

## **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 nonlinear and parameterized 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, bio-micromachined devices, aircraft, and biomolecules. In the sections below, we describe these activities in more detail.

### **Model Order Reduction**

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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[3,4].

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[5]. Our most recent efforts have been to combine the trajectory approach with improved methods of model reduction based on truncated balance realizations. We demonstrated that such methods can produce more accurate models for a given order, but issues of stability require more careful attention[6,7].

## **Numerical Techniques for Integral Equations**

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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 are 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[8]

## **Simulation Tools for Bio-Micromachined Device Design**

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### **Research Staff**

Carlos Coelho, Dmitry Vasilyev, Jongyoon Han, Joel Voldman 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

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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[9,10]. 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.

Our most recent work has been focused on improving tools for designing microfluidic devices which operate on cells. Detailed time domain analysis of three dimensional microfluidic structures requires dealing with the stiffness of the differential equations associated with the motion of cells in viscous fluids and with updating the solver grids. We developed an approach which minimizes the gridding problem by using a boundary element method which only requires discretizing and updating two dimensional surface meshes. In addition, we addressed the stiffness issue by introducing a velocity implicit time stepping scheme that has much better stability than the explicit Forward Euler scheme and that has a much lower computational cost than a fully implicit scheme[11].

## Tools for High Frequency Integrated Circuit Design

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### Research Staff

Luca Daniel, Xin Hu, Dmitry Vasilyev, 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 Synopsys 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[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 (<http://www.rle.mit.edu/cpg>). 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 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 cannot 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]. 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[15,16]. We also demonstrated that the frequency-dependent basis functions could be used in the surface formulation[17].

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. We recently developed an extremely fast method for substrate analysis which is based on a multidomain surface integral formulation and an extremely fast FFT-based solver[18]. The technique can analyze a substrate with 100,000's of contacts in a few minutes on a workstation.

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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].

Designers of communication integrated circuits test their designs using extremely complicated input patterns. Accurately simulating the response of a nearly thousand transistor circuit to these complicated input patterns is extremely time-consuming. We have developed a novel approach to automatically generating low-order models of these many transistor circuits that retain high accuracy while being orders of magnitude faster to evaluate[5,6,7]. We are currently working with Cadence Design System's Neolinear division and National Semiconductor to demonstrate that our approach can dramatically accelerate the simulation of realistic circuits.

### **Numerical Techniques for Aircraft Analysis**

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David Willis, Karen Willcox, Jaime Peraire, Jacob White

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[20].

### **Tools for Biomolecule and Cellular Analysis**

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#### **Research Staff**

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Computer simulation is growing in importance as a tool for improving biomolecule design and in developing an understanding of the networks used to model signal transduction and regulation in cells. As the simulation scenarios become more complicated, the issue of computational efficiency rises in priority. We have been investigating adapting the fast solver and model-order reduction techniques developed for integrated circuit design to problems in biomolecule design and cellular network analysis.

In designing certain types of drugs, the problem can be restated as designing a ligand biomolecule to optimize its likelihood of binding with a target receptor biomolecule. Electrostatic considerations are part of that optimization, but the computational cost of electrostatic optimization has been too high to use the results of the optimization to screen candidate ligands.

We have developed a combination of a fast integral equation solver for biomolecules and an implicit-Hessian optimization technique which reduces the cost of optimization by more than two orders of magnitude for realistic biomolecules[21,22,23].

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