Computational Prototyping Group

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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 areas of model-order reduction, fast methods for solving integral equations, and efficient algorithms for coupling differential equation solution with robust optimization. The applications we are currently using to drive our methodological efforts include design tools for: integrated circuits, electrical interconnect, nanophotonic structures, micro- and nano-devices, aircraft, and biomolecules. We describe these activities in more detail in the sections below.

1. Fast Solver Development for 3-D Nanophotonics

Sponsors
Defense Advanced Research Projects Agency, MARCO Interconnect Focus Center

Project Staff
J.H. Lee, L. Zhang, S. Johnson, and J. White

Fast integral equation solvers seem to be ideal approaches for simulating 3-D nanophotonic devices, as these devices generate fields in both an interior channel and in the infinite exterior domain. However, many devices of interest, such as ring resonators or optical couplers, have channels that can not be terminated without generating numerical reflections. Generating absorbers for these channels is a new problem for integral equation methods, as integral equation methods were initially developed for problems with finite surfaces. We have demonstrated that the obvious approach for eliminating reflections, making the channel mildly conductive outside the domain of interest, is quite inaccurate. Instead, we developed a new method which uses a gradually varying surface conductivity to act as an absorber. Experiments are presented to demonstrate that this new method is orders of magnitude more effective than a volume absorber, and is easily incorporated in an fast integral equation solver. Results below from a prototype implementation demonstrate the several orders of magnitude improvement in absorption.

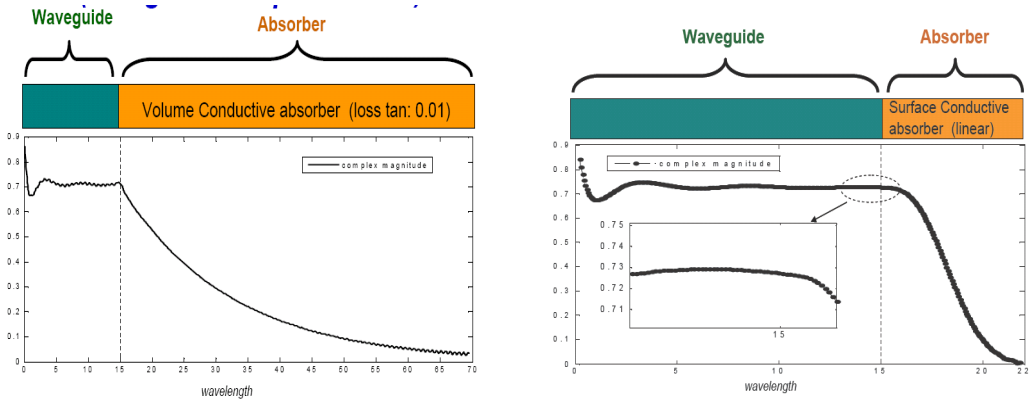

Figure: On the left is a graph of the complex magnitude of the steady-state light in a photonic waveguide computed using a standard long volume absorber, and on the right is the same computation using our new surface absorber. Notice that the oscillation in amplitude near the absorber is much smaller in the surface absorber case. Computation reveals that the new absorber reduces reflected power more than four orders of magnitude better than volume absorbers.

2. New Results for Linear and Nonlinear Reduction Methods

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

Project Staff
D. Vasilyev, J. H. Lee, X. Song, J. White

Finding reliable methods for automatically extracting low-order dynamically-accurate models from detailed physical simulation is becoming increasingly important as designers attempt to investigate the system impact of emerging technology. We have been developing methods for extracting such models from PDE-based descriptions, a challenging problem because spatially discretized PDE's generate systems with millions of states, but the extracted model of the system should be reduced to a few dozen states. Recently, we developed a new linear model order reduction method, one that 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. The application of the modified AISIAD method to bioMEMS devices was studied, and a particularly interesting example was a problem of electro-osmotic flow in a microfluidic channel. We considered injection of a (marker) fluid into such system We have found that this wave-like problem could be easily reduced using the modified AISIAD method.

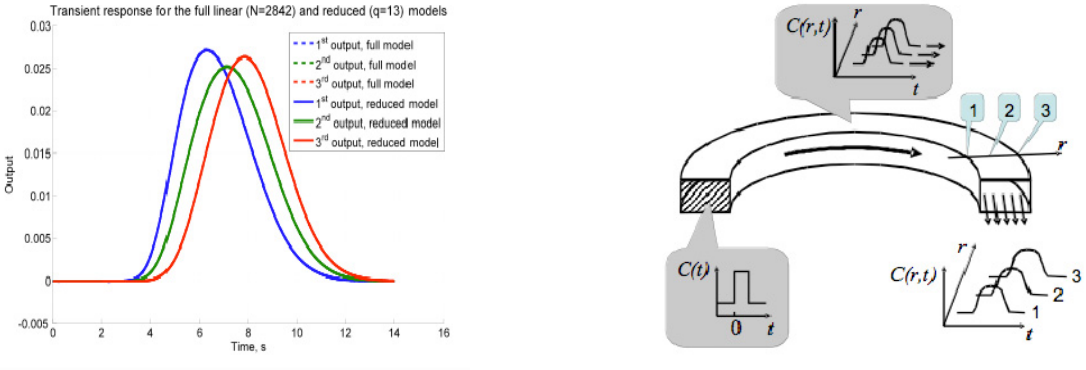

Figure: Results using ASAID-based model reduction to generate a 13-state model of a microfluidic channel described by a discretized 3-dimensional time-dependent convection-diffusion equation. The reduced model correctly captures the dispersion and spatial distribution of a pulse of injected marker in to the channel.

3. 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):

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

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

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.

4. Efficient tools for analyzing cell motions in microfluidic devices

Sponsors
Singapore-MIT Alliance (SMA)

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

In air-packaged surface micromachined devices and microfluidic devices the surface to volume ratio is such that drag forces play a very important role in device behavior and performance. Especially for surface micromachined devices, the amount of drag is greatly influenced by the presence of the nearby substrate. In this thesis precorrected FFT accelerated boundary element method specialized for calculating the drag force on structures above a substrate is presented. The method uses the Green's function for Stokes flow bounded by an infinite plane to implicitly represent the device substrate, requiring a number of modifications to the precorrected FFT algorithm. To calculate the velocity due to force distribution on a panel near a substrate an analytical panel integration algorithm was developed. Computational results demonstrate that the use of the implicit representation of the substrate reduces computation time and memory while increasing the solution accuracy. The results also demonstrate that surprisingly, and unfortunately, even though representing the substrate implicitly has many benefits it does *not* completely decouple discretization fineness from distance to the substrate. To calculate the dynamic behavior of micromechanical and microfluidic systems, a stable velocity implicit time stepping scheme coupling the precorrected FFT solver with rigid body dynamics was introduced and demonstrated. The ODE library was integrated with the solver to enable the simulation of systems with collisions, contacts and friction. Several techniques for speeding up the calculation of each time step were presented and tested. The time integration algorithm was successfully used to simulate the behavior of several real microfluidic devices.

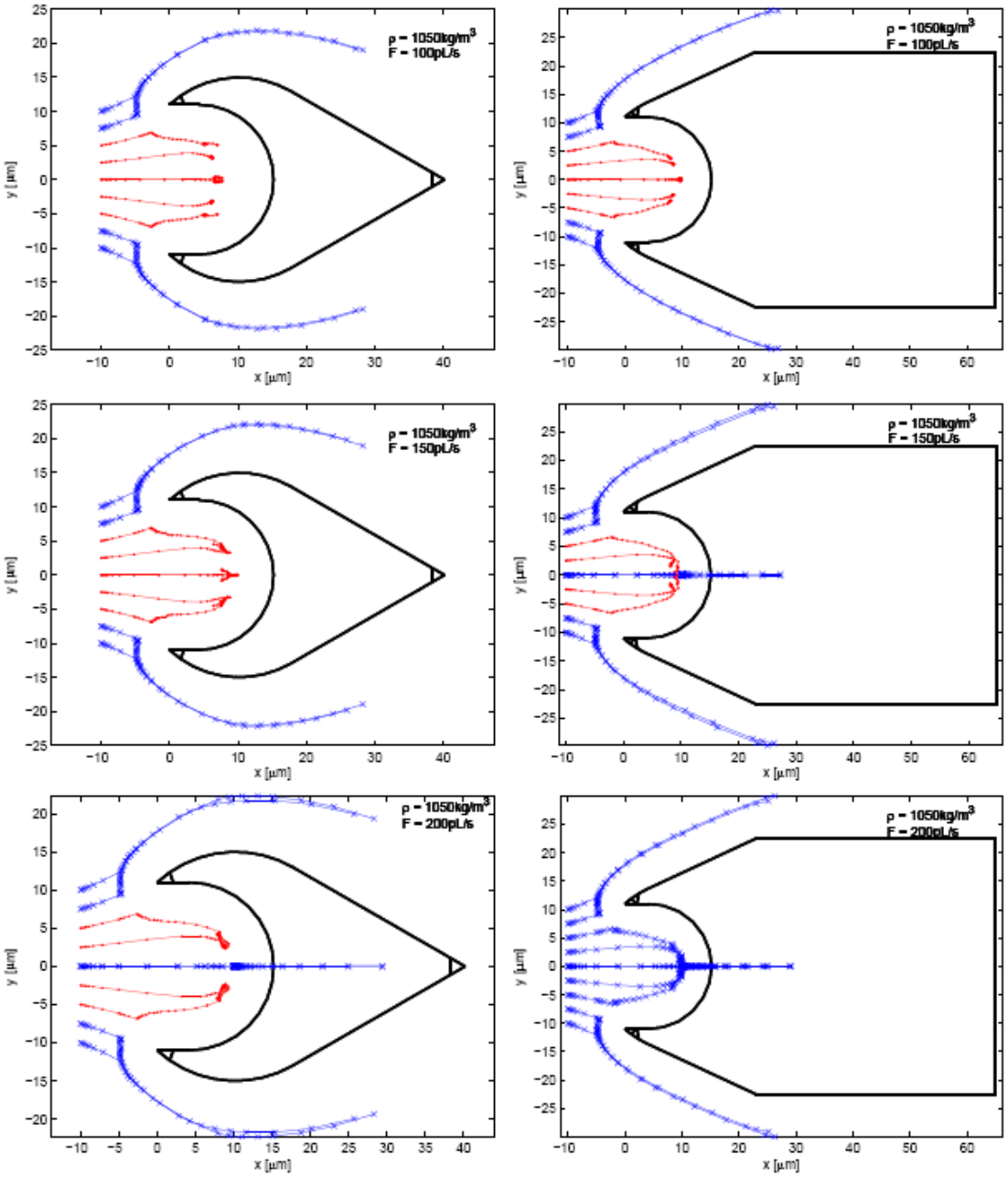

Figure: Characterization of the trapping region for pachinko trap model 1, on the left, and pachinko trap model 4, on the right. The curves in red, with the dot marker, represent situations where the bead was trapped; the curves in blue, with the cross marker, represent situations where the bead was not captured.

5. 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.

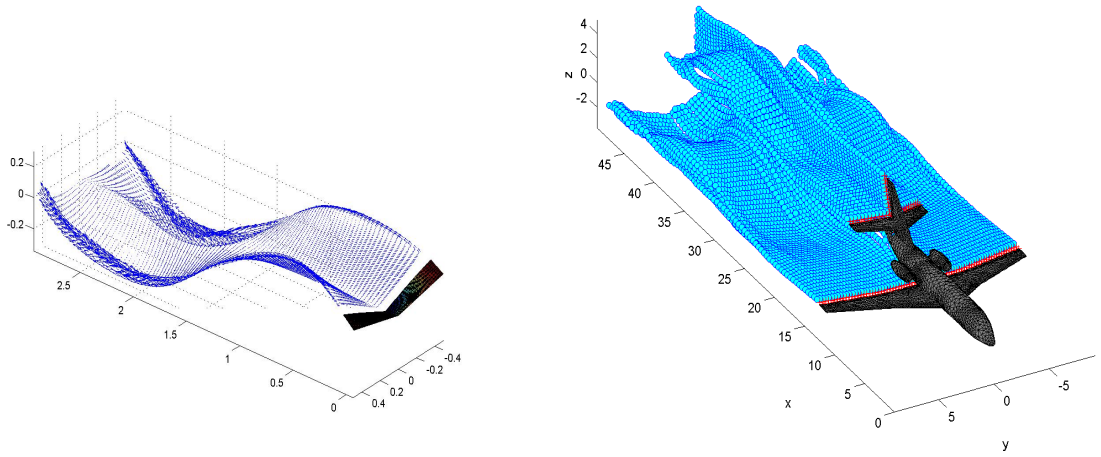

Figure: The above figures illustrate the combined boundary element method-vortex particle method approach for solving complex unsteady flows. The vortex particle representation of the lifting surface trailing vorticity is shown. The image on the left illustrates a flapping wing geometry, while the image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

6. Modeling Nanoscale Effects using Fast Integral Equation Methods

Sponsors
MARCO Interconnect Focus Center

Project Staff
H. Reid, S. Johnson, 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 $C_G \approx 3.2$ aF, to be compared with the experimentally estimated value of 4.3 aF.

For nanoscale structures, it is known that quantum fluctuations in the electromagnetic field can produce an attractive force between electrically neutral conductors, a force known as the Casimir force. For nanoscale devices, this force can become significant, but there are no reasonably efficient tools for computing these forces on arbitrary geometries. We have been working on a fast solver for computing Casimir forces. Our new method is orders of magnitude faster than the FDTD methods that have been applied to this problem, and we are now working on making the method more numerically reliable. In particular, the approach used in our method solves integral formulations of Maxwell's equations at imaginary frequencies, and reliably evaluating integrals for the exponentially decaying kernels associated with imaginary frequencies over a range of wavelengths has proved challenging.

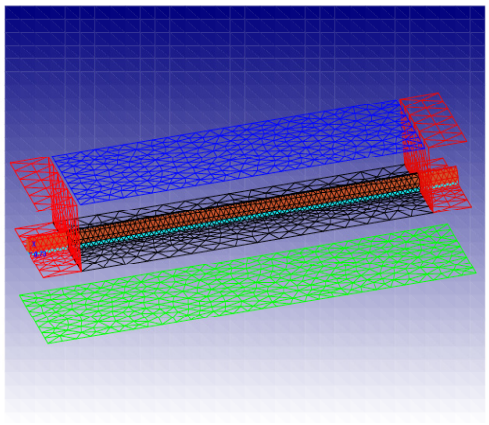

Figure 1. Discretized geometry of a 50-nm dualgate CNTFET. Green panels: bottom gate. Cyan panels: Si02–air interface. Black panels: High- K dielectric interface. Red panels: Source/Drain metallization. Blue panels: Top gate. Orange panels: Carbon nanotube. Note that our discretization accurately captures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

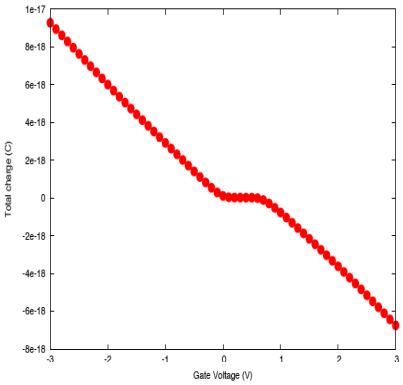

Figure 2. Total charge on nanotube surface versus gate voltage for a 50-nm dual-gate CNTFET. From this plot we estimate a total gate capacitance of 3.2 aF.

7. Numerical Methods for Biomolecule Electrostatic Analysis and Optimization

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

Project Staff
J. Bardhan, S. Kuo, M. Altman, B. Tidor, J. White

We developed a PDE-constrained approach to optimizing the electrostatic interactions between two biomolecules. These interactions play important roles in the determination of binding affinity and specificity, and are therefore of significant interest when designing a ligand molecule to bind tightly to a receptor. Using a popular continuum model and physically reasonable assumptions, the electrostatic component of the binding free energy is a convex, quadratic function of the ligand charge distribution. Traditional optimization methods require exhaustive pre-computation, and the expense has precluded a full exploration of the promise of electrostatic optimization in biomolecule analysis and design. We developed an approach in which the electrostatic simulations and optimization problem are solved simultaneously; unlike many PDEconstrained optimization frameworks, the proposed method does not incorporate the PDE as a set of equality constraints. This co-optimization approach can be used by itself to solve unconstrained problems or those with linear equality constraints, or in conjunction with primal–dual interior point methods to solve problems with inequality constraints. Model problems demonstrate that the co-optimization method

is computationally efficient and that it can be used to solve realistic problems.

For use in the co-optimization, we also developed a boundary-element method (BEM) implementation for accurately solving problems in biomolecular electrostatics using the linearized Poisson-Boltzmann equation. Motivating this implementation is the desire to create a solver capable of precisely describing the geometries and topologies prevalent in continuum models of biological molecules. This implementation is enabled by the synthesis of four technologies developed or implemented specifically for this work. First, molecular and accessible surfaces used to describe dielectric and ion-exclusion boundaries were discretized with curved boundary elements that faithfully reproduce molecular geometries. Second, we avoided explicitly forming the dense BEM matrices and instead solved the linear systems with a preconditioned iterative method (GMRES), using a matrix compression algorithm (FFTSVD) to accelerate matrix{vector multiplication. Third, robust numerical integration methods were employed to accurately evaluate singular and near-singular integrals over the curved boundary elements. Finally, we developed a general boundary-integral approach capable of modeling an arbitrary number of embedded homogeneous dielectric regions with differing dielectric constants, possible salt treatment, and point charges. A comparison of the presented BEM implementation and standard finite-difference techniques demonstrates that for certain classes of electrostatic calculations, such as determining absolute electrostatic solvation and rigid-binding free energies, the improved convergence properties of the BEM approach can have a significant impact on computed energetics. We also demonstrated that the improved accuracy offered by the curved-element BEM is important when more sophisticated techniques, such as non-rigid-binding models, are used to compute the relative electrostatic effects of molecular modifications. In addition, we show that electrostatic calculations requiring multiple solves using the same molecular geometry, such as charge optimization or component analysis, can be computed to high accuracy using the presented BEM approach, in compute times comparable to traditional finite-difference methods.

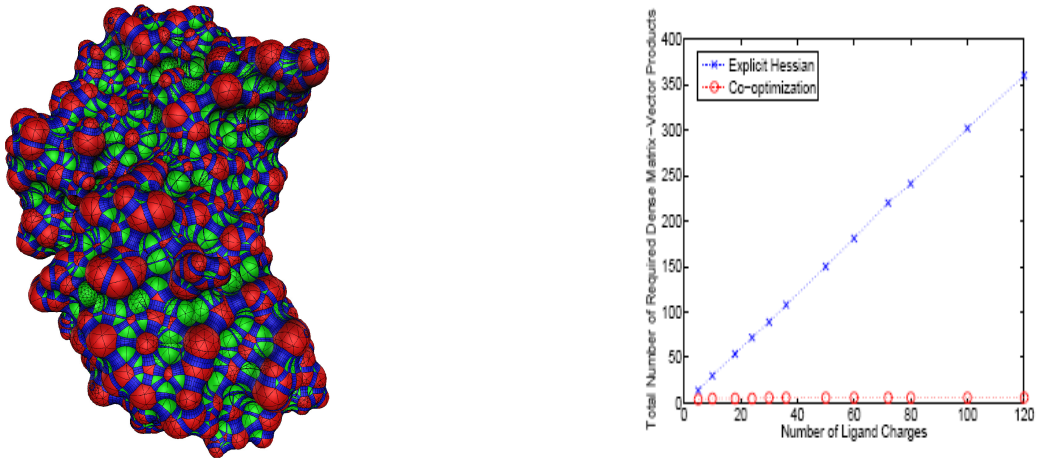

Figure: On the left is the molecular surface of the Barnase-Barstar receptor-ligand complex easily analyzed with our new fast solver, and on the right is a graph comparing the computational cost of explicit-Hessian versus our new co-optimization approach. Note that the cost of the co-optimization approach scales very slowly with the number of ligand charges, and can be orders of magnitude faster than the explicit-Hessian approach for problems with as few as several hundred ligand charges.

8. Higher Order Methods for Analyzing Molecular Surface Electrostatics

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

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

Electrostatic analysis involving complicated molecular surfaces arise in a number of nanotechnology applications including: biomolecule design, carbon nanotube simulation, and molecular electron transport. Molecular surfaces are typically smooth, without the corners common in electrical interconnect problems, and are therefore candidates for methods with higher order convergence. We developed and demonstrated a spectrally accurate integral equation method for electrostatic analysis of problems with molecular surfaces, where the surface is described using only a collection of surface points; that is, without resorting to generating a mesh. The entire method is a synthesis of a number of techniques including: spherical harmonic surface interpolation, spectral-element-like integral equation discretization, integral desingularization via variable transformation, and matrix-implicit iterative matrix solution. The spectral accuracy of this combined method is verified using analytically solvable sphere and ellipsoid problems, and then demonstrated numerically by solving capacitance and coupled Poisson/Poisson-Boltzmann problems associated with a molecule in solution. The results demonstrate that for a tolerance of 0.1%, this new approach reduces the number of unknowns by as much as two orders of magnitude over the more commonly used flat panel methods.

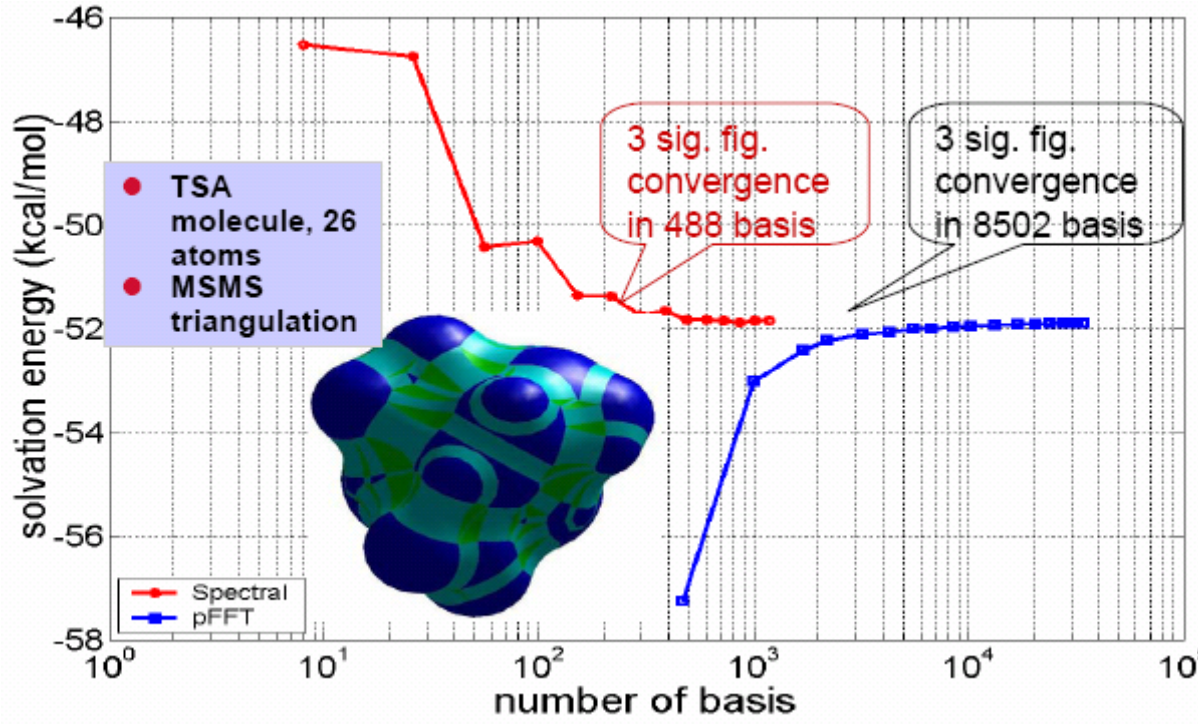

Figure: The graph above demonstrates that for a TSA molecule (whose molecular surface is shown in the lower left corner of the graph), our new higher-order method reduces, by a factor of nearly 20, the number of unknowns required to achieve 0.1% accuracy in the computed electrostatic contribution to solvation energy.

9. Robust Parameterization of Biological Networks

Sponsors
NIH Integrated Cancer Biology Program, Singapore-MIT Alliance

Project Staff
B. S. Kim, B. Tidor, 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.

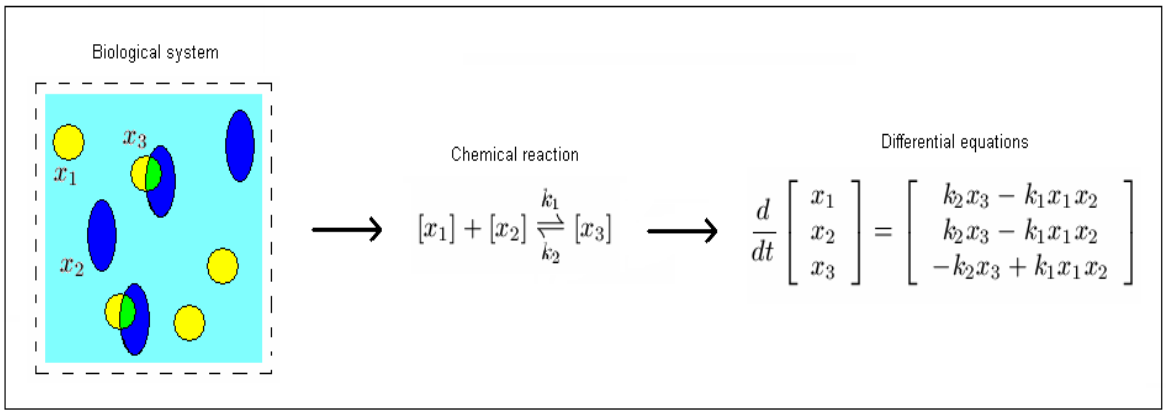

Figure: Basic illustration of modeling a biological system with differential equations.

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.

10. FastMaxwell: A Fast Impedance Extraction Solver for 3D Conductor Structures over Substrate

Sponsors
Semiconductor Research Corporation, MARCO-Interconnect Focus Center

Project Staff
T. Moselhy, X. Hu, L. Daniel

Interconnect-aware timing analysis and mixed-signal simulation rely on tools for extracting accurate low-order models for interconnect electrical behavior. Models should be physics-based to enable efficient modeling of 2D and 3D effects on interconnects with their statistics and variations. As a first step toward our goal we have been focusing on the development of a very efficient 3D parasitic extractor for the deterministic analysis of a large collection of interconnects. FastMaxwell, is a program for wideband electromagnetic extraction of complicated 3D conductor structures over substrate. It is based on the integral domain mixed potential integral equation (MPIE) formulation, with a 3D full-wave substrate dyadic Green's function kernel. Two dyadic Green's functions are implemented: a traditional Green's function and an alternative Green's function that can lead to computational cost reduction in most practical applications. Most importantly, the alternative

Green's function allows the use of dipoles (i.e., filaments) in arbitrary orientations, and it helps providing symmetric positive semidefinite matrices, hence facilitating the passive model order reduction of distributed systems. The pre-corrected Fast Fourier Transform (pFFT) algorithm has been extended and optimized to accelerate the fullwave substrate Green's function within FastMaxwell.

The accuracy and efficiency of FastMaxwell and the implemented acceleration algorithms have been verified against measurements of fabricated devices by a variety of examples, some as large as 100,000 unknowns, using less than 400MB of memory and a few hours of computation time. The pFFT computational complexity of O(N log N) in overall solver time and O(N) in memory usage has been observed from our results, leading to a scalable software for very large collection of interconnects.

FastMaxwell is public domain and can be downloaded at: http://www.rle.mit.edu/cpg/fastmaxwell

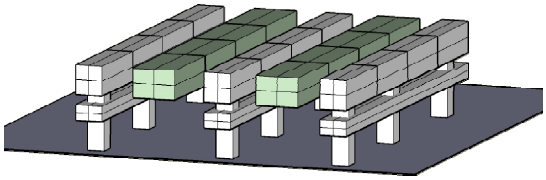

Figure 1: FastMaxwell discretization of a two-wire transmission line on top of a substrate and shielded by a 3D cage structure. The cage is connected to ground through vertical vias. (Figure is rescaled and edited for clarity.)

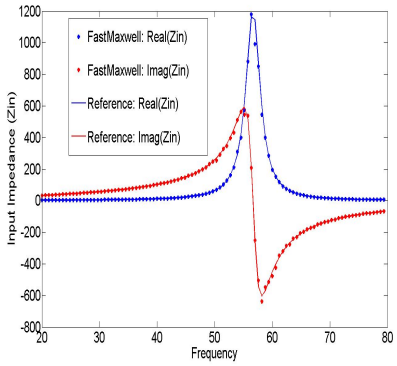

Figure 2: Real and imaginary components of the input impedance of a two-wire transmission line. Results obtained by FastMaxwell are within 2% of those obtained by reference simulator IE3D.

11. A Stochastic Integral Equation Solver for Efficient Variation-aware Interconnect Extraction

Sponsors
MARCO-Interconnect Focus Center, Cadence Design Systems.

Project Staff
T. Moselhy, L. Daniel.

On-chip and off-chip fabrication processes may typically generate interconnect structures of irregular geometries. Such irregularities are not deterministic, and are produced by several different manufacturing steps such as etching, chemical mechanical polishing (CMP), electro-deposition, and photolithography. However, as a result of technology scaling, such manufacturing uncertainties are now beginning to play a major role in determining the electrical characteristics of the interconnect structures. Consequently, variation-aware interconnect extraction is becoming increasingly important.

In this research we have developed a new methodology to solve large stochastic linear systems typically appearing during variation aware extraction. We have derived a new theorem to compute the coefficients of the multivariate Hermite expansion using only low dimensional integrals, resulting in a time complexity that is independent of the number of variables and only dependent on the order of the expansion. Practically speaking, for a typical large multivariate expansion the new theorem provides an improvement in the computation time by 86 orders of magnitude as compared to the standard tensor product rule, or by 10 orders of magnitude as compared to the state of the art (Monte Carlo integration or sparse grid integration). Such a theorem is not only useful for our methodology but it can also be applied to any algorithm that relies on expanding a random process, such as the stochastic finite element method (SFE). We have also provided a new stochastic simulation technique by merging both the Neumann expansion and the polynomial chaos expansion. The main advantages of the resulting technique are the compact size of the system at any time (unlike SFE) and the ease of calculating the statistics of the high order terms (unlike Neumann expansion). In addition, the new simulation algorithm is parallizable and can therefore take advantage of the state of the art in processor design. We have demonstrated the computational efficiency of the new methodology by solving problems that were completely intractable before. We have demonstrated that our algorithm can be used to compute the complete probability density function of the input impedance of very large problems (up to 400 random variables) in less then 8 hours using Matlab on a standard 4-core machine and using only 121MB RAM.

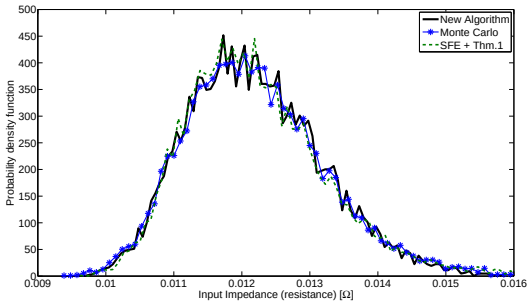

Figure 1: Comparison between the probability density function of the microstrip line obtained from our new algorithm and the reference Monte Carlo simulation.

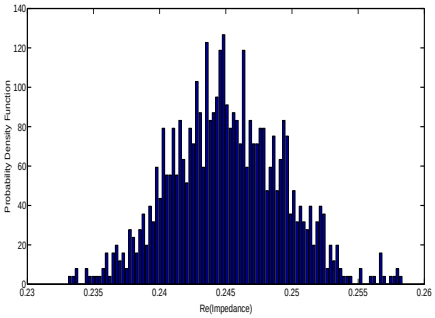

Figure 2: Probability density function of the real part of the input impedance at 1GHz for correlation length Lc = 50μm. The resistance of the non-rough surface is 11.3% smaller than the mean of the obtained distribution.
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12. A Quasi-Convex Optimization Approach to Parameterized Model Order Reduction of Linear Dynamical Systems

Sponsors
MARCO Interconnect Focus Center

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

In this project 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.

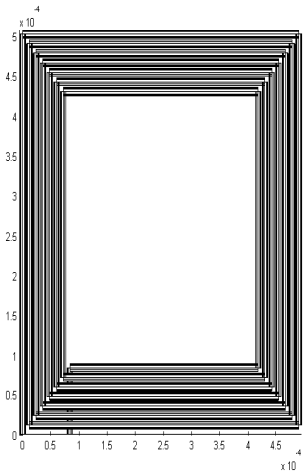


Figure 1: 7 turn RF inductor for which a parameterized (with respect to wire width and wire separation) reduced model has been constructed.

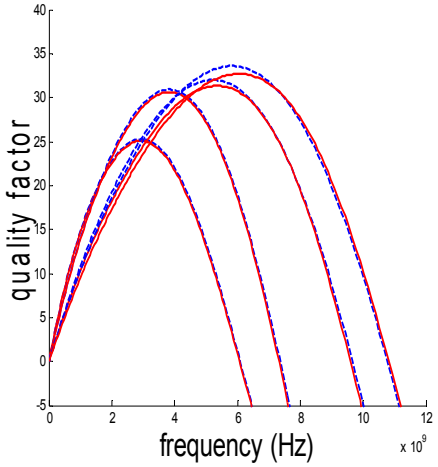


Figure 2: Matching of quality factor of 7 turn RF inductor when wire width = 16.5 um, wire separation = 1,5,18,20 um. Blue: Full model. Red: ROM.

13. A Piecewise-Linear Moment Matching Approach to Parameterized Model Order Reduction for Highly Non-Linear Dynamical Systems

Sponsors
National Science Foundation

Project Staff
B. Bond, L. Daniel

The automatic extraction of parameterized macromodels for modern mixed signal System-on-Chips is an extremely challenging task due to the presence of several nonlinear analog circuits and Micro-Electro-Mechanical (MEM) components. The ability to generate Parameterized Reduced Order Models (PROM) of nonlinear dynamical systems could serve as a first step toward the automatic and accurate characterization of geometrically complex components and subcircuits, eventually enabling their synthesis and optimization.

Our approach to this problem combines elements of a non-parameterized trajectory piecewise linear method for nonlinear systems with a moment matching parameterized technique for linear systems. By building on these two existing methods, we have created an algorithm 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.

In addition, we have proposed a model-construction procedure in which we approximate the system sensitivity to parameters of interest for the purpose of efficiently sampling important regions of the parameter space. 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 at several parameter values.

Typical PROMs constructed in this manner can be accurately reduced in size by a factor of 10 yielding a speedup of a factor of 10 in general. For further details on parameter-space accuracy and cost of the algorithms see.

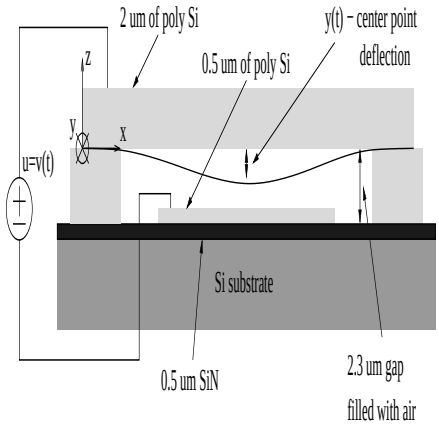


Figure 1: Application example: MEM switch realized by a polysilicon beam fixed at both ends and suspended over a semiconducting pad and substrate expansion.

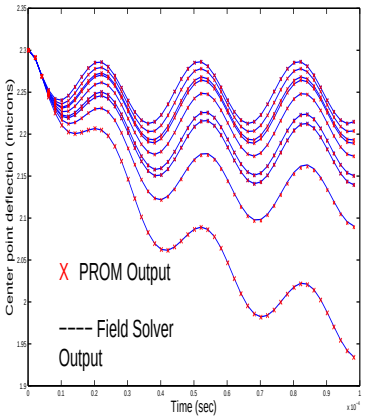


Figure 2: Center point deflection predicted by our parameterized reduced model (crosses) at a series of parameter values, compared to a finite difference detailed simulation (solid lines).

14. Preserving Stability in Model-Order Reduction for Highly Non-Linear Dynamical Systems

Project Staff
B. Bond, L. Daniel

The ability to generate accurate reduced-order models (ROMs) of nonlinear dynamical systems, such as analog circuits and micro-electro-mechanical systems (MEMS), is a crucial first step in the automatic design and optimization of such systems. One popular approach to model order reduction (MOR) of highly nonlinear systems employs trajectory-based methods, such as the piecewise-linear (PWL) approach. Despite substantial recent interest in such methods, trajectory-based models (TBMs) have failed to gain widespread acceptance due to a lack of theoretical statements concerning the accuracy of the resulting ROMs. In this work we address one such theoretical issue – guaranteed stability. Specifically, we present a scheme for preserving stability in PWL models whose system matrices possess a certain structure. We also propose a projection scheme and set of weighting functions, which together allow us to extend some of these stability results to systems composed of arbitrary unstructured matrices.

The stability of nonlinear systems is determined by the existence of a Lyapunov function. Our stabilizing scheme ensures stability by constructing the projection matrices such that there exists a Lyapunov function for the resulting ROM. In the case where a system's Jacobians all possess a certain structure, we present a projection routine that guarantees the existence of a quadratic Lyapunov function for both the large PWL model and the In the case where the system's Jacobians have no structure, and it is not known whether a Lyapunov function exists for the large model, we

utilize a new nonlinear projection and new set of interpolation functions to create a collection of stable nonlinear systems. The final ROM will switch between the various stable nonlinear One example of a system that produces unstructured Jacobians, and thus potentially unstable TBMs, is a MEMS switch. The Figure below shows a sample output from the MEMS switch, a stable TBM generated by our approach, and an unstable TBM generated by the traditional approach.

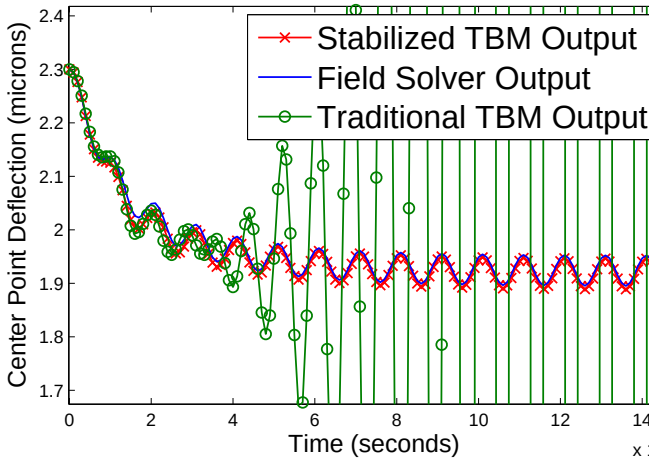
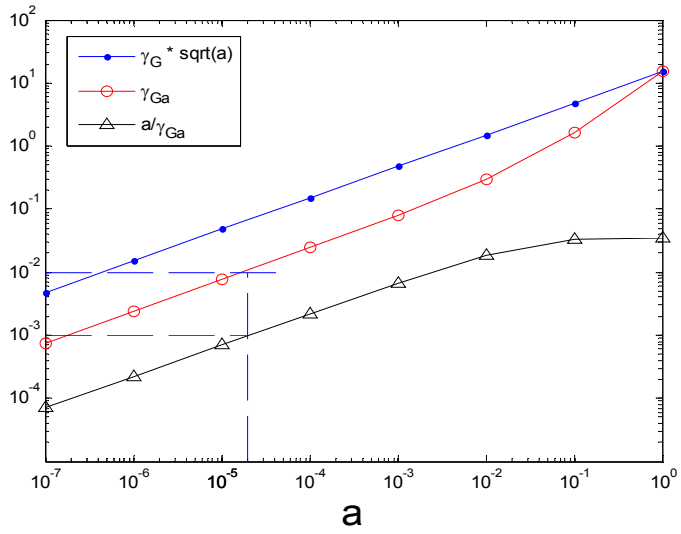


Figure 3: Center point deflection predicted by our stabilized reduced model (red crosses), compared to a finite difference detailed simulation (solid blue lines) and the traditional TBM approach (green circles).

15. Bounding L2 Gain System Error Generated by Approximations of the Nonlinear Vector Field in Model Order Reduction of Non-Linear Dynamical Systems

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

Typical nonlinear model order reduction approaches need to address two issues: reducing the order of the model, and approximating the vector field. In this project we focus exclusively on the second issue, and seek results characterizing the repercussions at the system level of vector field approximations. The error assessment problem is formulated as the L2 gain upper bounding problem of a scaled feedback interconnection. Applying the small gain theorem in the proposed setup, we prove that the L2 gain of the error system is upper bounded by the L2 gain of the vector field approximation error, provided it is small. In addition, in this project with have developed a numerical procedure, based on the IQC/LMI approach, to perform the error estimation task with less conservatism. A example is given below to demonstrate the practical implications of the presented results.



In this figure, the uppermost line (dots) represents the theoretical upper bound for the example considered. The middle line (circles) is used as the upper bound for the L2 gain of error system. The bottom line (triangles) is the quantity determines the maximum vector field error in order for the small gain theorem to hold. Figures of this type can easily be produced by our theoretical error bound and numerical procedure, and can be used to identify the maximum allowable nonlinear vector field error for a specific system error before any simulation is performed.

16. Convex Relaxation Approach to the Identification of the Wiener-Hammerstein Model for Modeling of Non-Linear Analog Circuit Blocks

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

Analog and mixed/signal VLSI circuits exhibit an ever-increasing and pressing need for automatic and accurate characterization of their non-linear components and subcircuits, in order to enable synthesis and optimization. While non-linear model order reduction has already been attempted using several types of clever linearizations or parametric approximation, in this project we are instead attempting a completely orthogonal approach. Specifically, this work proposes an input/output system identification technique for the Wiener-Hammerstein model and its feedback extension. In the proposed framework, the identification of the nonlinearity is non-parametric. The identification problem can be formulated as a non-convex quadratic program (QP). A convex semi-definite programming (SDP) relaxation is then formulated and solved to obtain a sub-optimal solution to the original non-convex QP. The convex relaxation turns out to be tight in most cases. When the relaxation idea is combined with the use of local search, high-quality solutions to the Wiener-Hammerstein identification can frequently be found. We identify randomly generated Wiener-Hammerstein models as examples of the application. Furthermore, we are attempting to use our method to identify small analog circuit blocks such as operational amplifiers. This work has been accepted for publication and will be presented at the Conference on Decision and Control in December 2008.

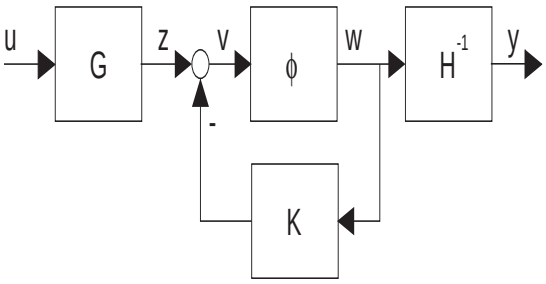


Figure 1: Wiener-Hammerstein Model to be identified.

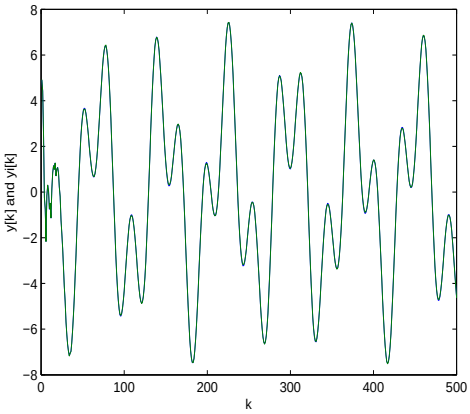


Figure 2: Matching of outputs of the original system and the identified system.

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