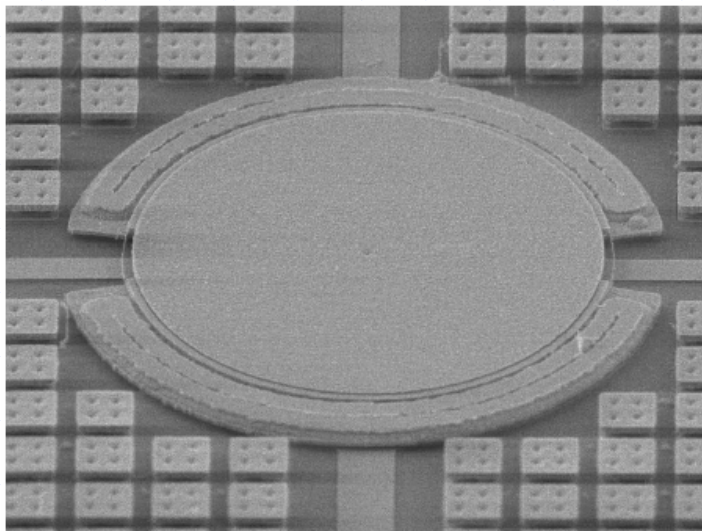


Solving generalized complex-symmetric eigenvalue problems arising from resonant MEMS simulations with PETSc

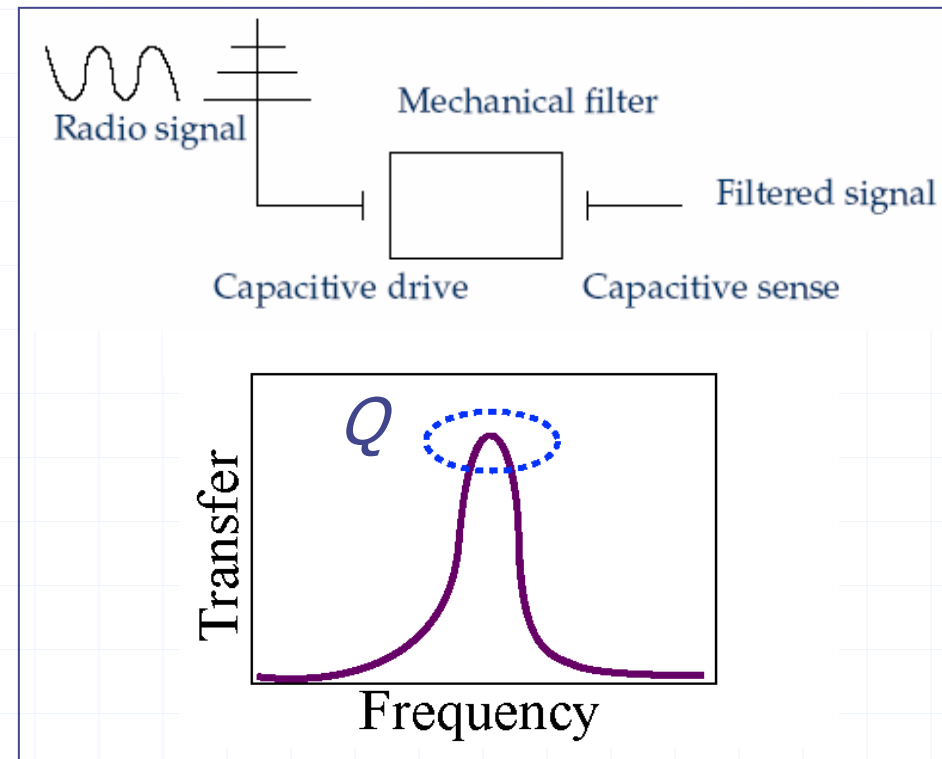
Tsuyoshi Koyama
Prof. Dr. Sanjay Govindjee
Center for Mechanics, IMES, ETHZ

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)**

Existing
Software
and Methods

?

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



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

$$\omega = \omega_R + i\omega_I$$

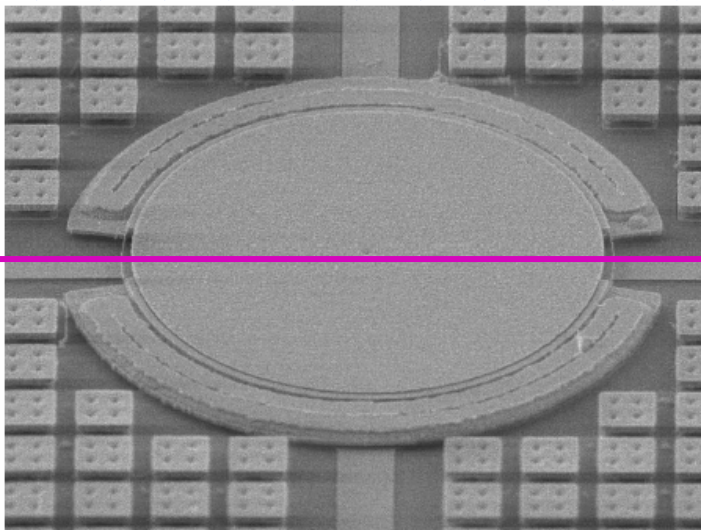
$$Q = \frac{|\omega|}{2\omega_I}$$

Overview

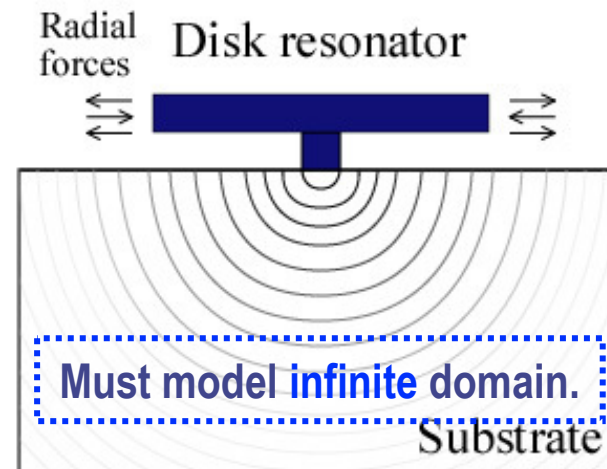
- ◆ Characteristics of the eigenvalue problem
 - Complex symmetry and interior eigenvalues
- ◆ Solution method
 - Projection methods
 - Jacobi-Davidson method (JDQZ)
 - Modified multigrid for the correction equation (JDQZ)
- ◆ Software architecture
- ◆ Numerical example of a 2D beam
- ◆ Conclusions

Disk resonator (Anchor loss)

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



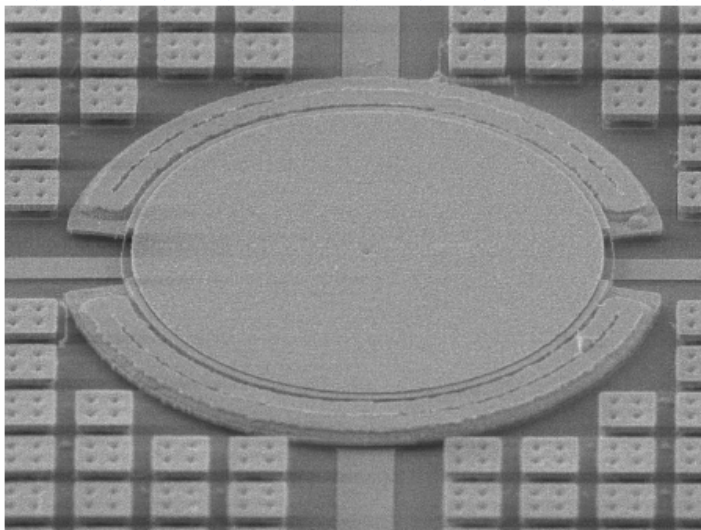
SEM of 41.5 μm radius poly-SiGe disk resonator



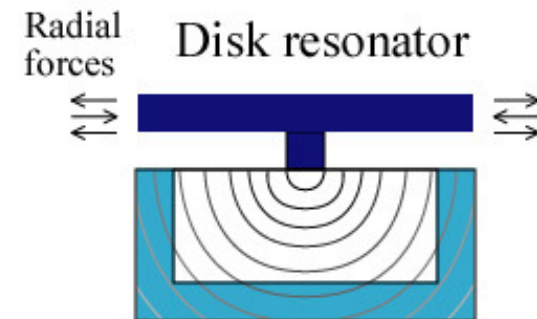
Section of disk resonator

Perfectly Matched Layers (PML)

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



SEM of 41.5 μm radius poly-SiGe disk resonator

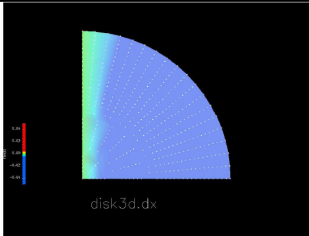
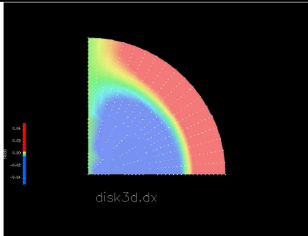
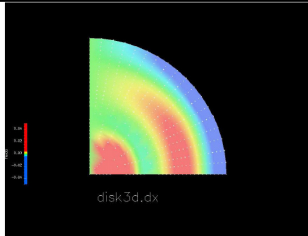
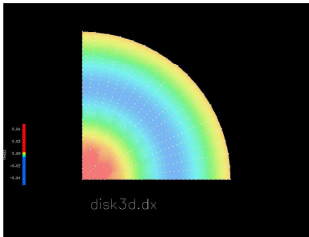
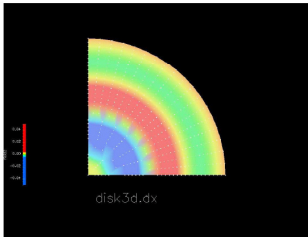
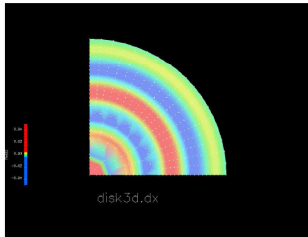
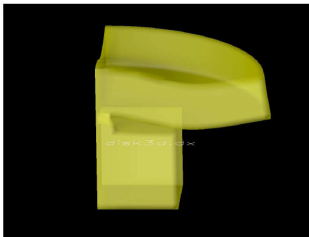
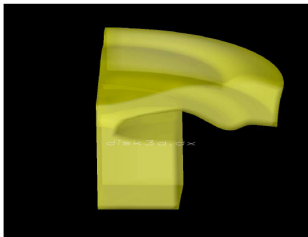
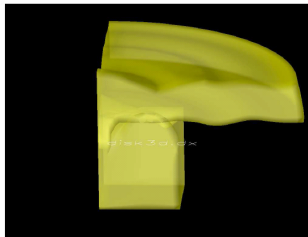


Perfectly Matched Layer

Outgoing waves are absorbed with **zero impedance** mismatch at PML boundaries.

Complex valued, Non-Hermitian matrices

Modes of vibration

Radial mode	1st	2nd	3rd
x disp.			
z disp.			
Shape			
Freq.[MHz]	289	759	1494
Nth mode	24	92	250-300

Difficulties

- ◆ PML implementation and high modes:

Generalized complex symmetric eigenvalue problem

$$\mathbf{K}\mathbf{x} = \omega^2 \mathbf{M}\mathbf{x}$$

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 $\mathbf{K} - \omega^2 \mathbf{M}$

Projection methods

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

$$(\mathbf{K} - \omega^2 \mathbf{M}) \mathbf{x} \perp \mathcal{W}$$

- ◆ Galerkin projection (Ritz values, vectors) $\mathcal{W} = \mathcal{V}$
- ◆ Petrov-Galerkin projection $\mathcal{W} \neq \mathcal{V}$

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

$$\mathcal{W} = (\mathbf{K} - \omega_0^2 \mathbf{M}) \mathcal{V}$$

Jacobi-Davidson(JDQZ)

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

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

1. Find approximate eigenpair $((\alpha, \beta), \mathbf{u})$

$$\mathbf{u} \in \mathcal{V} \quad (\beta \mathbf{K} - \alpha \mathbf{M}) \mathbf{u} \perp \mathcal{W}$$

2. Solve **correction equation** for \mathbf{t}

3. Expand subspace

$$\mathcal{V}_{\text{new}} = \mathcal{V} \oplus \text{span}\{\mathbf{t}\}$$

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

(Fokkema, Sleijpen, and van der Horst, 1998)

Correction equation

$$(\mathbf{I} - \mathbf{p}\mathbf{p}^*) (\beta\mathbf{K} - \alpha\mathbf{M}) (\mathbf{I} - \mathbf{u}\mathbf{u}^*) \mathbf{t} = -\mathbf{r}$$

$$\begin{aligned} \mathbf{r} &= (\beta\mathbf{K} - \alpha\mathbf{M}) \mathbf{u} \\ \mathbf{p} &= (\beta_0\mathbf{K} - \alpha_0\mathbf{M}) \mathbf{u} \in \mathcal{W} \end{aligned}$$

◆ 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

$$\Rightarrow \mathbf{P}_{\text{MG}} \approx (\beta_0\mathbf{K} - \alpha_0\mathbf{M})$$

(Vanek, Mandel, and Brezina, 1995)

Correction equation

$$(\mathbf{I} - \mathbf{p}\mathbf{p}^*) \mathbf{P}_{\text{MG}} (\mathbf{I} - \mathbf{u}\mathbf{u}^*) \mathbf{t} = -\mathbf{r}$$

$$\begin{aligned} \mathbf{r} &= (\beta \mathbf{K} - \alpha \mathbf{M}) \mathbf{u} \\ \mathbf{p} &= (\beta_0 \mathbf{K} - \alpha_0 \mathbf{M}) \mathbf{u} \in \mathcal{W} \end{aligned}$$

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

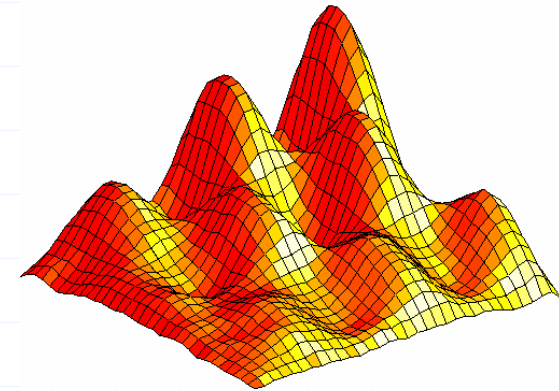
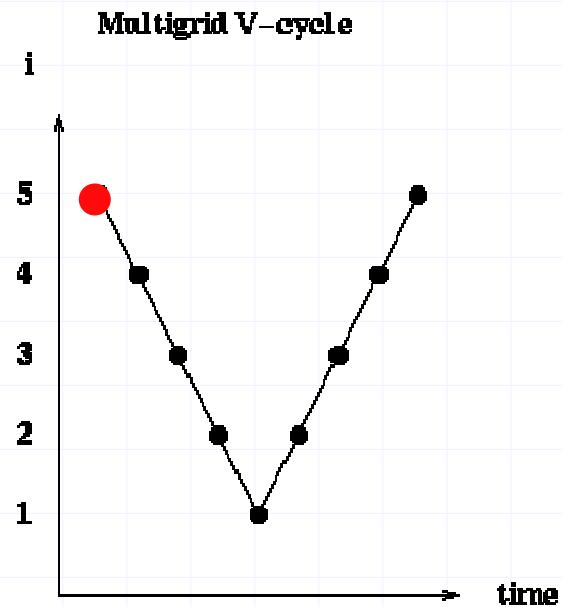
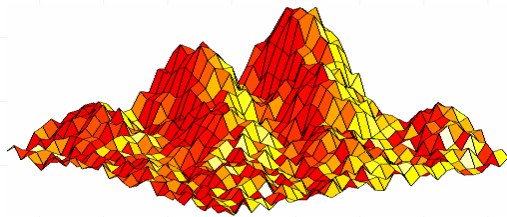
Use Smooth Aggregation Multigrid

→ $\mathbf{P}_{\text{MG}} \approx (\beta_0 \mathbf{K} - \alpha_0 \mathbf{M})$ Not S.P.D.

(Vanek, Mandel, and Brezina, 1995)

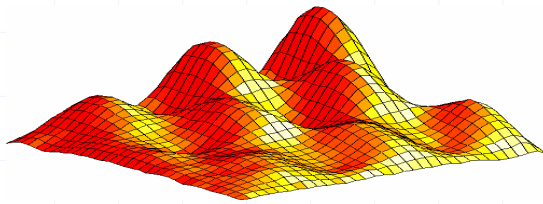
Algebraic Multigrid

◆ Smoothed aggregation algebraic multigrid



Algebraic Multigrid

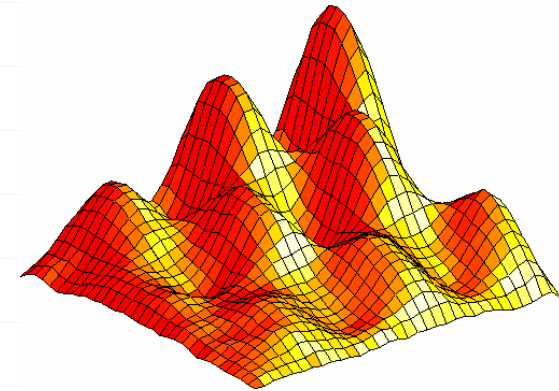
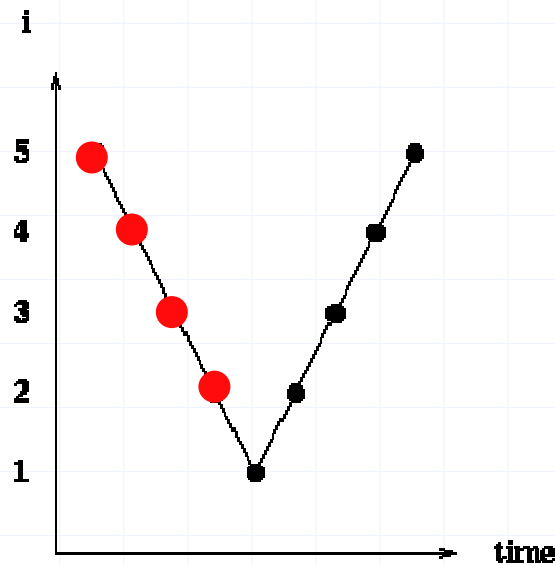
◆ Smoothed aggregation algebraic multigrid



Smoother

Remove error with large eigenvalue

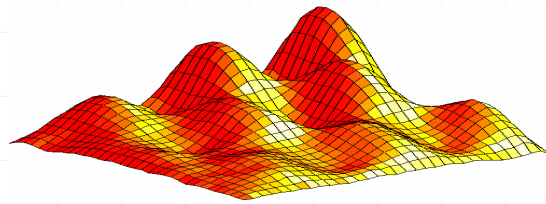
Multigrid V-cycle



(Demmel, Parallel Computing Notes)

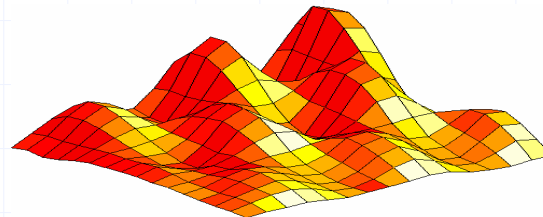
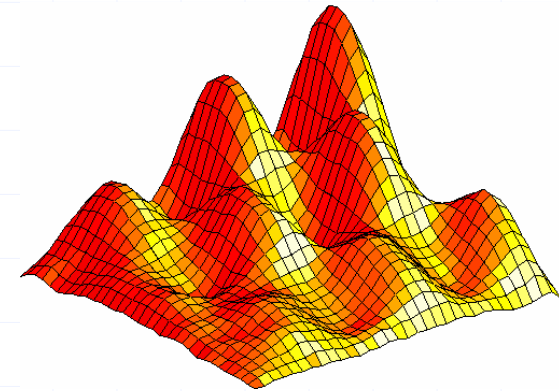
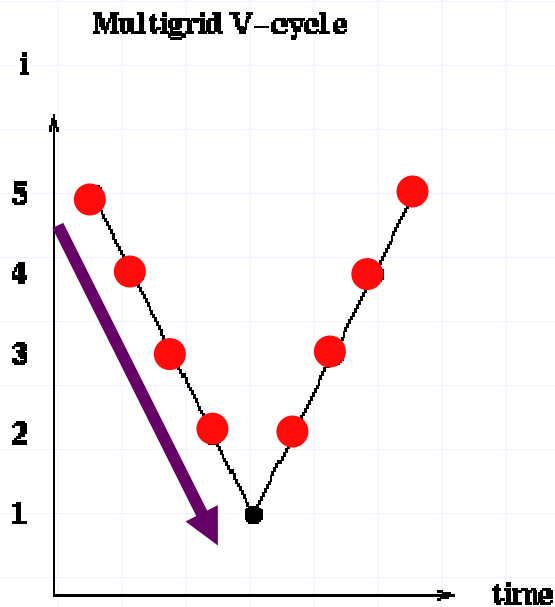
Algebraic Multigrid

◆ Smoothed aggregation algebraic multigrid



Smoother

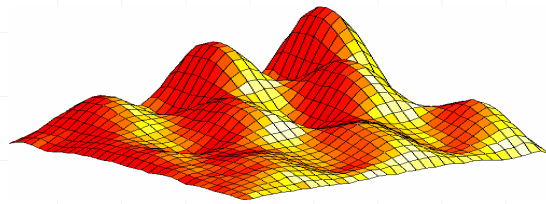
Remove error with large eigenvalue



(Demmel, Parallel Computing Notes)

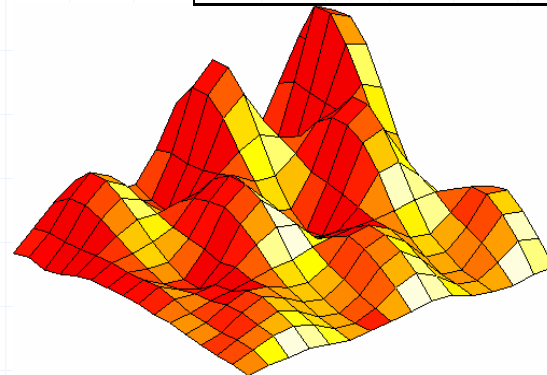
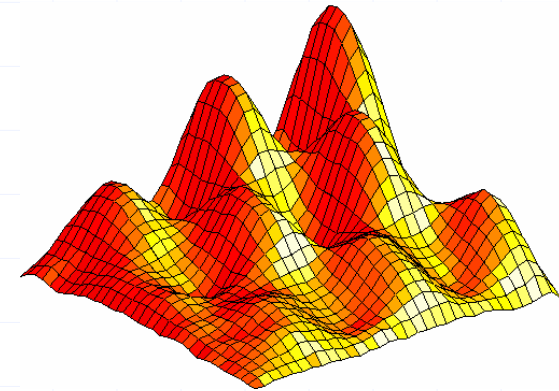
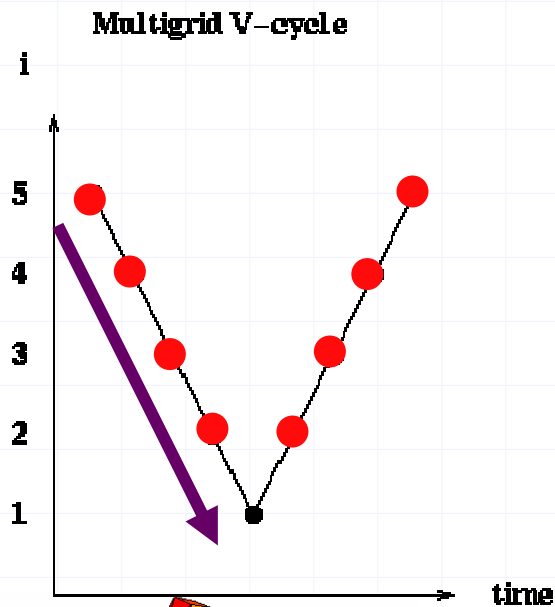
Algebraic Multigrid

◆ Smoothed aggregation algebraic multigrid



Smoother

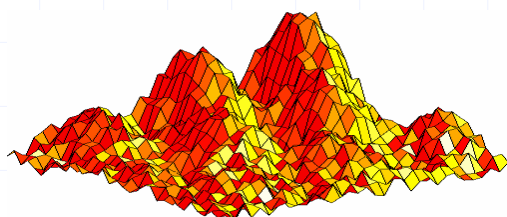
Remove error with large eigenvalue



(Demmel, Parallel Computing Notes)

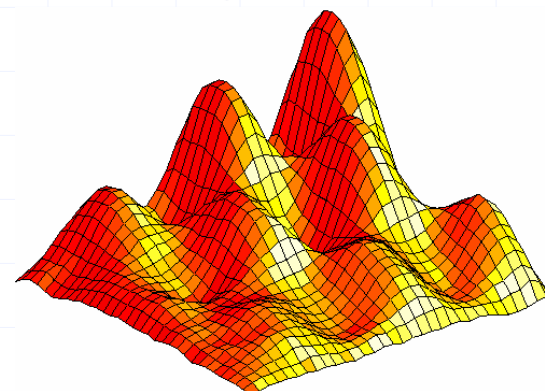
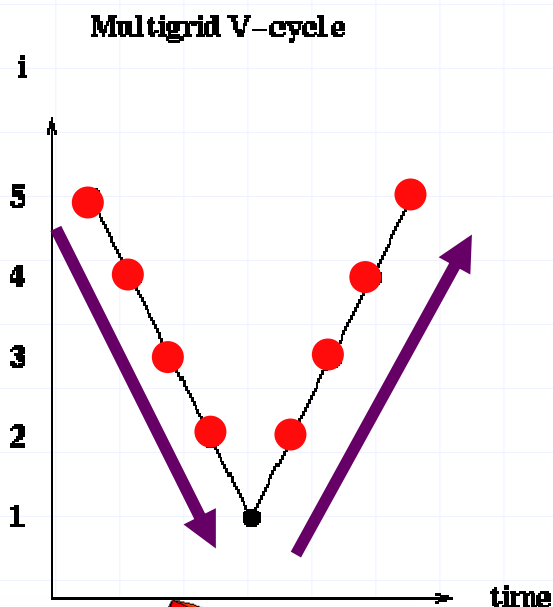
Algebraic Multigrid

◆ Smoothed aggregation algebraic multigrid



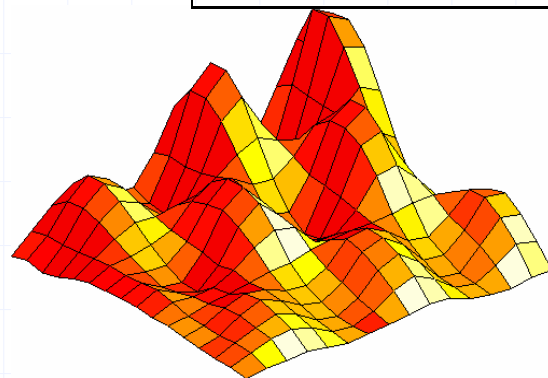
Smoother

Remove error with large eigenvalue



Coarse grid correction (Prolongator)

Remove error with small eigenvalue



(Demmel, Parallel Computing Notes)

Smoother for $\mathbf{Ax} = \mathbf{b}$

◆ Gauss-Seidel

Does not converge and smooth for indefinite case.

◆ Row projection method (Kaczmarz, 1937)

Gauss-Seidel

$$\mathbf{AA}^* \mathbf{y} = \mathbf{b}$$

$$\mathbf{A}^* \mathbf{y} = \mathbf{x}$$

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

Parallel version (Gordan and Gordon, 2005)

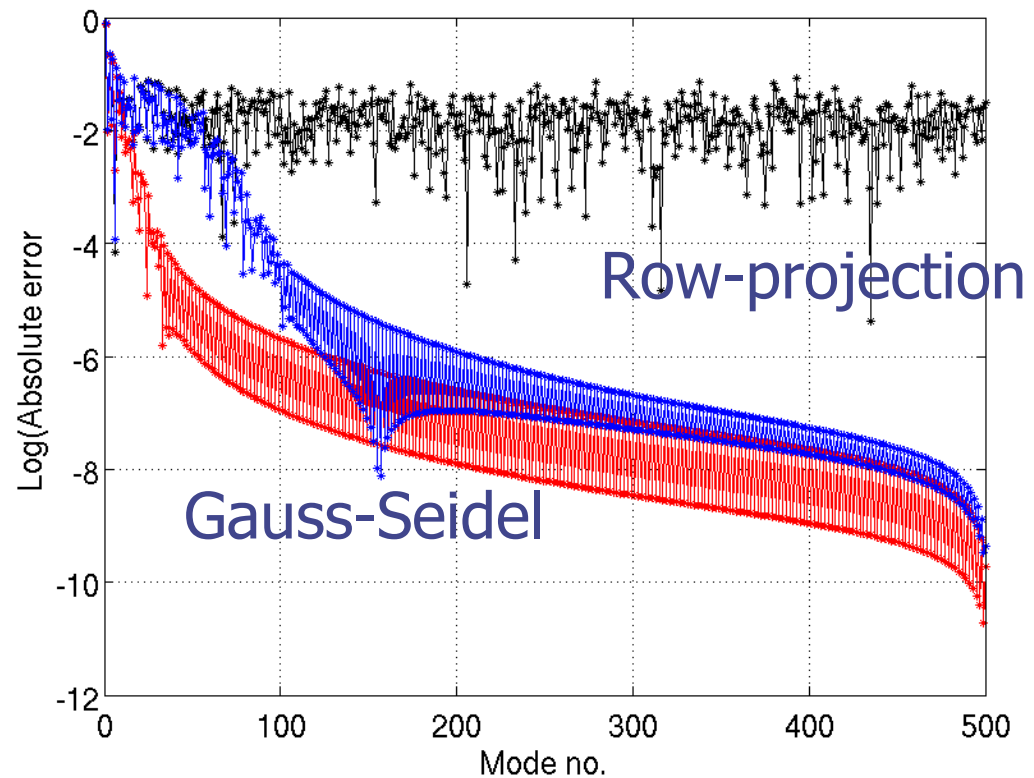
Smoother performance (SPD)

◆ 1-D Helmholtz fixed boundaries

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

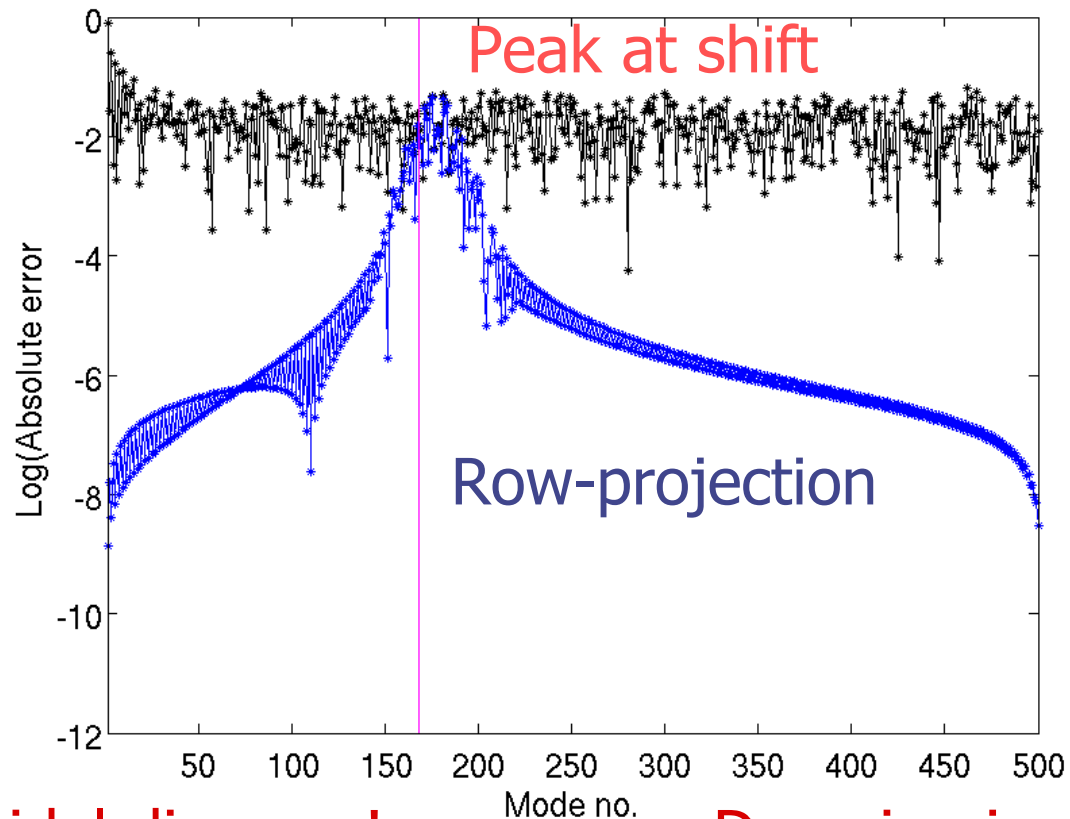
$$\mathbf{A}\mathbf{x} = 0$$

$$\mathbf{x} = \text{rand}$$



Smother performance (indefinite)

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



Gauss-Seidel diverges!

Damping is not superior
but does work!

Prolongators

◆ Vectors based on near null space of operator \mathbf{K}

$$\mathbf{V}_{\text{Null}} = [\mathbf{v}_1, \mathbf{v}_2, \dots, \mathbf{v}_N]$$

Real to complex formulation

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

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

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

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

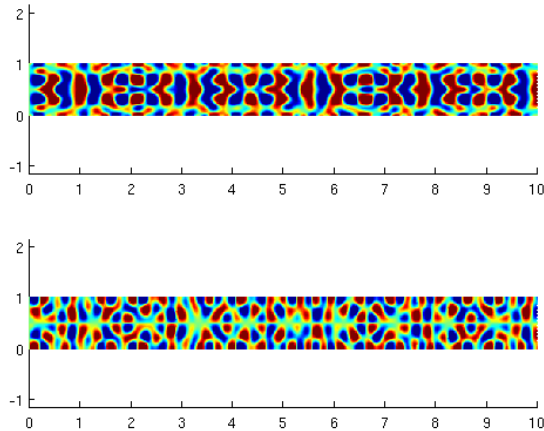
Flexibility

- Generates the mass, stiffness matrix data.

Symmetric indefinite problem

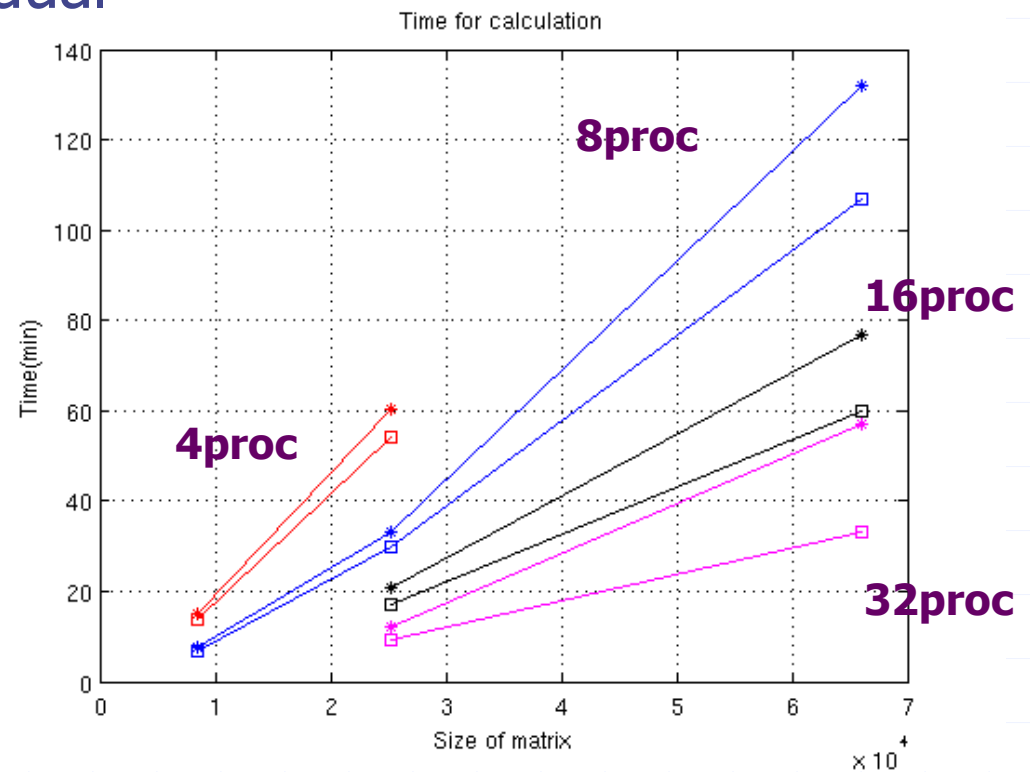
◆ 2D elastic beam

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



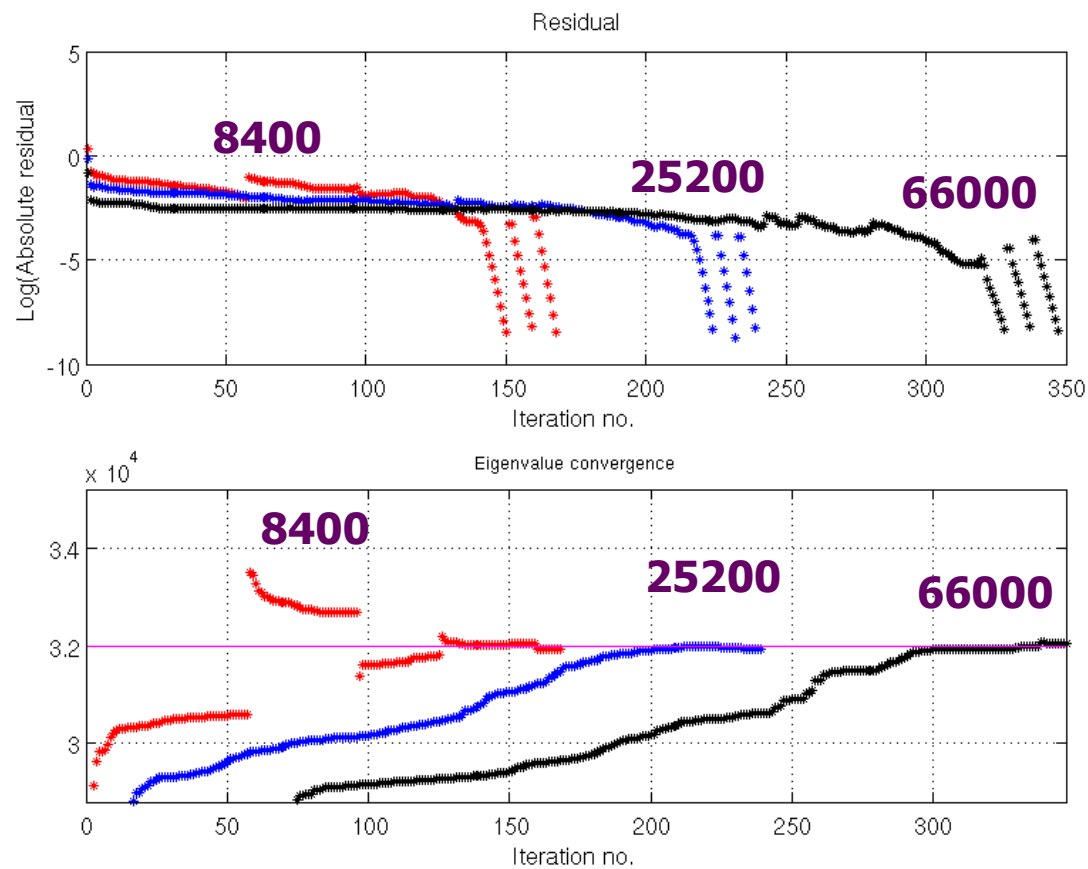
$$\mathbf{P}_{MG} \approx (\beta_0 \mathbf{K} - \alpha_0 \mathbf{M})$$

s.p.d



Convergence behavior

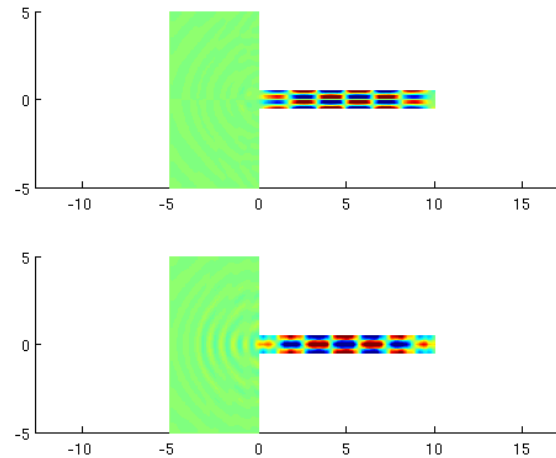
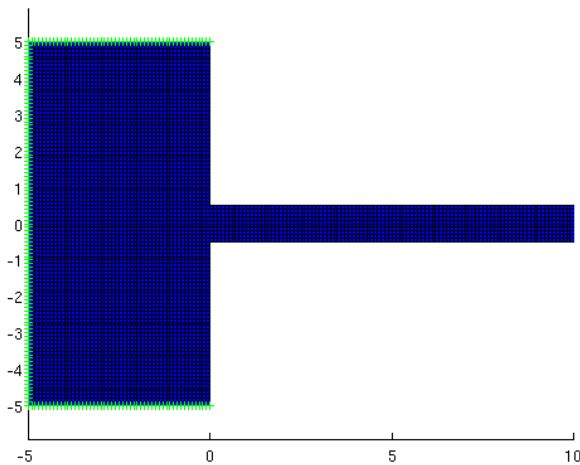
- ◆ Comparison of 8 proc for different discretizations.



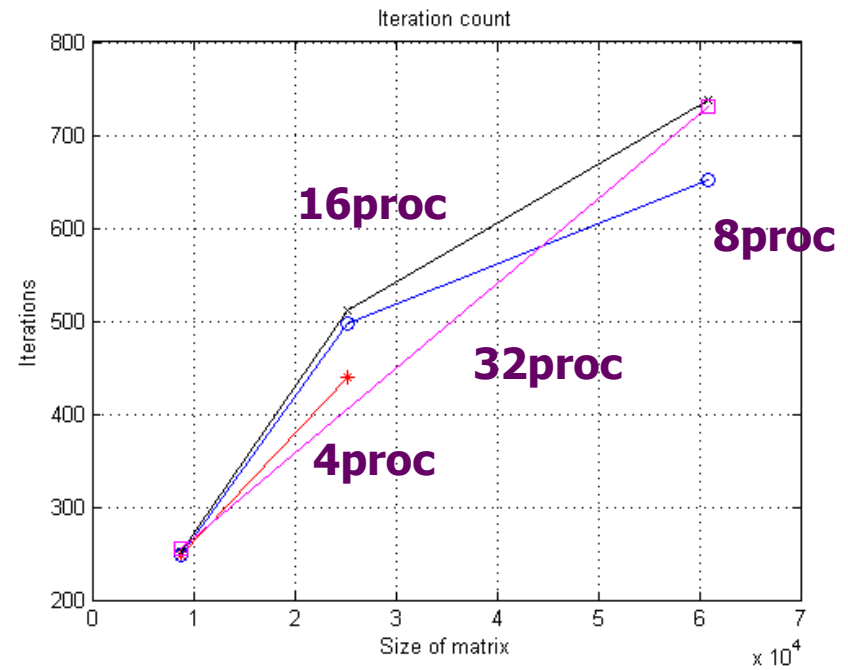
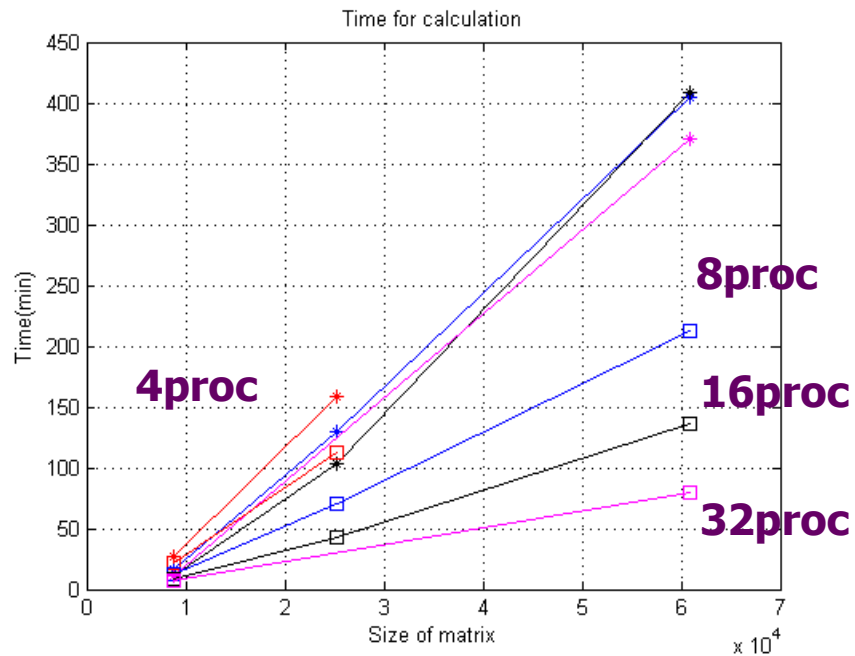
Complex symmetric problem

◆ 2D elastic beam with PML $\mathbf{P}_{MG} \approx (\beta_0 \mathbf{K} - \alpha_0 \mathbf{M})$
complex sym

Search for 3 eigenvalues near 500th
from bottom.



Convergence behavior



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>