Research Statement

1 INTRODUCTION

Over the past few decades, the increase of computing power has fueled a tremendous progress in the area of computational mechanics. In terms of hardware, the average desktop of today can conduct more floating point operations per second than some of the super computers 20 years ago. In terms of software, industrial strength Finite Element Method (FEM) packages such as *Abaqus* [1] and educational packages such as *MATLAB* [45] greatly facilitate the accessibility to the subject. Though the environment surrounding computational mechanics has changed in this way, the fundamental procedure one must go through in using computational mechanics as a tool for understanding behavior of physical systems has not changed at all. The numerical modeling procedure one must go through can be stated as,

1. understand the physical phenomenon of interest correctly,
2. develop a model reflecting the correct physics,
3. compute the behavior of the phenomenon efficiently.

This procedure of numerical modeling must be closed in a loop with verification with actual experimental observations or results. Lack in any of the steps can lead to utterly wrong results and unbelievably inefficient use of computational resources.

As a graduate student at the University of California, Berkeley, I have been a member of SUGAR [21], a multidisciplinary research group involved in constructing computer aided design (CAD) tools for the simulation of Microelectromechanical systems (MEMS). The group consists of members from Mechanical Engineering, Civil and Environmental Engineering, Math, and Computer Science and also collaborates with people from Electrical Engineering. From those constructing MEMS devices in the Mechanical and Electrical Engineering Department I have learned the difficulties and importance of experimentation. From those in the Math and Computer Science Department I have learned and gained mathematical insight along with skills in efficient programming.

In this environment I have extensively trained myself not only in mechanics but also in mathematics, which has lead to my M.A. in Math with an emphasis on Numerical Linear Algebra. I have also acquired software development skills, contributing to the development of a resonant MEMS simulation software *HiQLab* [9] written in C++, *LUA*, and *MATLAB*. *HiQLab* can run on a serial computer as well as a multiple processor machine. In this code, I have implemented the efficient methods for simulating MEMS devices which I have developed, requiring the procedure of numerical modeling I have outlined above.

In Section 2, I will present my contributions as well as my research interests in the context of simulation of MEMS resonators, which has been the focus of my research at the University of California, Berkeley. In Section 3, I will present my future goals based on these research interests.

2 SIMULATION OF DAMPING IN MEMS RESONATORS

MEMS is the broad term used to describe micron-sized devices that interact not only with the electrical and mechanical domain, but also with the thermal and fluidic domain [43]. Within MEMS, the focus of my research has been on understanding and simulating devices called resonant MEMS, which have applications in radio frequency (RF) wireless technology as potential replacements for off-chip bulky components, reducing the total size, cost, and energy consumption of devices like wireless transceivers [40, 39]. The performance of these devices are defined by the quality factor, Q, which is defined as the maximum stored energy divided by the energy dissipation per radian of oscillation. High Q values are desired, but can be limited by energy dissipation mechanisms such as anchor loss [25], thermoelastic damping [16, 2, 54, 42, 25, 55], air damping [25, 12], material losses, and ohmic loss. The design process of these MEMS resonators can be accelerated significantly by accurate and efficient numerical simulations which can predict the amount of damping in the system, and ultimately Q.

Below I have categorized my contributions, their importance, and how they are related to my current and future research interests.

2.1 Thermoelastic damping: Reduced-order modeling

Thermoelastic damping is the mechanism in which energy is dissipated through the coupling between the mechanical and thermal domain. Mechanical oscillation couples into the thermal domain via volumetric expansion causing local temperature gradients. This in turn produces heat flow in the system leading to energy dissipation. This mechanism has been experimentally observed to be a prominent source of damping in micromechanical beam resonators. Despite its recognition, the MEMS community has been restricted to analyzing this mechanism for resonators of beam type, solely because the only accessible closed formula solution is applicable to only this type of geometry [57].

I have modeled this phenomenon by solving the coupled linearized balance of linear momentum and linearized heat equation through a finite element discretization. Though this approach is not necessarily new [20, 14, 33, 56], what I have focused on is observing the structure of the underlying equation. The linear system of equations that one must solve has a block structure with symmetry, as well as a perturbative structure. In the course of evaluating the quality factor Q of a resonant system, one must either solve for the eigenvalues of the system or evaluate a transfer function. Evaluation of the transfer function can be extremely expensive for a large scale system, since one must solve a linear system of equations at each step. To circumvent this, I have developed a structure preserving Krylov-subspace based model reduction method based on the second-order system which is capable of computing the transfer function model up to 60 times faster than a full finite element discretization and yet is still as accurate. The simulation of real fabricated devices confirms the validity of our proposed method [29]

The feature of my reduced-order model (of the second-order system), which allows good accuracy, is its moment-matching property of the transfer function. The moments are defined as the coefficients of the power series expansion of the transfer function around a specified point. The standard approach to obtaining matching moments for second-order systems is to convert to an equivalent first-order system and conduct standard Krylov subspace model reduction techniques [4, 35]. What I have done is to prove a general moment-matching theorem applicable to second-order and higher-order systems in their original form without a conversion step to an equivalent first-order system [31, 32]. This can facilitate proofs for moment-matching as well as construction of structure preserving reduced-order models for various higher-order linear dynamical systems such as the modeling of many physical systems: electromagnetics, mechanical or structural, thermal, and those coupling any number of these systems.

2.2 Anchor loss: Numerical linear algebra, Parallel computing

Resonant MEMS devices are fabricated on top of a Silicon or other semi-conductor substrate orders of magnitudes larger than the device and thus the substrate can be considered a semi-infinite half domain. As the MEMS device resonates, this motion couples with the underlying substrate through its anchors, sending non-returning waves into the substrate. This energy dissipation mechanism, called "anchor loss" in the MEMS community, has been experimentally observed to be prominent in resonant MEMS at high-frequencies, larger than the MHz range.

To model this damping phenomenon arising from an infinite domain behavior with a finite domain, we employ boundary conditions which are called radiation boundary conditions. Among the various types of radiation boundary conditions [22], we have chosen the Perfectly Matched Layer

(PML) absorbing boundary condition which was developed by Bérenger [7] for solving Maxwell's equation and later adapted in a displacement based finite element method setting by Basu [6]. The choice was made due to its ability to preserve the sparsity structure of the resulting finite element matrices. An issue that has been addressed frequently in the application of PMLs is the optimal selection of PML parameters for a desired accuracy in approximating the radiation boundary condition [13, 23]. It is crucial that one be able to know this from a users standpoint. I have developed heuristics for selecting optimal parameters in the PML for a 1D scalar wave problem, extending the work of Bindel [8], and have confirmed them in higher dimensions [29]. Here, optimality is defined in terms of the least computational effort required for a desired accuracy in the solution.

The application of PMLs to a linear elastic problem changes the structure of the discretized finite element mass and stiffness matrices drastically from a positive definite pencil to a complex-valued symmetric pencil. This has large consequences in solving linear systems involving a linear combination of these matrices as well as eigenvalue problems. To evaluate the quality factor Q of a resonant MEMS device, one can solve for the complex-valued eigenfrequencies of the system. The imaginary part of the eigenfrequency arises from the existence of damping. For devices with very small damping, the imaginary part of the complex-valued eigenfrequency can be orders of magnitude smaller than the real part. To obtain sufficient accuracy in the imaginary part to which the accuracy of the quality factor depends on, one is faced with a fine discretization. This leads to a large scale generalized eigenvalue problem. An added difficulty can arise when the eigenvalue corresponding to the mode shape of interest of the device is not at the exterior of the eigenvalue spectrum but in the interior of the spectrum.

Standard methods due not exist for the computation of interior eigenvalues of a generalized complex-symmetric large scale eigenvalue problem. The difficulties lie in the following reasons. Most large scale eigenvalue methods concentrate on Hermitian positive definite problems, and solving for interior eigenvalues of Hermitian positive definite systems can already be difficult due to the required step of solving large scale indefinite linear systems [17, 3] in the eigenvalue computation procedure. This situation greatly contradicts the current needs, since any system with a damping component is no longer Hermitian positive definite. To solve the generalized complex-symmetric eigenvalue problem arising from the application of PMLs, I have developed a geometric-multigrid [49] preconditioned Jacobi-Davidson QZ [19] method [29]. To the best of my knowledge, this is the first successful attempt in applying geometric multigrid to these linear systems. This is also the first application of the Jacobi-Davidson QZ solver to problems on the order of millions of degrees of freedom. I have successfully applied this to simulate a class of MEMS disk resonators that are fabricated for a high-operating frequency [51].

In order to compute the generalized eigenvalues of a complex-symmetric system on the order of millions of degrees of freedom, I have also had to employ parallel computing techniques. To facilitate the management of parallel linear algebra objects such as vectors and matrices, I have used the linear solver package *PETSc* [5] as well as *Trilinos* [24]. These packages have been used through the software *HiQLab* mentioned in a subsequent section.

2.3 Electromechanically coupled systems: Reduced-order modeling

In the design of a resonant MEMS device as a component in an electrical circuit, the engineer is interested in the behavior of the mechanical device at a specific frequency and mode of vibration, namely at resonance. The device at this frequency can be modeled by a single degree of freedom system through lumped mechanical parameters. From an analogy between a single degree of freedom mechanical and electrical system, these lumped mechanical parameters can be translated to equivalent circuit model parameters [28, 47, 48]. The engineer can then use these few parameters to effectively model the complex mechanical resonator and subsequently simulate the entire response of the circuit including the mechanical system with ease to evaluate the quality factor Q.

In many papers, one encounters formulas to evaluate equivalent circuit parameters, but in most cases they are either based on parallel plate assumptions [53, 11] or derived for other special geometries [52, 15, 44, 41]. As the geometry of the devices become more complex such assumptions may not apply, and numerical evaluation is necessary. In the area of piezoelectric bulk acoustic wave resonators, finite element methods have been applied to develop a process to extract equivalent circuit parameter expressions [34, 38]. Unfortunately this type of approach has not been extended into the MEMS computational domain.

As opposed to the ad hoc parameter extraction process presently used in resonant MEMS design, I have developed a systematic parameter extraction process based on a variational framework for modeling electrostatic and piezoelectric electromechanically coupled systems. The new framework allows one to treat systems with general geometry and to incorporate the electromechanical coupling effect into the mechanical modes of vibration. The extracted equivalent circuit model parameters produce a transfer function with relatively accurate behavior near the resonance frequency with much less computation time than the full model, and also represents features that cannot be obtained by current simplifying parallel plate assumptions [29]. By using this method to simulate a resonator excited by electromechanical forces across a dielectric material (Internal Dielectric Drive [37, 26]), I have been presented with one of the two best presentation awards at the Berkeley Sensor and Actuator Center (BSAC) Industrial Advisory Board meeting.

2.4 HiQLab

HiQLab [9] is a finite element tool for simulating resonant MEMS that Bindel [10] initiated and continues to develop in collaboration with our research group SUGAR [21] at the University of California, Berkeley. The software's aim is to be able to make available a tool for accurately modeling damping behavior in resonators, since the current widely available CAD tools are able to simulate the resonance frequencies but are not able to model the damping well. *HiQLab* is written mainly in C++, with an interface to the scripting language *LUA* [27] and the popular commercial software *MATLAB* [45].

I have made contributions in developing the software [30] which include but are not restricted to implementation of thermoelastic elements, electrical circuit elements, and interfaces to the parallel numerical libraries *Trilinos* [24] and *PETSc* [5]. All the simulations I have conducted have been with this software.

3 FUTURE RESEARCH DIRECTIONS

MEMS simulation and design. I would like to continue working in the modeling of RF MEMS, simulating other sources of damping and further developing the simulation software *HiQLab*. In my current research I have only addressed two sources of damping, but this does not imply that other sources are not of importance. The effect of air damping which behaves viscously in the lower-frequency regime and has well known damping models such as squeeze film and Couette damping have a different behavior in the high-frequency regime. For high-frequency disk resonators, the performance in air and in vacuum have been experimentally observed to be close, but the reason for this is not clear [52, 50]. This can be attributed to the complex interaction between the surface of the resonator moving only nanometers in stroke at very high-frequencies with the discrete nature of the air molecules surrounding it. I would like to investigate this phenomenon through methods which can take into account the discreteness of the air molecules, either through the Molecular Gas Lubrication Method (a continuum type of approach) or the the Direct Simulation Monte Carlo Method (a quasimolecular approach). By understanding this phenomenon and producing an accurate model to simulate it, the requirement of packaging resonators in vacuum for high-sensitivity can be reduced, leading to a huge reduction in costs.

The success in development and fabrication of resonant MEMS has introduced a new paradigm regarding the originally individual stand-alone MEMS devices as hierarchical building blocks for more complex and integrated structures. This approach is similar to the process in which integrated circuitry (IC) has developed. By combining individual MEMS devices either mechanically, electronically, or by both, in quantities ranging from 2 to 60, successful filter designs with low insertion and improved band-width have been constructed [36]. I would like to investigate the construction of reduced-order models of resonator components in the format of a library. If this is possible, a designer who would like to make a complicated device consisting of hundreds of individual resonators can essentially pick required components from this library, similarly to how circuit design is done today without having to solve the electromagnetic field equations. Such a framework can facilitate the design of complex devices making it systematic, straightforward, and economically feasible.

Reduced-order modeling and eigenvalue problems. In my research, to prove moment-matching properties in model reduction of higher-order linear dynamical systems, I have introduced the notion of higher-order Krylov subspaces, which are generalization of standard Krylov subspaces. I have been able to show a connection between the higher-order Krylov subspace of the higher-order linear dynamical system with the standard Krylov subspace of the equivalent first-order form. I would like to further investigate this higher-order Krylov subspace in terms of polynomial eigenvalue problems, and whether they are more or less suitable for computing eigenvalues compared to the standard method of computing eigenvalues from companion forms. Should they turn out to be advantageous, they can lead to new and improved methods for computing eigenvalues of polynomial eigenvalue problems.

I am also interested in the advantage of structure preservation in model reduction. As I have been able to identify the advantage of structure preservation for increased efficiency in the linear thermoelastic problem, I would like to investigate if there are other coupled-physics problems which give rise to structure which one can exploit for more efficient computation.

Radiation boundary conditions and solution methods. I have studied the behavior of PMLs and its accuracy as well as developed a method to solve the generalized complex-symmetric eigenvalue problem arising from its discretization. Since PMLs is not the only type of radiation boundary condition, I would like to investigate other types of existing methods such as absorbing boundary conditions (e.g., local BGT and globalDtN) and infinite elements (e.g., Burnett, Astley-Leis elements) [22, 46] to see how they effect the structure of the systems of equations one must solve and how they compare in terms of computation efficiency and performance to PMLs. The method I have selected as a preconditioner to the generalized complex-symmetric eigenvalue problem was a multigrid method. I would also like to investigate the effect that the complex-symmetry imposed by the PML has on the performance of domain decomposition methods as preconditioners, such as FETI [18], for large scale systems.

The results obtained from this analysis have broad implications since the use of radiation boundary conditions is not restricted to simulation of small MEMS devices but to scattering of electromagnetic and acoustic waves on large aircrafts and elastic wave propagation in earthquakes. Understanding which radiation boundary is the most efficient for each case and which solution method is suitable can be invaluable.

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