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

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In the operation of high frequency resonators in micro electromechanical systems(MEMS), there is a strong need to be able to accurately determine the energy loss rates or alternatively the quality of resonance. The resonance quality is directly related to a designers ability to assemble a high fidelity system response for signal filtering, for example. This has implications on robustness and quality of electronic communication and also strongly influences overall rates of power consumption in such devices - i.e. battery life. An index of the quality of resonance Q is inversely proportional to the amount of energy loss existing in the system, and can be defined in terms of the complex-valued eigenvalues ω of the system as, $Q = \frac{|\omega|}{2\mathrm{Im}[\omega]}$. In this presentation, we examine methods for accurately simulating energy loss using the direct modeling of acoustic radiation via perfectly matched layer (PML) technology for 3-D structures, which results in complex-symmetric mass and stiffness matrices. Thus it is crucial that one is able to accurately compute eigenvalues of a complex-symmetric system. 3-D modeling increases the number of degrees of freedom and complexity in obtaining the solution, resulting in a requirement for more computing power and memory which can only be supplied by parallel computing methods. The simulations are conducted through the MEMS simulation software HiQLab in combination with the parallel numerical libraries PETSc and Trilinos. A modified smoothed aggregation algebraic multigrid method for solving a linear system of equations is combined with a Jacobi-Davidson method to solve for desired eigenvalues.

1 Introduction

The performance of high frequency MEMS resonators is determined by the quality factor or Q, which measures the sharpness of a resonance peak and is inversely related to the amount of damping in the system. A large Q value is desired for high performance. Since Q can be related with the complex eigenfrequencies ω of the system through the equation, $Q = \frac{|\omega|}{2\mathrm{Im}(\omega)}$, the problem of evaluating Q can be replaced with computing the eigenvalues of the system. HiQLab[1], the code that we have developed to simulate high frequency resonators, discretizes the governing equations of motion for the system by the finite element method to obtain stiffness and mass matrices $(\mathbf{K}, \mathbf{M})$ from which eigenvalues are computed through the generalized eigenvalue problem, $\mathbf{Kx} = \omega^2\mathbf{Mx}$.

There exist many different mechanisms which can contribute to damping or Q, but among these it has been observed that in high frequency resonators (MHz-GHz), a prominent source is acoustic loss. Acoustic loss is the mechanism in which energy is lost from the resonating system in the form of outgoing propagating waves. To model this phenomenon numerically, one must truncate the domain finitely and apply proper boundary conditions at the domain boundary to mimic the infinite domain behavior. The method selected is a technology called Perfectly Matched Layers(PML)[2].

The difficulty of solving for eigenvalues of the system above are due to the application of the PML, the sensitivity of acoustic loss to the system design, and the modes of interest. Application of the PML results in complex-valued symmetric non-Hermitian mass and stiffness matrices and finer meshes are required for accurate computation. The magnitude of acoustic loss is sensitive to the geometric design of the device, and in certain cases 2-D models of the actual 3-D device may not serve as accurate models to estimate damping. The eigenvalues corresponding to modes of interest may not be at the exterior of the spectrum. Thus to obtain accurate solutions, one requires a method to compute interior generalized eigenvalues of large-scale complex symmetric matrices through parallel computing. To ease parallel computation, HiQLab is combined with well established efficient libraries, namely PETSc[5] and Trilinos[4], built on top of MPI.

2 Eigenvalue computation

JDQZ[3], a Jacobi-Davidson method tailored to compute interior eigenvalues through a harmonic-Ritz projection method, is selected to solve the problem due to its capability of approximating interior eigenvalues as well as the lack in requiring linear solves accurate to the precision of those obtained from direct methods. This allows the use of iterative methods which are the only choice available for large systems. The JDQZ method is as follows. Given matrices $(\mathbf{K}, \mathbf{M})$ and a target eigenvalue $\omega_0^2 = \frac{\alpha_0}{\beta_0}$, one continuously expands subspaces $\mathcal{V}, \mathcal{W} := (\beta_0\mathbf{K} - \alpha_0\mathbf{M})\,\mathcal{V}$ from which eigenvalues are extracted by a Petrov-Galerkin projection.

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1. Find approximate eigenpair $((\alpha, \beta), \mathbf{u})$, such that $\mathbf{u} \in \mathcal{V}$ and $(\beta\mathbf{K} - \alpha\mathbf{M})\,\mathbf{u} \perp \mathcal{W}$.
2. Solve correction equation, $(\mathbf{I} - \mathbf{p}\mathbf{p}^*)(\beta\mathbf{K} - \alpha\mathbf{M})(\mathbf{I} - \mathbf{u}\mathbf{u}^*)\,\mathbf{t} = -\mathbf{r}$, for $\mathbf{t}$,
where $\mathbf{r} = (\beta\mathbf{K} - \alpha\mathbf{M})\,\mathbf{u}$ and $\mathbf{p} = (\beta_0\mathbf{K} - \alpha_0\mathbf{M})\,\mathbf{p}$.
3. Expand subspace, $\mathcal{V}_{\text{new}} = \mathcal{V} \oplus \text{span}\,\{\mathbf{t}\}$, $\mathcal{W}_{\text{new}} = \mathcal{W} \oplus \text{span}\,\{(\beta_0\mathbf{K} - \alpha_0\mathbf{M})\,\mathbf{t}\}$.

The solution of the correction equations require a linear solve of the form $\mathbf{A}\mathbf{x} = \mathbf{b}$, where $\mathbf{A} = (\beta\mathbf{K} - \alpha\mathbf{M})$, but this is not required to be accurate to machine precision, allowing the use of iterative methods. One observes that an additional difficulty in the solve is the indefiniteness and non-Hermitian property of the matrix $\mathbf{A}$, which prohibits the use of the vast iterative solution technology developed for positive definite matrices.

For the iterative solution of mechanical problems, methods such as multigrid preconditioned GMRES have been observed to be effective. In the presented method, a smooth aggregation algebraic multigrid[4] is selected to solve the linear system. Just as in the symmetric positive definite case, the smooth aggregation multigrid for this indefinite and non-Hermitian $\mathbf{A}$ consists of two components, the smoother and the coarse grid correction that is defined by the prolongator. The smoother is designed to reduce the part of the error of the solution corresponding to large eigenvalues and the coarse grid correction to small eigenvalues. For the smoother, the unconditionally convergent stationary method of row projections, which is equivalent to applying Gauss-Seidel on the equation $\mathbf{A}\mathbf{A}^*\mathbf{y} = \mathbf{b}$ where $\mathbf{x} = \mathbf{A}\mathbf{y}$, is used since standard smoothers such as Jacobi and Gauss-Seidel may no longer be effective in reducing the error when eigenvalues lie in the complex plane and are not positive real. Since the near-null space of the shifted matrix $\mathbf{A} := (\beta_0\mathbf{K} - \alpha_0\mathbf{M})$ is unclear, the prolongators are constructed from the near-null space of the unshifted operator $\mathbf{K}$, which is still not Hermitian positive definite for the case with PML. The use of the unshifted operator for prolongator construction is justified by the fact that the shift (α, β) is not too deep into the spectrum.

The JDQZ method is most effective with an adapting pair (α, β), but for reduction in computation of reconstructing the multigrid operator for each solve, it is only formed once with the target pair (α_0, β_0) such that $\mathbf{P}_{\text{MG}} \approx (\beta_0\mathbf{K} - \alpha_0\mathbf{M})^{-1}$ is used to obtain $\mathbf{x}_{\text{approx}} = \mathbf{P}_{\text{MG}}\mathbf{b}$.

3 Numerical example of a 2D elastic beam

The model of a 2D cantilever including the support governed by the equations for linear elasticity is analyzed. The beam has an aspect ratio of 10 and is modeled by linear elements. 3 levels of discretization are tested, 8.4k, 25k, and 66k degrees of freedom(DOF) on 4,8,16, and 32 processors for both the case without PML(real symmetric matrices) and with PML(complex-symmetric matrices). Figures 1 and 2 show the time required to compute 3 eigenvalues approximately 500th smallest in magnitude. The white bar inside the colored bars, represent the amount of time spent in applying the multgrid operator $\mathbf{P}_{\text{MG}}$. Not all combinations are listed, since combinations such as the 2 processor case for the 66k DOF system was not feasible. One observes that for the real symmetric case there is close to linear speed up with respect to problem size and good scalability in terms of processors. Processor scalability is due to the fact that most of the time is spent in applying the preconditioner. In the complex symmetric case, one does not see as good behavior as the real symmetric case. This lack in processor scalability is due to the increase in the number of iterations, leading to a larger dimension approximation subspace $\mathcal{V}, \mathcal{W}$, which increases the size of the matrix that is serially Schur factorized in the method. To avoid this problem, one must incorporate a restart to keep the subspace sizes small.

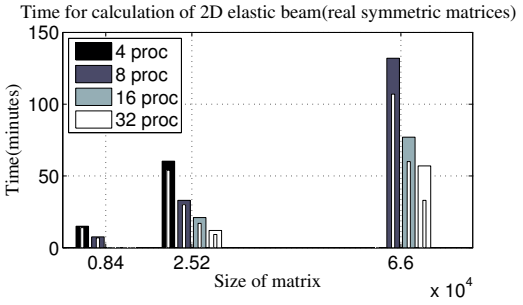

Fig. 1 Real symmetric case

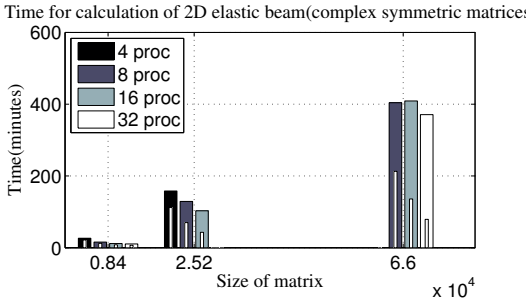

Fig. 2 Complex symmetric case

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