Solving generalized complex-symmetric eigenvalue problems arising from resonant MEMS simulations with PETSc

Tsuyoshi Koyama
Prof. Dr. Sanjay Govindjee
Center for Mechanics, IMES, ETHZ
High-frequency MEMS resonators (MHz-GHz)

Applications as small size, low energy consuming frequency references, filters, and sensors

SEM of 41.5 um radius poly-SiGe disk resonator
Resonator simulation

- Design requires knowledge of:
  - Frequency
  - Quality factor ($Q$)

$$Q = \frac{\text{Maximum Stored Energy}}{\text{Energy Loss per radian}} \approx \frac{1}{\text{Damping}}$$

Tools and methods for evaluating damping in resonant MEMS
Mathematical problem

Equation of motion discretized with FEM under harmonic assumption

Quadratic eigenvalue problem.

\[
\left(-\omega^2 M + i\omega C + K\right)x = 0
\]

Complex eigenfrequency

\[
\omega = \omega_R + i\omega_I
\]

\[
Q = \frac{|\omega|}{2\omega_I}
\]
Overview

- Characteristics of the eigenvalue problem
  - Complex symmetry and interior eigenvalues

- Solution method
  - Projection methods
  - Jacobi-Davidson method (JDQZ)
  - Modified multigrid for the correction equation (JDQZ)

- Software architecture

- Numerical example of a 2D beam

- Conclusions
Disk resonator (Anchor loss)

Mechanism: Energy loss from radiating waves escaping into the substrate.

SEM of 41.5 um radius poly-SiGe disk resonator

Section of disk resonator

Must model infinite domain.
Perfectly Matched Layers (PML)

Mechanism: Energy loss from radiating waves escaping into the substrate.

SEM of 41.5 um radius poly-SiGe disk resonator

Complex valued, Non-Hermitian matrices
Modes of vibration

<table>
<thead>
<tr>
<th>Radial mode</th>
<th>1st</th>
<th>2nd</th>
<th>3rd</th>
</tr>
</thead>
<tbody>
<tr>
<td>$x$ disp.</td>
<td><img src="disk3d.ux" alt="Image" /></td>
<td><img src="disk3d.uy" alt="Image" /></td>
<td><img src="disk3d.uz" alt="Image" /></td>
</tr>
<tr>
<td>$z$ disp.</td>
<td><img src="disk3d.ux" alt="Image" /></td>
<td><img src="disk3d.uy" alt="Image" /></td>
<td><img src="disk3d.uz" alt="Image" /></td>
</tr>
<tr>
<td>Shape</td>
<td><img src="disk3d.ux" alt="Image" /></td>
<td><img src="disk3d.uy" alt="Image" /></td>
<td><img src="disk3d.uz" alt="Image" /></td>
</tr>
<tr>
<td>Freq. [MHz]</td>
<td>289</td>
<td>759</td>
<td>1494</td>
</tr>
<tr>
<td>Nth mode</td>
<td>24</td>
<td>92</td>
<td>250-300</td>
</tr>
</tbody>
</table>
Difficulties

- PML implementation and high modes:

  Generalized complex symmetric eigenvalue problem

\[ Kx = \omega^2 Mx \]

1. Matrices are complex valued, Non-Hermitian

2. Desired modes are not the exterior of the spectrum but interior

Must deal with iterative methods for indefinite systems

\[ K - \omega^2 M \]
Projection methods

- Find eigen pair \((\omega^2, x \in \mathcal{V})\) such that

\[
(K - \omega^2 M) x \perp \mathcal{W}
\]

- Galerkin projection (Ritz values, vectors)
- Petrov-Galerkin projection

Select harmonic-Ritz projection for better approximation of interior eigenvalues.

\[
\mathcal{W} = (K - \omega_0^2 M) \mathcal{V}
\]
Jacobi-Davidson (JDQZ)

**Harmonic JD method for** \((K, M)\) **target** \(\omega_0^2 = \frac{\alpha_0}{\beta_0}\)

Given subspace \(\mathcal{V}, \mathcal{W} = (\beta_0 K - \alpha_0 M) \mathcal{V}\)

1. Find approximate eigenpair \(((\alpha, \beta), u)\)
   
   \(u \in \mathcal{V} \quad (\beta K - \alpha M) u \perp \mathcal{W}\)

2. Solve correction equation for \(t\)

3. Expand subspace

   \[
   \mathcal{V}_{new} = \mathcal{V} \oplus \text{span}\{t\}
   \]

   \[
   \mathcal{W}_{new} = \mathcal{W} \oplus \text{span}\{((\beta_0 K - \alpha_0 M) t\}
   \]

   *(Fokkema, Sleijpen, and van der Horst, 1998)*
Correction equation

\[
(I - pp^*) (\beta K - \alpha M) (I - uu^*) t = -r
\]

\[
\begin{align*}
    r &= (\beta K - \alpha M) u \\
    p &= (\beta_0 K - \alpha_0 M) u \in \mathcal{W}
\end{align*}
\]

Accurate solve is not required.

For large scale problems, iterative methods such as GMRES with Multigrid preconditioning is known to be effective for mechanical problems.

Use Smooth Aggregation Multigrid

\[ P_{MG} \approx (\beta_0 K - \alpha_0 M) \]

(Vanek, Mandel, and Brezina, 1995)
Correction equation

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(I - pp^*) P_{MG} (I - uu^*) t = -r
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Algebraic Multigrid

Smoothed aggregation algebraic multigrid

Multigrid V-cycle

(Demmel, Parallel Computing Notes)
Algebraic Multigrid

Smoothed aggregation algebraic multigrid

Smoother
Remove error with large eigenvalue

(Demmel, Parallel Computing Notes)
Algebraic Multigrid

Smoothed aggregation algebraic multigrid

Smoother
Remove error with large eigenvalue

(Demmel, Parallel Computing Notes)
Algebraic Multigrid

- Smoothed aggregation algebraic multigrid

Smoothen

Remove error with large eigenvalue

(Demmel, Parallel Computing Notes)
Algebraic Multigrid

- Smoothed aggregation algebraic multigrid

- Smoother: Remove error with large eigenvalue

- Coarse grid correction (Prolongator): Remove error with small eigenvalue

(Demmel, Parallel Computing Notes)
Smoother for\[ Ax = b \]

Gauss-Seidel

Does not converge and smooth for indefinite case.

Row projection method (Kaczmarz, 1937)

\[ AA^*y = b \]
\[ A^*y = x \]

Converges if \( b \in \text{range}(A) \) (Tanabe, 1971)

Parallel version (Gordan and Gordon, 2005)
Smoother performance (SPD)

1-D Helmholtz fixed boundaries

\[ A = \text{tridiag}[-1, 2, -1] \]

\[ Ax = 0 \]

\[ x = \text{rand} \]
Smoothing performance (indefinite)

- Shift into $\frac{1}{4}$ of the spectrum 
  $$(A - \sigma I)x = 0$$

- Gauss-Seidel diverges!
- Row-projection diverges!
- Damping is not superior but does work!
Prolongators

Vectors based on near null space of operator $K$

$$\mathbf{V}_{\text{Null}} = \begin{bmatrix} \mathbf{v}_1, \mathbf{v}_2, \cdots, \mathbf{v}_N \end{bmatrix}$$

Real to complex formulation

$$\mathbf{A} := \mathbf{K} - \omega_0^2 \mathbf{M} = \mathbf{A}_r + i \mathbf{A}_i$$

$$\hat{\mathbf{A}} = \begin{bmatrix} \mathbf{A}_r & -\mathbf{A}_i \\ \mathbf{A}_i & \mathbf{A}_r \end{bmatrix}$$

$$\hat{\mathbf{V}}_{\text{Null}} = \begin{bmatrix} \mathbf{v}_1 & 0 & \mathbf{v}_2 & 0 & \cdots & \mathbf{v}_N & 0 \\ 0 & \mathbf{v}_1 & 0 & \mathbf{v}_2 & \cdots & 0 & \mathbf{v}_N \end{bmatrix}$$
Hybrid software architecture

- **Petsc**
  - Fast implementation
  - Linear algebra objects (vector, matrices), solvers, and related operations.

- **Trilinos**
  - User friendly architecture
  - ML (MultiLevel) package for algebraic multigrid.

- **HiQLab**
  - Flexibility
  - Generates the mass, stiffness matrix data.
Symmetric indefinite problem

- 2D elastic beam

Search for 3 eigenvalues near 500\textsuperscript{th} from bottom with residual tol 1e-8.

\[ P_{MG} \approx (\beta_0 K - \alpha_0 M) \]

s.p.d
Convergence behavior

Comparison of 8 proc for different discretizations.
Complex symmetric problem

2D elastic beam with PML

\[ P_{MG} \approx (\beta_0 K - \alpha_0 M) \]

Search for 3 eigenvalues near 500\textsuperscript{th} from bottom.

\[ P_{MG} \approx (\beta_0 K - \alpha_0 M) \]

complex sym
Convergence behavior

![Graphs showing convergence behavior](image)
Closure and Outlook

We have presented a scalable method based on JDQZ and Modified Multigrid to iteratively compute interior eigenvalues of real symmetric generalized systems. The complex symmetric case still requires analysis.

Modifications and further analysis for faster computation, and verification of effectiveness for 3D calculations is required.
HiQLab group and Software

- **PIs:** Prof. Sanjay Govindjee (ETHZ)
  Prof. James Demmel (CS and Math, Berkeley)
  Prof. Roger Howe (Stanford)

- **Post doctoral students:**
  Dr. David Bindel (Courant Institute, NYU)
  Dr. Emmanuel Quevy (Electrical Eng., Berkeley)

- **Graduate students:**
  Wei He (Civil Engineering, Berkeley)

Members of the SUGAR group

- **HiQLab: Resonant MEMS Simulator**
  - [http://www.cims.nyu.edu/~dbindel/hiqlab](http://www.cims.nyu.edu/~dbindel/hiqlab)