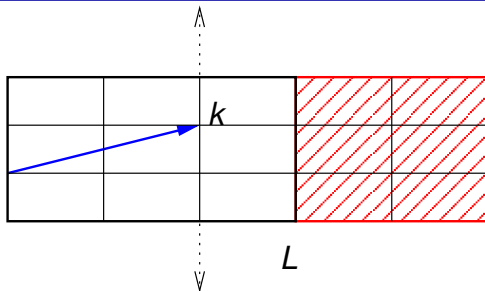
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Reflection Analysis



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

Rate of stretching:

$$\beta h^p$$

Elements per wave:

$$(k_x h)^{-1} \text{ and } (k_y h)^{-1}$$

Elements through the PML:

$$N$$

Nondimensionalization

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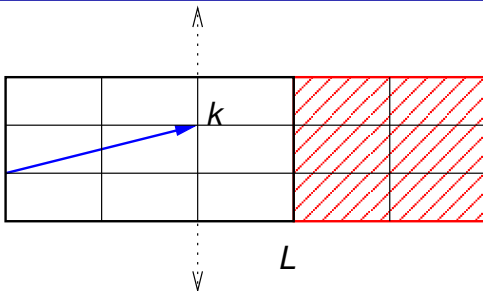
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Reflection Analysis



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

Rate of stretching:

$$\beta h^p$$

Elements per wave:

$$(k_x h)^{-1} \text{ and } (k_y h)^{-1}$$

Elements through the PML:

$$N$$

Discrete reflection behavior

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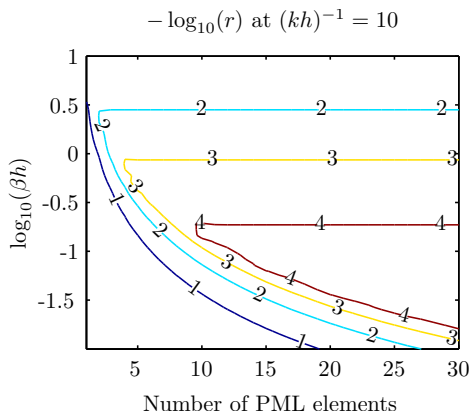
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Reflection Analysis



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

Discrete reflection decomposition

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Reflection Analysis

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

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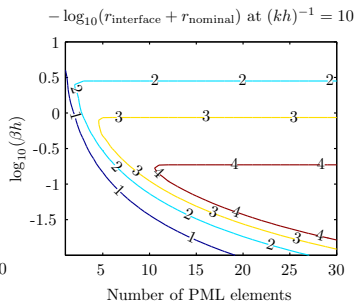
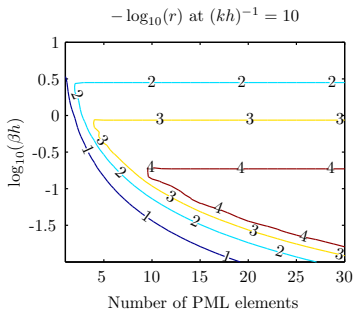
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Reflection Analysis



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

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Reflection Analysis

- 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 β based on interface reflection at $k_x^{\max}$
 - Choose length based on far-end reflection at $k_x^{\min}$