Computational Prototyping

Academic and Research Staff
L. Daniel, EECS and RLE, K.M. Lim, SMA Faculty Affiliate, J. Peraire, EECS and Aero-Astro, A. Megretski, EECS and LIDS, B. Tidor, EECS, Bioengineering Division, and CSAIL, J. White, EECS and RLE

Graduate Students
J. Bardhan, Research Assistant, EECS, B. Bond, Research Assistant, EECS, C. Coelho, Research Assistant, EECS, T.A.E. Moselhy, Research Assistant, EECS, X. Hu, Research Assistant, EECS (Graduated) S. Kuo, Research Assistant, EECS, J.H. Lee, Research Assistant, EECS, N.S. Ngoyen, SMA Student, L. Proctor, Research Assistant, ME, H. Reid, Research Assistant, Physics, K.C. Sou, Research Assistant, EECS, L.H. Tan, SMA Student, D. Vasilyev, Research Assistant, EECS, D. Willis, Research Assistant, Aero-Astro, L. Zhang, Research Assistant, EECS

Support Staff
C. Collins, Administrative Assistant

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

1. Development of Specialized Basis Functions and Efficient Substrate Integration Techniques for Electromagnetic Analysis of Interconnect and RF Inductors

Sponsors
Semiconductor Research Corporation, MARCO Gigascale Systems Research Center, National Science Foundation

Project Staff
X. Hu, T.A.E. Moselhy, J. White, L. Daniel

The performance of several mixed-signal and RF-analog platforms depends on substrate effects that need to be represented in a library of models which have field solver accuracy. For instance, substrate-induced currents in RF inductors can severely affect quality and hence RF filter selectivity. We have developed an efficient approach to full-wave impedance extraction that accounts for substrate effects through the use of two-layer-media Green's functions in a mixed-potential-integral-equation (MPIE) solver. In particular, we have developed accelerated techniques for both volume and surface integrations in the solver.

In this work, we have also introduced a technique for the numerical generation of basis functions that are capable of parameterizing the frequency-varying nature of cross-sectional conductor current distributions. Hence skin and proximity effects can be captured using many fewer basis functions in comparison to the prevalently-used piecewise-constant basis functions. One important characteristic of these basis functions is that they only need to be pre-computed once for a frequency range of interest per unique conductor cross-sectional geometry, and they can be stored off-line with a

minimal associated cost. In addition, the robustness of these frequency-independent basis functions is enforced using an optimization routine.

The cost of solving a complex interconnect system using our new basis functions can be more than two orders faster than using piecewise-constant basis functions over a wide range of operating frequencies. Furthermore our volume and surface integration routines result in an additional efficiency improvement of a factor of up to 9.8 as shown in [1]. Our solver accuracy is validated against measurements taken on fabricated devices.

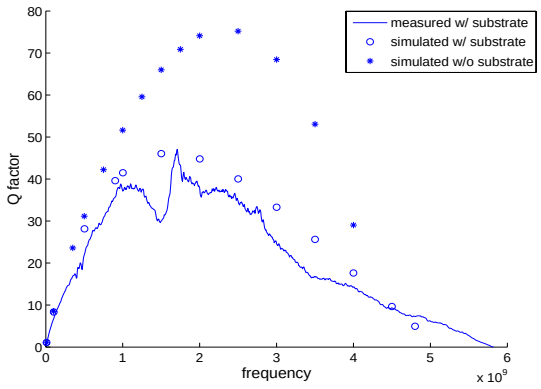


Figure 1: Measured and simulated Q-factors for a square RF inductor with an area of 15mm x 15mm and surrounded by a ground ring.

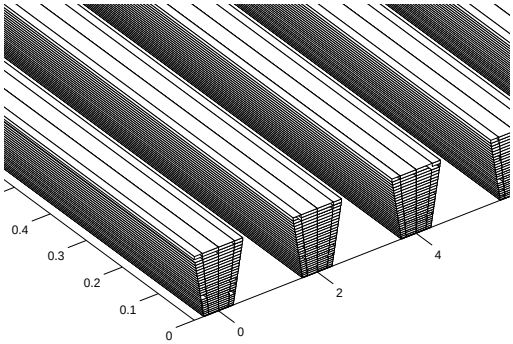


Figure 2: Our basis functions avoid the expensive cross-sectional discretization shown in figure necessary to account for trapezoidal cross-sections or skin and proximity effects.

References

[1] X. Hu, J.H. Lee, J. White, and L. Daniel, "Analysis of full-wave conductor-system-impedance over substrate using novel integration techniques," in *Proc. of the IEEE/ACM Design Automation Conference*, June 2005.

2. A Quasi-Convex Optimization Approach to Parameterized Model Order Reduction

Sponsors

MARCO Gigascale Systems Research Center, Semiconductor Research Corporation, National Science Foundation

Project Staff

K. C. Sou, L. Daniel, A. Megretski

In this work an optimization based model order reduction (MOR) framework is proposed. The method involves setting up a quasi-convex program that explicitly minimizes a relaxation of the optimal H-infinity norm MOR problem. The method generates guaranteed stable and passive reduced models and it is very flexible in imposing additional constraints. The proposed optimization approach is also extended to parameterized model reduction problem (PMOR). The proposed method is compared to existing moment matching and optimization based MOR methods in several examples. For example, a 32nd order parameterized reduced model has been constructed for a 7 turn RF inductor with

substrate (infinite order) and the error of quality factor matching was less than 5% for all design parameter values of interest.

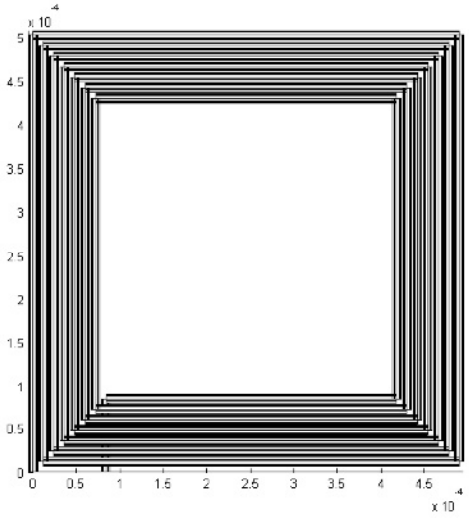


Figure 1: 7 turn RF inductor for which a parameterized (with respect to wire width and wire separation) reduced model has been constructed.

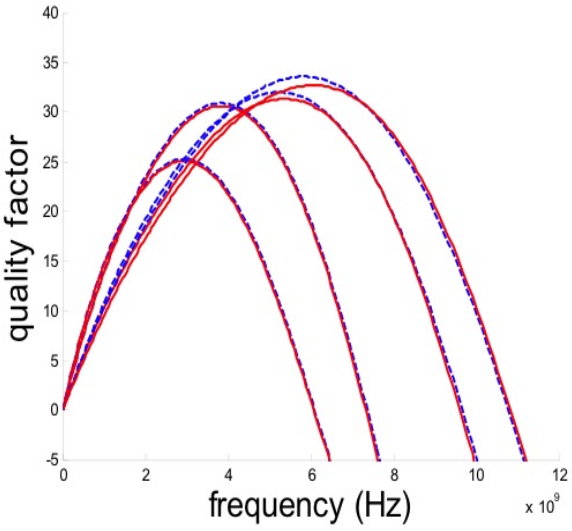


Figure 2: Matching of quality factor of 7 turn RF inductor when wire width = 16.5 um, wire separation = 1,5,18,20 um. Blue: Full model. Red: ROM.

References

Sou, K, Megretski, A, Daniel, L, A Quasi-Convex Optimization Approach to Parameterized Model Order Reduction. IEEE/ACM Design Automation Conference, Anaheim, CA, (2005)

3. Fast Solver Development for 3-D Nanophotonics

Sponsors

Defense Advanced Research Projects Agency, MARCO Interconnect Focus Center

Project Staff

J.H. Lee, L. Zhang, Y. Avniel, J. White

We have been developing a fast solver for analysis of general photonic waveguides as a part of the robust optimization for nanotechnology project. As an example, quasi-periodic dielectric waveguides can be used to generate light-delay elements with a small volume factor, and will be an integral part of integrated photonics. An example of such a waveguide is shown in Figure 1.

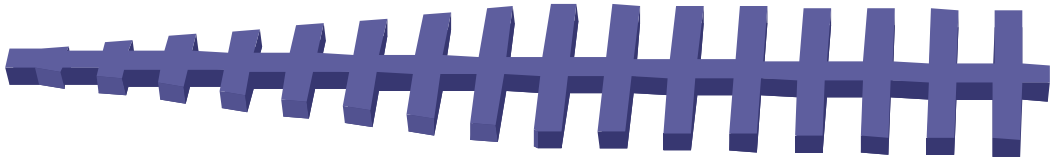


Figure 1: A taper transition from uniform waveguide to a slow light waveguide

We have developed (a) a full-wave integral equation solver using the PMCHW(T) formulation; (b) circulant preconditioner-based acceleration techniques for long periodic waveguides; and (c) absorbers to terminate waveguides with small reflection. As shown in Figure 2, the simulate field inside a dielectric slab terminated by a low-loss absorber has almost no reflections.

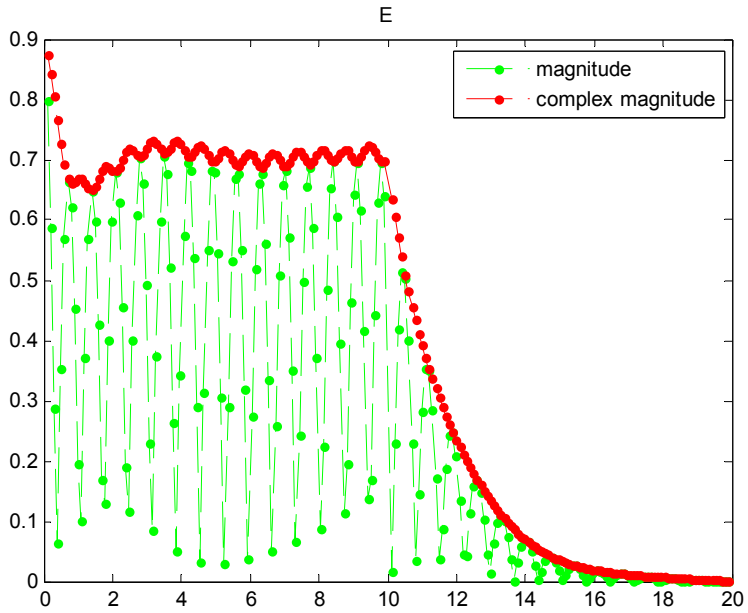


Fig. 2: The electrical field of a dielectric waveguide followed by an absorbing layer

The next phase of our project is to develop (a) a more efficient absorber; (b) an acceleration technique for non-periodic structures using the precorrected-FFT algorith; and (c) techniques to couple the accelerated solver with robust optimization to tackle practical design optimization problems.

4. Parameterized Model Order Reduction of Nonlinear Circuits and MEMS

Sponsors
MARCO Gigascale Systems Research Center, National Science Foundation

Project Staff
B. Bond, L. Daniel

The presence of several nonlinear analog circuits and Micro-Electro-Mechanical (MEM) components in modern mixed signal System-on-Chips (SoC) makes the fully automatic synthesis and optimization of such systems an extremely challenging task. Our research focuses on the development of techniques for generating Parameterized Reduced Order Models (PROM) of nonlinear dynamical systems. These reduced order models could serve as a first step towards the automatic and accurate characterization of geometrically complex components and subcircuits, eventually enabling their synthesis and optimization.

Our approach combines elements of a non-parameterized trajectory piecewise linear method [1] for nonlinear systems with a moment matching parameterized technique [2] for linear systems. Building upon such methods, we have created four different algorithms for generating PROMs for *nonlinear*

systems. The algorithms were tested on three different systems: a MEM switch, shown in Figure 1, and two nonlinear analog circuits. All of the examples contain distributed strong nonlinearities and possess some dependence on several geometric parameters.

The reduced order models can be constructed to posses strong local or global accuracy in the parameter-space depending on which algorithm is used. Figure 2 shows the output of one PROM created for the example in Figure 1 and compared to the field solver output of the full nonlinear system. In this example the system was parameterized in the width of the device, and simulated at a parameter value different from the values at which the model was created. We found that in general the best algorithm is application specific, but the PROMs are very accurate over a practical range of parameter values. For further details on parameter-space accuracy and cost of the algorithms see [3].

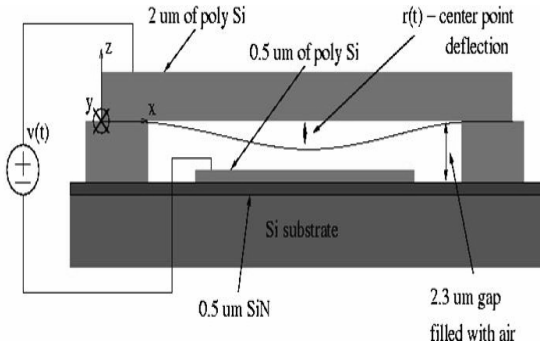


Figure 1: Application example: MEM switch realized by a polysilicon beam fixed at both ends and suspended over a semiconducting pad and substrate expansion.

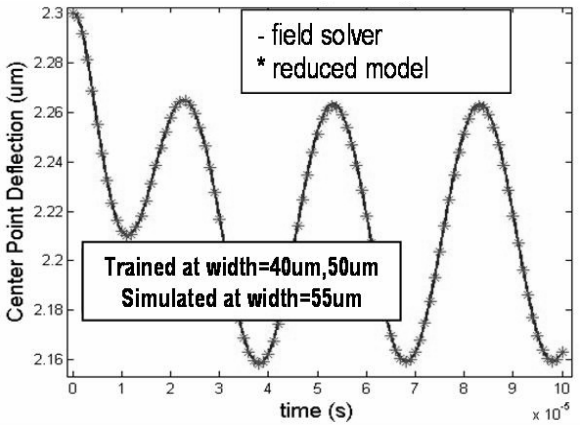


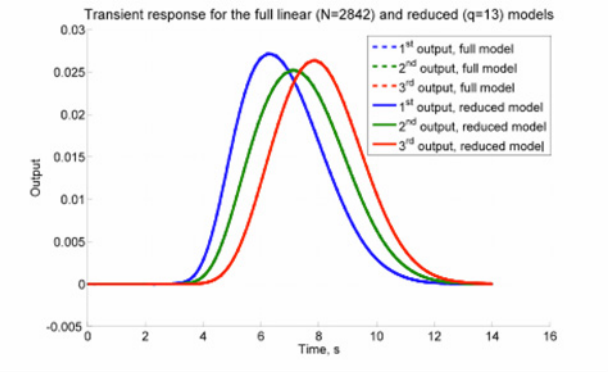
Figure 2: Center point deflection predicted by our parameterized reduced model of order 40, compared to a finite difference detailed simulation.

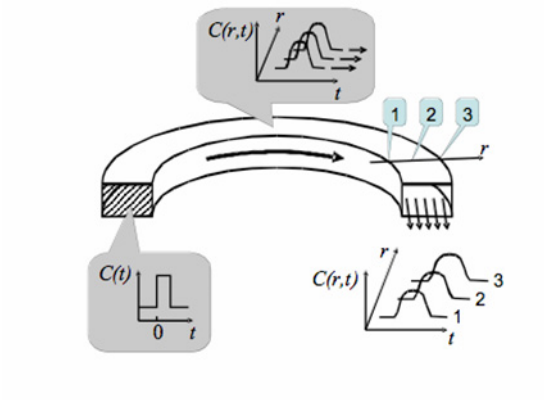
References

[1] M. Rewienski and J. K. White. A trajectory piecewise-linear approach to modle order reduction and fast simulation of nonlinear circuits and micromachined devices. In *Proc. Of IEEE/ACM International Conference on Computer Aided-Design,* pages 252-7, San Jose, CA, USA, Novermber 2001.

[2] L.Daniel, C.S. Ong, S.C. Low, K.H. Lee, and J.K. White. A multiparameter moment matching model reduction approach for generating geometrically parameterized interconnect performance models. *IEEE Trans. On Computer-Aided Design of Integrated Circuits and Systems*, 23(5):678-93, May 2004.

[3] B. Bond and L. Daniel, Parameterized Model Order Reduction of Nonlinear Dynamical Systems, *Proc. Of the IEEE Conference on Computer-Aided Design*, San Jose, 2005.





5. New Results for Linear and Nonlinear Reduction Methods

Sponsors
National Science Foundation, MARCO Interconnect Focus Center, Singapore-MIT Alliance (SMA)

Project Staff
D. Vasilyev, J. White

A new linear model order reduction method was developed, which is applicable to large sparse nonsymmetrical dynamical systems. This method is a modification of the AISIAD method (approximate implicit subspace iteration with alternate directions), and aims at approximating the balanced-truncation method. The developed method is preferable if the system has completely different most *observable* and most *controllable* states. For several test cases, this modified AISIAD method showed either similar or superior accuracy compared to other approximations to balanced truncation model reduction method [1].

Application of trajectory piecewise-linear model order reduction (TPWL MOR) to bioMEMS devices was studied [2]. Particularly interesting example was a problem of electro-osmotic flow in a microfluidic channel. We considered an injection of a (marker) fluid into such system We have found that nonlinear wave-like solutions present a significant challenge for TPWL nonlinear reduction methods, whereas linear modified AISIAD reduction was quite successful.

References

[1] Dmitry Vasilyev and Jacob White: A more reliable reduction algorithm for behavioral model extraction, ICCAD: Proc. IEEE/ACM Int. Conf. Computer-Aided Design, San Jose CA, Nov. 2005, pp. 813-820

[2] Dmitry Vasilyev, Michal Rewienski, Jacob White: Macromodel Generation for BioMEMS Components Using a Stabilized Balanced Truncation Plus Trajectory Piecewise-Linear Approach. IEEE Trans. on CAD of Integrated Circuits and Systems 25(2): 285-293 (2006).

6. Modeling Ion Flow in a Nanochannel

Sponsors
Singapore-MIT Alliance (SMA)

Project Staff
L. Proctor, L. Tan, J. Han, K. Lim, J. White

A nanofluidic filtration device has been manufactured in which proteins, which are initially in such small concentrations that they cannot be tested, are filtered and increased up to 100 million times in concentration. The purpose of this project is to do computational simulations of the filtration device in order to better understand its behavior and optimize its design. Presently, the simulation uses a Finite-Volume approach combined with a Scharfetter-Gummel discretization technique. Future work will be to accelerate the simulation using Integral Equation Methods. The equations modeled are the Poisson-Nernst-Planck equations (or the Drift-Diffusion Equations):

$$\varepsilon^2 \nabla^2 \Psi = (C_N - C_P) F \tag{1}$$

$$\nabla \cdot \left(-DC_a - z_a \mu F C_a \nabla \Psi \right) = 0, \quad a = \{N, P\}. \tag{2}$$

These equations model the continuous ion flow through the device. The nanochannel is capable of blocking ion flow resulting from an overlapping double layer produced by a surface electric charge on the walls of the device. Currently, this surface charge effect is modeled as a Neumann boundary condition on the potential which, essentially, models the potential drop across the compact Stern layer. The double layer produces another phenomenon, known as concentration polarization, a decrease in concentration with a decrease of distance to the wall while maintaining electroneutrality – this will occur in the diffuse part of the double layer. This decrease in concentration, subsequently, produces a larger Debye length (a general measure of the double layer). The idea is that the Debye length actually extends out of the nanochannel and is capable of blocking ion flow through an adjoining microchannel. This is the major mechanism needed for the filtration.

7. Efficient tools for the calculation of drag forces on planar microelectromechanical systems

Sponsors
Singapore-MIT Alliance (SMA)

Project Staff
C. P. Coelho, N. Nguyen, J. Voldman, K. Lim, J. White

Steady state and time-domain simulation are essential tools for robust design and optimization of micromechanical devices. We are working on improving the current state of the art accelerated boundary element methods for calculating damping forces in planar MEMS structures. We propose to improve previous work for the important case of planar MEMS structures, such as comb-drives and accelerometers, that lie at a short distance above a flat substrate. For these structures, the drag force between the device and the substrate is one of the largest contributions to the total drag force and the presence of the substrate cannot be ignored. General purpose solvers require that the substrate be discretized into a large number of panels which limits the size of the problems that can be simulated. In our work, we represent the substrate implicitly by using a Stokes flow Green's function that automatically satisfies the no-slip, no-penetration boundary conditions at the substrate. By using this ground plane Green's function we eliminate the need to discretize the substrate and to consider the forces on the substrate.

The boundary element method relies on the calculation of panel-to-panel interactions. We have extended the analytical integration scheme and we are now capable of accurately calculating the integrals of polynomial distributions over odd powers of the distance between the panel and an observation point. Using our integration scheme we are capable of calculating the velocity and force distributions due to polynomial force distributions on a flat panel. Our integration scheme can also be used to calculate the effects due to force dipoles and higher order singularities.

Within the Computational Prototyping Group we have setup a Matlab framework for the precorrected Fast Fourier Transform (pFFT) algorithm. The pFFT has been used as the basis of an accelerated boundary element solver for Stokes flow. We have applied the pFFT algorithm to the case of the ground plane Green`s function, which is not space-invariant along the direction normal to the substrate by splitting the kernel into a set of space invariant kernels associated with the force distribution and the force moment distribution. The method we used to apply the pFFT algorithm to the case of space varying kernels can be reused with other non-space invariant kernels. Furthermore, we have improved upon the previous implementations of the pFFT algorithm by exploiting the symmetry of the Green function kernels to reduce the computation time and memory usage of the algorithm by a factor of eight.

In order to extract the most performance from the pFFT algorithm we have also developed several strategies that rely on the application of the pFFT algorithm in the plane parallel to the substrate and that use non-FFT accelerated convolution along the direction normal to the substrate. Currently we are collecting results and characterizing the accuracy of the algorithms we have developed.

8. An Unsteady, Accelerated High Order Panel Method with Vortex Particle Wakes

Sponsors
Singapore-MIT Alliance, National Sciences Foundation, Natural Sciences and Engineering Research Council of Canada, National Science Foundation

Project Staff
D. Willis, J. Peraire, J. White

In this work a computational tool for rapid aerodynamic analysis of three dimensional, unsteady, morphing-body, potential flows is being developed. A combined boundary element method-vortex particle approach is considered. The method is made computationally tractable through the use of iterative solvers and matrix vector product acceleration routines. Furthermore, the use of the combined boundary element method-vortex particle method approach permits hands off vorticity generation and evolution in the domain. The resulting simulation tool is effective and efficient for simulating complex aerodynamics problems such as flapping flight and unsteady aircraft maneuvers.

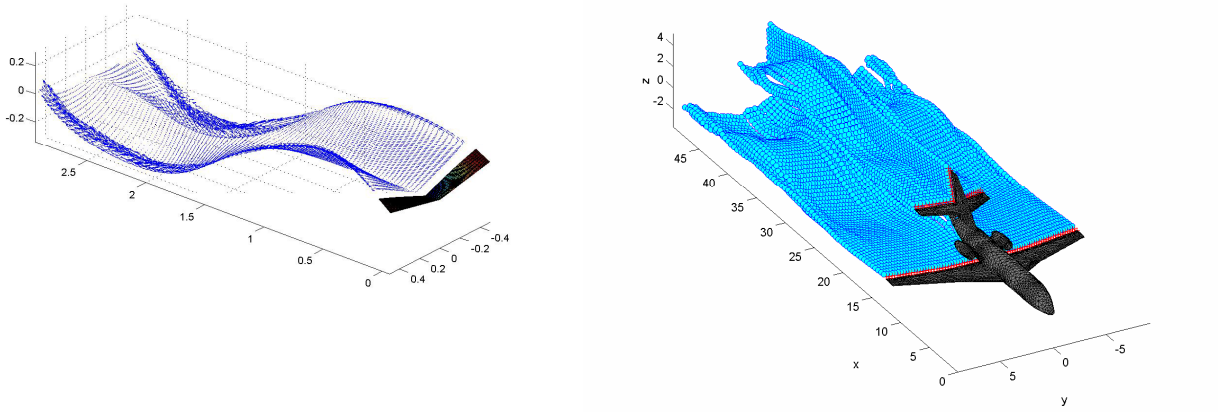


Figure: The above figures illustrate the combined boundary element method-vortex particle method approach for solving complex unsteady flows. The vortex particle representation of the lifting surface trailing vorticity is shown. The image on the left illustrates a flapping wing geometry, while the image on the right illustrates a rapidly heaving business jet.

References

[1] Willis, D.J., Peraire, J., and White, J.K., 'A Combined pFFT-multipole tree code, unsteady panel method with vortex particle wakes', AIAA Paper 2005-0854, Reno, NV, Jan. 2005.

[2] Willis, D.J., Peraire, J., and White, J.K., 'A quadratic basis function, quadratic geometry, high order panel method' presented at 44th AIAA Aerospace Sciences Meeting, AIAA-2006-1253, Reno, Nevada, 2006.

[3] Willis, D.J., "An Unsteady, Accelerated, High Order Panel Method with Vortex Particle Wakes", MIT PhD. Thesis, Department of Aeronautics and Astronautics

9. Boundary-Element Modeling Of Nanoscale Device Electrostatics

Sponsors

Network for Computational Nanotechnology, MARCO Interconnect Focus Center

Project Staff

H. Reid, J. White

Accurate electrostatic modeling is an essential tool for the design of electronic devices. Yet the complex topologies of modern nanoscale devices pose severe challenges for traditional finite-difference or finite-element (FDM/FEM) simulators, which scale poorly with system size and only approximately account for effects at material interfaces. To remedy these inadequacies, we have introduced a boundary element method (BEM) that discretizes surfaces instead of volumes. In addition to capturing the correct physics at material interfaces, our method reduces the complexity scaling from $< L^3$ to $< L^2$, where L is a characteristic length. We combine our BEM electrostatic solver with accurate quantum-statistical-mechanical modeling of electronic states in nanoscale devices, achieving an accurate and efficient modeling framework for predicting capacitances and IV curves of device geometries whose complexity would otherwise render direct simulations intractable. We apply our methods to study recently reported carbon nanotube field-effect transistors (CNTFETs), plotting

charge distributions, potential profiles, and electronic band diagrams for the devices. For a dual gate CNTFET device with a 50 nm channel length and both standard and high-κ gate dielectrics, we calculate a total gate capacitance of CG ≈ 3.2 aF, to be compared with the experimentally estimated value of 4.3 aF.

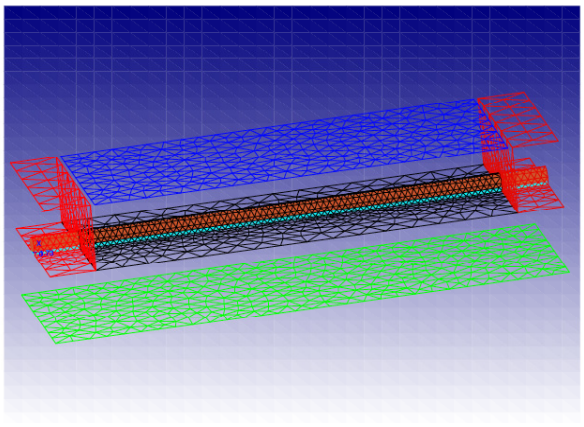


Figure 1. Discretized geometry of a 50-nm dualgate CNTFET. Green panels: bottom gate. Cyan panels: Si02–air interface. Black panels: High- K dielectric interface. Red panels: Source/Drain metallization. Blue panels: Top gate. Orange panels: Carbon nanotube. Note that our discretization accurately captures the immersion of the nanotube in the Pd source/drain contacts and in the high-K material in the channel region.

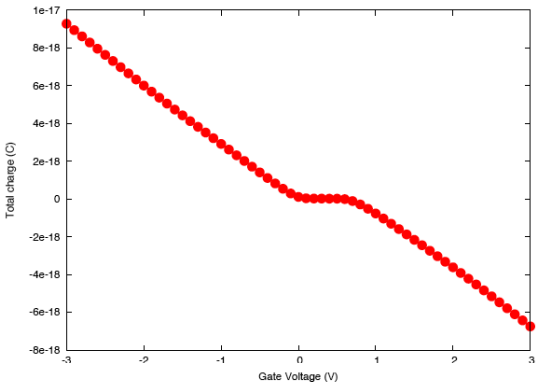


Figure 2. Total charge on nanotube surface versus gate voltage for a 50-nm dual-gate CNTFET. From this plot we estimate a total gate capacitance of 3.2 aF.

10. Numerical Methods for Biomolecule Electrostatics

Sponsors

Singapore-MIT Alliance (SMA), NIH Integrated Cancer Biology Program

Project Staff

J. Bardhan, M. Altman, J. White, B. Tidor

Electrostatic interactions play important roles in biomolecule structure and function. In contrast to hydrogen bonding and van der Waals interactions, however, electrostatic interactions act over much longer distances. This long-range nature significantly complicates computational modeling.

Since computational expense prohibits explicitly modeling the many solvent molecules surrounding a biomolecule of interest, approximate models have been introduced that capture solvent effects in an average way. In these models, macroscopic laws of electrostatics are assumed to hold in the molecular interior and in the solvent region exterior; the charge distribution in the molecule is assumed to be a set of discrete point charges located at the atom centers, and the potential satisfies the Poisson equation in this region. In the solvent exterior, mobile water molecules and salt ions screen charges and the Poisson--Boltzmann equation governs the electrostatic potential.

Even these simplified models, however, require large quantities of computer time and memory. In

this project we focus on designing new, more efficient numerical techniques for computing the electrostatic interactions between biomolecules and surrounding solvent.

Finite difference methods (FDM) are one of the most popular approaches for molecular electrostatics; in these methods, a grid is laid down over the problem domain, and one finds a set of electrostatic potentials at the grid points that approximately solve the underlying partial differential equations. The finite difference approach is straightforward to understand and implement, but suffers from several sources of error. First, the irregular molecule-solvent interface cannot be accurately resolved on a regular grid. Second, the point charges that represent the molecular charge distribution must be spread to nearby grid points. Finally, the mathematical model has an infinite domain, which the finite difference method is forced to truncate.

The boundary element method (BEM) is another technique that can be used to model molecular electrostatics. The partial differential equations governing the potential throughout space are converted to an integral equation, or set of integral equations, over the molecular surface. The transformation therefore reduces the dimensionality of unknowns from three to two. In addition, the integral equation suffers from none of the grid-based inaccuracies inherent to finite difference methods: boundary conditions at infinity are treated exactly, point charges can be treated exactly, and the molecular surface can be represented much more accurately.

The linear systems that arise in the BEM are dense. Solving these systems by Gaussian elimination therefore has memory requirements that grow quadratically in time with respect to the number of unknowns, and time requirements grow cubically. For large systems, such cost is prohibitive, and we use Krylov subspace iterative methods such as GMRES instead. Using Krylov methods allows us to avoid the cubic time cost, but the dense matrix-vector multiply still limits performance. We therefore use techniques that compute the matrix-vector product approximately but in much less time and memory.

We have shown, for instance, that the precorrected-FFT algorithm can be used to solve the BEM formulation of the biomolecule electrostatics problem. To reduce memory requirements, we have developed a new algorithm, which we call FFTSVD, for biomolecule electrostatics and bioMEMS simulations [1]. The algorithm is based on compressing long-range interactions using an approximate singular value decomposition (SVD), and then quickly computing the interactions using the FFT.

The boundary element method holds significant promise for improving the accuracy and speed of biomolecule electrostatics simulations. We have already demonstrated the viability of a fast solver approach. We believe that the FFTSVD algorithm and future techniques will allow us to dramatically reduce the memory and time requirements for these calculations.

References

[1] M. D. Altman, J. P. Bardhan, B. Tidor, and J. K. White. FFTSVD: A Fast Multi-Scale BEM Algorithm Suitable for BioMEMS Design. *submitted to IEEE Transactions on Computer-Aided Design of Integrated Circuits and Systems*.

11. Higher Order Methods for Analyzing Biomolecules in Ionic Solutions

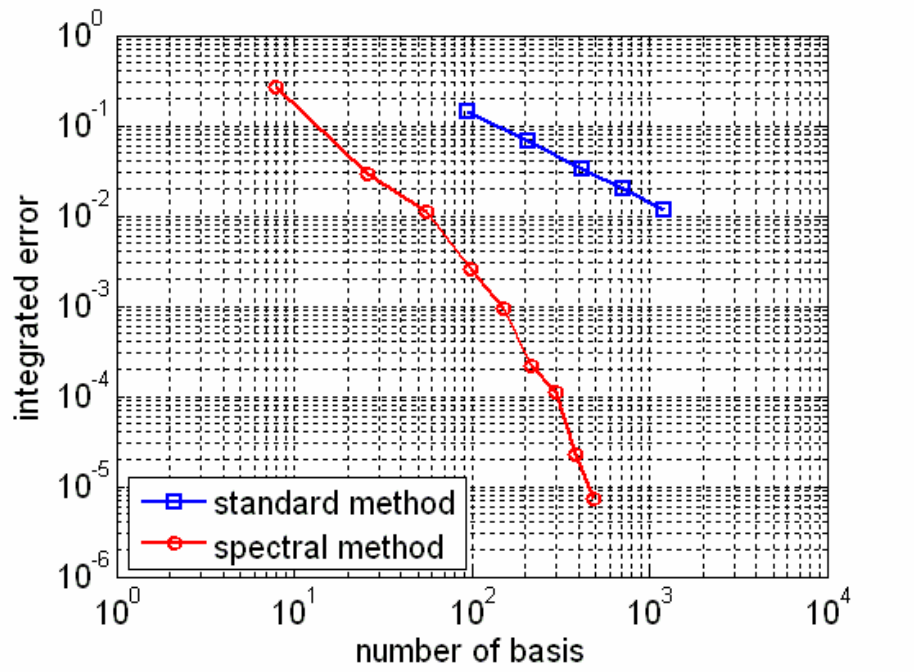
Project Staff
S.-H. Kuo, J. White

Sponsors

When boundary element methods are used to solve Laplace or Helmholtz problems associated with complicated three-dimensional geometries, a piecewise constant basis on a triangular mesh is typically used to discretize the associated integral equation:

$$\varphi(\vec{r}) = \int_{\Omega} G(\vec{r},\vec{r}\,')\sigma(\vec{r}\,')dS'$$

where $G(\vec{r},\vec{r}\,')$ is Green's function (e.g. $1/|\vec{r}-\vec{r}\,'|$, $e^{k|\vec{r}-\vec{r}\,'|}/|\vec{r}-\vec{r}\,'|$) and Ω is the surface boundary of a three-dimensional region of interest on which one would like to solve for the unknown quantity σ given an arbitrary φ. However, piecewise-constant bases are low order, and therefore large numbers of unknowns are needed to achieve high accuracy. In this research, a spectrally accurate approach is proposed for analyzing molecular surfaces described by a collection of surface points. The method is a synthesis of several techniques, starting by generating a high order spherical harmonic surface representation using least-squares fitting to the given points. Then this analytic representation is used to construct a map and map Jacobian for a mapping to a cube. A quadrature scheme is used to generate an orthogonal basis on the rectangular cube surfaces, and a change of variables is used to desingularize the required integrals of products of basis functions and Green's function. Finally, an efficient method for solving the discretized system using a matrix-implicit scheme is developed. Figure 1 demonstrates convergence behaviors of the standard method and the proposed method. More details and computational results can be found at [1, 2].



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12. Robust Parameterization of Biological Networks

Sponsors
NIH Integrated Cancer Biology Program, Singapore-MIT Alliance

Project Staff
B. S. Kim, J. K. White

As biological systems are being increasingly investigated from the networks point of view, there is an escalated demand for computational models that quantitatively characterize those systems. As is the case with modeling any system, accurate and precise models that can both represent and predict their respective biological systems' behaviors are desired.

An essential task in building such a model involves effective calibration of the parameters that define the model. With respect to biological systems, which are often modeled using differential equations derived from the chemical reactions that take place within the systems (basic illustration provided in Figure 1 below), the task entails finding reaction rates (such as k_1 and k_2 in Figure 1) or initial conditions that lead to outputs that match experimental measurements.

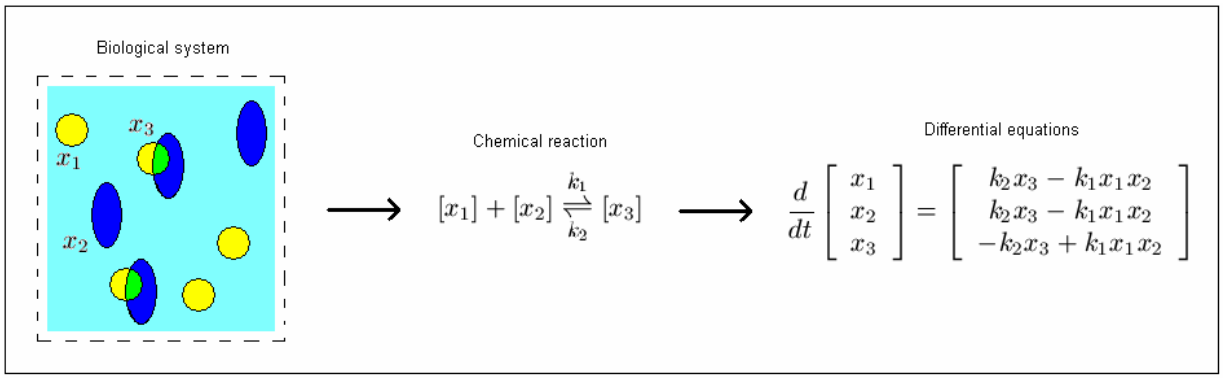

Figure 1: Basic illustration of modeling a biological system with differential equations.

A major barrier to successful calibration is the limited amount of available experimental data, rising from the irreplaceable and unsteady nature of biological systems. This leads to the existence of multiple possible sets of parameters that could potentially result in outputs that match the data. We explore robust optimization to develop computational methods that would enable us to select out the correct parameter set among the many, with the goal of being able to perform the task without the need for qualitative system-specific information.

Research thus far has been conducted primarily in the context of signaling pathways, including the mitogen-activated protein kinase and Fas signaling pathways.

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