

## **Computational Prototyping Tools and Techniques**

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Our research group uses several engineering design applications to drive research in simulation and optimization algorithms and software. Recent efforts have focused on the fundamentals of model-order reduction, matrix-implicit methods, and fast techniques for solving integral equations. The applications currently being examined to drive those fundamental investigations include design tools for integrated circuit interconnect, micromachined devices, aircraft, and biomolecules. In the sections below, we describe these activities in more detail.

### **1. Model Order Reduction**

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#### **Project Staff**

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Designers of very complicated systems, be it hardware or software, often design using a combination of top-down or bottom-up decomposition strategies. In a top-down approach, designers decompose their systems into easily understood blocks with well-defined interfaces, and in a bottom-up approach, designers develop a complicated system by combining existing blocks. For designers of systems which are expensive to construct; such as aircraft, automobiles, cell phones, chemical processing plants, or integrated circuits; it is necessary to ensure that a final design will meet performance objectives before construction, and this is often accomplished using computer simulation and optimization.

In order to make use of computer simulation and optimization, there must be accurate models for each of the blocks used in a given physical system design. And as these models are going to be evaluated many, many times, they must be easy to evaluate. For blocks corresponding to mature technology, such models usually already exist, but for designers hoping to take advantage of rapidly evolving technology, the situation can be quite different. For example, a designer exploiting micromachining technology to develop a single-chip chemical agent detector may be frustrated to discover that there are no dynamically accurate models for fundamental building blocks, such as micropumps and microvalves.

In this project we are developing numerical techniques for automatically generating dynamically accurate models for the blocks used in physical system designs. Our approach is based on assuming that the physical blocks, more commonly referred to as devices, can be characterized at a detailed level by a system of coupled ordinary and/or partial differential equations. Such detailed differential equation descriptions are too computationally expensive to use in system simulation and optimization, and so the challenge is to automatically extract dynamically accurate simplified models from the differential equation description. This kind of automatic numerical model extraction, referred to as model-order reduction, can enormously accelerate the transfer of new technology by making models immediately available to system designers.

Many problems of engineering interest can be approximated accurately by a linear time-invariant (LTI) systems of differential equations. For example, the electrical behavior of integrated circuit interconnect and packaging is accurately described by the innately linear Maxwell's equations, and many problems in three-dimensional fluid flow are accurately described by linearization. Our group has been working on computationally efficient techniques for generating low-order models for a number of years, and we have had several recent successes. Arnoldi methods, which generate reduced models by projecting on to a truncated Krylov subspace, were shown to be closely connected to a more classical reduction approach, referred to as frequency-domain principle orthogonal direction methods, and then the two methods were compared for a problem in turbomachinery[1].

We have also been investigating another approach to computing reduced order models for LTI systems, the truncated balanced realization (TBR) methods. These methods have largely been abandoned for large system model-order reduction, even though there is an optimality result for such models, because TBR requires the solution of two Lyapunov equations and is believed to be too computationally expensive to use on large problems. We recently developed two computationally efficient model reduction approaches which approximate the TBR-produced reduced models. The first is a two-level scheme in which an Arnoldi method is used to quickly reduce a large model to a medium-sized model, and then a TBR method is used to further reduce the medium-sized model.

We developed a computationally efficient model-reduction scheme that is a more direct application of the TBR methods. In particular, we developed a new efficient iterative technique for solving the Lyapunov equations associated with the TBR method, the Cholesky Factor Alternating Direction Implicit method (CFADI). The method is particularly effective when the system matrix is sparse, and makes the TBR algorithm comparable in cost to the Arnoldi algorithm. The CFADI method, when used in TBR-based model order reduction of symmetric systems, can be shown to be equivalent to multipoint Arnoldi methods and therefore makes the first theoretical connection between the two schemes for reduction[2].

Automatically-generated reduced-order models can make system simulation both accurate and efficient, but efficient system optimization requires that the reduced-order models be parameterized with respect to design variables. We have only recently begun to work on this problem, and have developed a multiparameter Arnoldi method for LTI systems where the parameters modify the underlying system of differential equations in a linear manner[3].

Research at many groups, including ours, has resulted in enormous progress in strategies for automatic model-reduction for linear problems, but these techniques have been difficult to extend to the nonlinear problems. We have had some recent success based on representing the nonlinear system with a piecewise-linear system and then reducing each of the piecewise-linear sections using an Arnoldi method. However, rather than approximating the individual components as piecewise-linear and then composing hundreds of components to make a system with exponentially many different linear regions, we instead generate a small set of linearizations about the state trajectory which is the response to a "training input". At first glance, such an approach would seem to work only when all the inputs are very close to the training input, but examples have shown that this is not the case. In fact, the method easily outperforms recently developed techniques based on quadratic reduction[4,5].

## **2. Numerical Techniques for Integral Equations**

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### **Project Staff**

Jay Bardhan, Luca Daniel, Xin Hu, Shihhsien Kuo, David Willis, Ben Song, Anne Vithayathil, Xin Wang, Zhenhai Zhu and Jacob White

Finding computationally efficient numerical techniques for simulation of three dimensional structures has been an important research topic in almost every engineering domain. Surprisingly, the most numerically intractable problem across these various disciplines can be reduced to the problem of solving a three-dimensional potential problem with a problem-specific Greens function. Application examples include electrostatic analysis of sensors and actuators; electromagnetic analysis of integrated circuit interconnect and packaging; drag force analysis of micromachined structures; and potential flow based analysis of off-shore structures.

Although the boundary element method is a popular tool to solve the integral formulation of many three-dimensional potential problems, the method becomes slow when a large number of elements are needed to be used. This is because boundary-element methods lead to dense matrix problems which are typically solved with some form of Gaussian elimination. Generating dense systems implies that the required memory grows quadratically and required computational resources grows cubically with the number of unknowns needed to accurately discretize the problem. Over the last fifteen years, a number of algorithms have been developed which can solve the dense systems associated with boundary-element methods in time and memory that grows only linearly with problem size. These fast algorithms typically combine iterative matrix solution methods with fast techniques for multiplying dense boundary-element matrices by vectors. Our recent work in this area has been to develop precorrected-FFT techniques, which can work for general Greens functions, and Wavelet based techniques, which generate extremely effective preconditioners which accelerate iterative method convergence[6].

The development of fast boundary-element based solvers has renewed interest in developing well-conditioned integral formulations for a variety of engineering problems. It is widely believed that most ill-conditioning problems in integral equations can be alleviated by deriving second-kind formulations, but for many applications the problems stem for a different difficulty. For interconnect analysis, the ill-conditioning problem arises from the jump in conductivity associated with crossing the air-conductor interface. Our recent results demonstrate that by explicitly enforcing a divergence free condition on the conductor-air interface, we can reduce the ill-conditioning problem to manageable levels[7]. In Stoke's flow analysis, the integral equation is fundamentally singular and this singularity must be removed. In the single body case, the problem is well-understood and can be resolved by avoiding a one-dimensional singular subspace. The multibody case presents two additional difficulties: the singular subspace is the same dimension as the number of bodies, and the correct solution includes nonzero components that are outside the range of integral operator for Stokes flow. We developed approaches for dealing with both problems, by combining a modified Krylov-subspace linear system solution method with a set of pressure constraints[8].

## **3. Simulation Tools for Micromachined Device Design**

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### **Research Staff**

Xin Wang, Carlos Pinto Coelho, Anne Vithayathil, and Jacob White

Researchers in almost every engineering and scientific discipline are examining ways to harness the ability to fabricate, at low cost, centimeter-sized systems with hundreds of thousands of mechanical parts and transistors. Micro-electro-mechanical system (MEMS), or more generally micromachined devices, are in ever increasing use. Computer displays now use integrated circuits with nearly a million micron-sized moving mirrors, and automobile air bags often use a micromechanical accelerometer to detect collisions. Active research on microfluidic valves, pumps and mixers may lead to single-chip chemical analysis systems which could be used to make “in-vitro” medical diagnostic equipment or pocket-sized chemical agent detectors. Research on microfabricated turbines and generators may lead to alternative portable power sources; and microfabricated parts small enough to capture and hold individual biological cells may accelerate progress in both medical and scientific research.

Over the last decade there has been extensive, and successful, research focused on developing and exploiting micromachining, though there are very few high-volume micromachined products. In addition, almost all the research in applying micromachining technology has been carried out by specialists with many years of focused training. In contrast, integrated circuit designers do not need such a high level of specialization. Instead, they rely on a coordinated suite of synthesis and verification tools that makes it possible to design an application-specific circuit with high confidence of first-pass success, even without becoming an expert in semiconductor fabrication. The current situation for micromachined device designers is very different. These designers must know the fabrication process intimately, and may even have to design their own process. In addition, the design tools available are often limited and provide only domain-specific simulation or rudimentary layout editing. The combination of inadequate computer-aided design tools and rapidly evolving process technology has created an expertise barrier that excludes nonspecialists who would bring important application expertise. Unless this expertise barrier is lowered, primarily through vastly improved computer-aided design tools, it seems unlikely that the potential of micromachining to impact so many different disciplines will be achieved.

Computing drag forces on geometrically complicated 3-D micromachined structures, such as an entire laterally moving comb resonator, is a challenging problem. The standard semi-analytic approach, based on assuming a regular flow patterns such as Couette or one-dimensional Stokes flow, results in a good rough estimate for the drag force but can be insufficiently accurate to correctly predict geometric sensitivities. Designers have not tried to improve the accuracy using numerical simulation because traditional finite-element based 3-D fluid simulation is too computationally expensive to use for such complicated geometries. However, the recently developed FastStokes solver, based on the precorrected-FFT accelerated iterative methods, has made it possible to perform fluid analysis of very complicated three dimensional micromachined structures, such as a comb drive resonator or a tilting mirror, in under twenty minutes on a personal workstation. We have compared results our FastStokes program to measurements of comb drive resonators and tilting micromirrors, and have demonstrated that drag force can be accurately predicted using 3-D simulation[9]. One particular interesting result from our comb drive resonator experiments was that a detailed examination of the results from 3-D simulation indicated that there is significant contribution to drag due to sidewall forces, and therefore structure levitation will not increase quality factor as dramatically as one would expect from Couette flow analysis alone. We have also extended our FastStokes solver for use in higher frequency applications. As excitation frequencies rise, fluid convection may still be small, but inertial effects rise linearly with frequency. Therefore, analyzing higher frequency resonances requires the unsteady Stokes equations, though the small excitation amplitudes typically involved make it possible to use frequency domain techniques. We have used the Green's function independent properties of the precorrected-FFT accelerated approach to extend FastStokes to the unsteady case. Finally, our most recent work is on extending the FastStokes solver to the incompressible fluid case. In particular, recent modeling and experimental work has demonstrated that the out-of-plane motion of certain micro-machined

devices is strongly influenced by fluid compression. For simple structures, such as a plate over a substrate, the fluid compression effects can be determined by solving the Reynolds equation but such an approach can not be extended to more geometrically complicated structures. Instead, we have developed a linearized compressible Stokes flow formulation and a corresponding boundary-element method. The formulation exploits the fact that the relative pressure variation in most air packaged micromachined devices is very small, allowing for a linearization. Computational using this model have demonstrated that fluid compression effects occur surprisingly infrequently[10].

#### **4. Tools for High Frequency Integrated Circuit Design**

##### **Sponsors**

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##### **Research Staff**

Luca Daniel, Xin Hu, Ben Song, Anne Vithayathil, Zhenhai Zhu, and J. White.

Designers of high-performance integrated circuits are paying ever-increasing attention to minimizing problems associated with interconnect. For example, in joint work with Synposys it was demonstrated that a commonly-used technique to minimize noise in electrical cables, differential signaling, is becoming an important strategy for minimizing crosstalk in integrated circuit interconnect[11,12,13]. Analysis techniques for integrated circuit interconnect has been revolutionized by the combination of model-order reduction methods and fast methods for solving integral equations, and our fundamental research in both of these areas is described above. Fast methods for solving integral equations, like the multipole-accelerated algorithms or the precorrected-FFT methods, have made it possible to extract accurate capacitances and inductance of complicated three-dimensional structures with hundreds of interacting conductors. Codes developed at MIT are widely used for fast capacitance (FASTCAP) and inductance (FASTHENRY) extraction, and manuals and source code for our programs are still available from our web site (<https://www.rle.mit.edu/vlsi>). The results from interconnect extraction can be compressed into low-order models suitable for simulation using model-order reduction techniques, and the FASTHENRY program includes an approach to model reduction. As a recent example of our work on an extraction/reduction strategy, an approach was developed for incorporating interconnect effects in static timing analysis, based on a easily updated reduced-order model of the interconnect[16].

As integrated circuit clock frequencies rise into the multiple gigahertz range, the interconnect can no longer be treated as a combination of lumped inductors, capacitors and resistors. Instead, the interconnect must be treated using electromagnetoquasistatic and full-wave analysis. For several years we have been trying to develop fast algorithms for these higher frequency analyses, but have always struggled with the problem of how to best treat the strongly frequency dependent current crowding, also known as the skin effect. Since integrated circuit interconnect models must treat a broad frequency range, one can not rely on high or low frequency limit cases. We now have two approaches for efficient simulation in the presence of skin effects. The first involves generating template solutions based on two dimensional numerical simulation of typical conductor geometries to generate frequency-dependent basis functions to use to represent the current in conductor interiors[14]. We also developed approaches for generating reduced order models in the presence of dielectrics for those conductor interior discretizing formulations[15]. Our second approach was to develop a purely surface formulation that did not require discretizing conductor interiors, therefore eliminating the impact of the skin effect. Our surface formulation for the interconnect problem

is the only one, as far as we are aware, that is well-conditioned over the entire frequency range of interest[16].

Also in this area, we have been investigating techniques for analyzing coupling problems in single chip mixed-signal systems, where both analog and digital functional blocks share a common substrate. A major challenge for mixed-signal design tools is the accurate modeling of the parasitic noise coupling through the common substrate between the high-speed digital and high-precision analog components. The main problem with substrate models is that every substrate contact is coupled to all the other contacts, generating a collection of interactions that grows like the number of contacts squared. We recently developed methods for generating a compressed representation of these interactions, which grows nearly linearly with the number of contacts. The methods developed use either a wavelet-like approach or a hierarchy of singular value decompositions to accomplish the compression[17,18].

Finally, as magnetic materials are becoming more readily available, there is an increasing need for accurate tools for analyzing frequency dependent inductances for geometries of conductors surrounded by highly permeable material. We recently completed the development of FASTMAG, a inductance extraction program which is based on a novel integral formulation for problems with highly permeable materials[19,20].

## **5. Numerical Techniques for Aircraft Analysis**

### **Sponsors**

Singapore-MIT Alliance  
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The fluid dynamic simulation tools for both aerodynamics and turbomachine analysis are still too slow to be useful in an iterative design optimization process. We have been investigating using model reduction to accelerate the analysis of turbomachine control loops [1] and we are investigating extending fast integral equation methods for potential flow to Navier-Stokes based aerodynamic analysis.

## **6. Tools for Biomolecule Design**

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### **Research Staff**

Jay Bardhan, Carlos Pinto Coelho, Shihhsien Kuo, Bruce Tidor, Jacob White

Computer simulation is an important tool for improving our understanding of biomolecule electrostatics, in part to aid in drug design. However, the numerical techniques used in these simulation tools do not exploit fast solver approaches widely used in analyzing integrated circuit interconnects. We have adapted one of the popular formulations used to analyze biomolecule electrostatics, and developed a fast integral-equation based method for computing the electrostatic forces[21]. We then used the integral formulation in a matrix-implicit optimization method for determining optimal charge distributions[22].

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