Computer Aided Design of Micro-Electro-Mechanical Systems

From Energy Losses to Dick Tracy Watches

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The Computational Science Picture

- 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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Outline

1. Resonant MEMS and models
2. HiQLab
3. Anchor losses and disk resonators
4. Thermoelastic losses and beam resonators
5. Conclusion
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
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!”

I’m On My Way
Disk Resonator

\[ V_{\text{in}} \]

\[ V_{\text{out}} \]
Disk Resonator

\[ V_{\text{in}} \]

\[ V_{\text{out}} \]

\[ L_x \]

\[ C_x \]

\[ R_x \]

\[ C_0 \]
Electromechanical Model

Assume time-harmonic steady state, no external forces:

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

Eliminate the mechanical terms:

\[
Y(\omega) \delta \hat{V} = \delta \hat{l}_{\text{external}}
\]

\[
Y(\omega) = i \omega C + G + i \omega H(\omega)
\]

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

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

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

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

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

To understand $Q$, we need damping models!
The Designer’s Dream

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

- 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

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
“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

- User interfaces (MATLAB, Lua)
- Solver library (C, C++, Fortran, MATLAB)
- Core libraries (C++)
- Element library (C++)
- Problem description (Lua)

- 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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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 Layer

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

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

\[
\hat{u} = c_{\text{out}} e^{-ik\tilde{x}} + c_{\text{in}} e^{ik\tilde{x}}
\]
Model with Perfectly Matched Layer Layer

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

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

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

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

Outgoing $\exp(-i\tilde{x})$

Incoming $\exp(i\tilde{x})$

Transformed coordinate

$\text{Re}(\tilde{x})$
Model Problem Illustrated

Outgoing $\exp(-i\tilde{x})$

Incoming $\exp(i\tilde{x})$

Transformed coordinate

$\text{Re}(\tilde{x})$

$\text{Im}(\tilde{x})$
Model Problem Illustrated

Outgoing exp\((-i\tilde{x})\)

Incoming exp\((i\tilde{x})\)

Transformed coordinate

Re(\(\tilde{x}\))
Model Problem Illustrated

Outgoing $\exp(-i\tilde{x})$

Incoming $\exp(i\tilde{x})$

Transformed coordinate

$\text{Re}(\tilde{x})$
Model Problem Illustrated

Outgoing $\exp(-i\tilde{x})$

Incoming $\exp(i\tilde{x})$

Transformed coordinate
Model Problem Illustrated

Outgoing $\exp(-i\tilde{x})$

Incoming $\exp(i\tilde{x})$

Transformed coordinate

Re($\tilde{x}$)
Finite Element Implementation

- Combine PML and isoparametric mappings

\[
\begin{align*}
\mathbf{k}^e &= \int_{\Omega^e} \mathbf{B}^T \mathbf{D} \mathbf{B} \mathbf{J} \, d\Omega \\
\mathbf{m}^e &= \int_{\Omega^e} \rho \mathbf{N}^T \mathbf{N} \mathbf{J} \, d\Omega
\end{align*}
\]

- Matrices are complex symmetric
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 $K_n$
- Compute with much smaller $V^* K V$ and $V^* M V$

Can we do better?
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 \( \Rightarrow \) Second-order accurate eigenvalues.

- Key: relation between left and right eigenvectors.
Accurate Model Reduction

- Build new projection basis from $V$:
  \[ W = \text{orth}[\text{Re}(V), \text{Im}(V)] \]

- $\text{span}(W)$ contains both $\mathcal{K}_n$ and $\bar{\mathcal{K}}_n$
  \[ \implies \text{double digits correct vs. projection with } V \]

- $W$ is a real-valued basis
  \[ \implies \text{projected system is complex symmetric} \]
Disk Resonator Simulations
Disk Resonator Mesh

- Axisymmetric model with bicubic mesh
- About 10K nodal points in converged calculation
Cubic elements converge with reasonable mesh density
Results from ROM (solid and dotted lines) nearly indistinguishable from full model (crosses)
Model Reduction Accuracy

| Frequency (MHz) | $|H(\omega) - H_{\text{reduced}}(\omega)|/H(\omega)|$
<table>
<thead>
<tr>
<th></th>
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<tbody>
<tr>
<td>45</td>
<td>$10^{-6}$</td>
</tr>
<tr>
<td>46</td>
<td>$10^{-4}$</td>
</tr>
<tr>
<td>47</td>
<td>$10^{-2}$</td>
</tr>
<tr>
<td>48</td>
<td>$10^{-4}$</td>
</tr>
<tr>
<td>49</td>
<td>$10^{-6}$</td>
</tr>
<tr>
<td>50</td>
<td>$10^{-2}$</td>
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</tbody>
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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
Interaction of two nearby eigenmodes
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Thermoelastic Damping (TED)
Thermoelastic Damping (TED)

\[ u \text{ is displacement and } T = T_0 + \theta \text{ is temperature} \]

\[
\begin{align*}
\sigma &= C\varepsilon - \beta \theta I \\
\rho \ddot{u} &= \nabla \cdot \sigma \\
\rho c_v \dot{\theta} &= \nabla \cdot (\kappa \nabla \theta) - \beta T_0 \text{tr}(\dot{\varepsilon})
\end{align*}
\]

- 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:**

\[
\begin{align*}
\sigma &= \hat{C}\epsilon - \xi \theta^1 \\
\ddot{u} &= \nabla \cdot \sigma \\
\dot{\theta} &= \eta \nabla^2 \theta - \text{tr}(\dot{\epsilon})
\end{align*}
\]

**Discrete equations:**

\[
\begin{align*}
M_{uu} \ddot{u} + K_{uu} u &= \xi K_{u\theta} \theta + f \\
C_{\theta\theta} \ddot{\theta} + \eta K_{\theta\theta} \theta &= -C_{\theta u} \dot{u}
\end{align*}
\]

- Micron-scale poly-Si devices: \(\xi\) and \(\eta\) are \(\sim 10^{-4}\).
- Linearize about \(\xi = 0\)
Perturbative Mode Calculation

Discretized mode equation:

\[
(-\omega^2 M_{uu} + K_{uu}) u = \xi K_{u\theta} \theta
\]
\[
(i\omega C_{\theta\theta} + \eta K_{\theta\theta}) \theta = -i\omega C_{\theta u} u
\]

First approximation about \( \xi = 0 \):

\[
(-\omega_0^2 M_{uu} + K_{uu}) u_0 = 0
\]
\[
(i\omega_0 C_{\theta\theta} + \eta K_{\theta\theta}) \theta_0 = -i\omega_0 C_{\theta u} u_0
\]

First-order correction in \( \xi \):

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

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.
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
Onward!

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

- **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 computing challenges

http://www.cims.nyu.edu/~dbindel
Concluding Thoughts

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

- 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 Simulation
- Frequency (Hz)
- Amplitude (dB)
- Phase (rad)
- Resonant MEMS and models
- HiQLab
- Anchor losses and disk resonators
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- Conclusion
- Backup slides
  - Checkerboard resonators
  - Nonlinear eigenvalue perturbation
  - Electromechanical model
  - Hello world!
  - Reflection Analysis
Checkerboard Measurement

Transmission (dB)

Frequency (MHz)

S. Bhave, MEMS 05
Contributions

- Built predictive model used to design checkerboard
- Used model reduction to get thousand-fold speedup – fast enough for interactive use
If \( w^* A = 0 \) and \( A v = 0 \) then

\[
\delta(w^* A v) = w^*(\delta A)v
\]

This implies

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

\[
w^*(\nu)A(\rho(\nu))\nu = 0.
\]

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

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

\[
w_0^*(A_\lambda \delta \lambda + A_\xi \delta \xi)v_0 = 0.
\]
Kirchoff’s current law and balance of linear momentum:

\[ \frac{d}{dt} (C(u)V) + GV = I_{\text{external}} \]

\[ Mu_{tt} + Ku - \nabla_u \left( \frac{1}{2} V^* C(u) V \right) = F_{\text{external}} \]

Linearize about static equilibrium \((V_0, u_0)\):

\[ C(u_0) \delta V_t + G \delta V + (\nabla_u C(u_0) \cdot \delta u_t) V_0 = \delta I_{\text{external}} \]

\[ M \delta u_{tt} + \tilde{K} \delta u + \nabla_u (V_0^* C(u_0) \delta V) = \delta F_{\text{external}} \]

where

\[ \tilde{K} = K - \frac{1}{2} \frac{\partial^2}{\partial u^2} (V_0^* C(u_0) V_0) \]
HiQLab’s Hello World

```lua
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

```
>> 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

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

\[ \frac{1}{\lambda} \frac{\partial}{\partial x} \left( \frac{1}{\lambda} \frac{\partial u}{\partial x} \right) + \frac{\partial^2 u}{\partial y^2} + k^2 u = 0 \]
Continuum 2D model problem

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

\[ \frac{1}{\lambda} \frac{\partial}{\partial x} \left( \frac{1}{\lambda} \frac{\partial u}{\partial x} \right) - k_y^2 u + k^2 u = 0 \]
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)
\[ \lambda(x) = \begin{cases} 
1 - i/\beta|x - L|^p, & x > L \\
1 & x \leq L.
\end{cases} \]

Rate of stretching: \( \beta h^p \)

Elements per wave: \( (k_x h)^{-1} \) and \( (k_y h)^{-1} \)

Elements through the PML: \( N \)
Nondimensionalization

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

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

\[ -\log_{10}(r) \text{ at } (kxh)^{-1} = 10 \]

![Graph showing discrete reflection behavior with logarithmic scale for the number of PML elements and \( \log_{10}(\beta h) \). The graph includes curves for different values of \( p = 1 \), with \( (kxh)^{-1} = 10 \). The graph indicates the behavior of reflection as the number of PML elements increases.

Quadratic elements, \( p = 1 \), \( (kxh)^{-1} = 10 \)
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

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