Computational Prototyping

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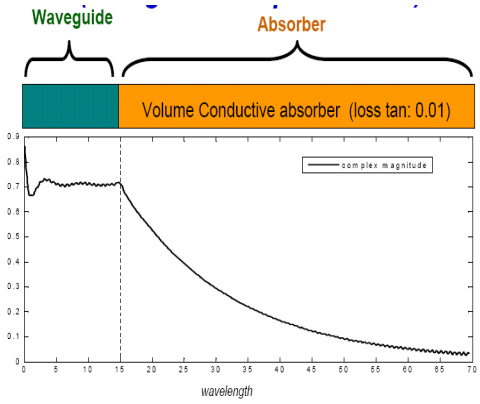
Group Summary
Our research group uses several engineering design applications to drive research in simulation modeling and optimization algorithms and software. Recent efforts have focused specifically in the areas of compact dynamical modeling, fast methods for solving deterministic and stochastic integral equations, and efficient algorithms for coupling differential equation solution with robust optimization. The applications we are currently using to drive our methodological efforts include: analog/mixed-signal/RF/microwave integrated circuits, electrical interconnect, micro-electro-mechanical devices, nano-photonic structures, nano-fluidic devices, aircraft, magnetic resonance imaging, the human cardiovascular system, biomolecules and biological networks. We describe these activities in more detail in the sections below.

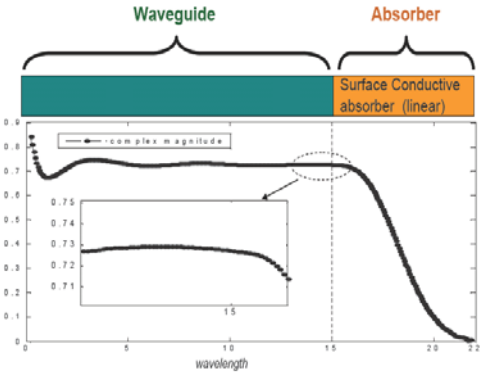
1. Fast Solver Development for 3-D Nanophotonics

Sponsors
Defense Advanced Research Projects Agency, MARCO Interconnect Focus Center, Singapore-MIT Alliance

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.





2. Continuum Modeling of Nano-fluidic devices for processing Bio-molecules.

Sponsors
Singapore-MIT Alliance (SMA)

Project Staff
P. Van Sang, J. Han, K. Lim, J. White

Modeling nano-scale devices that perform bio-molecular sieving, filtration, or preconcentration is a multi-scale, multi-physics problem, one that demands a collection of computational tools tailored to modeling different layers of complexities of the given problem. In this project we are investigating the effectiveness of modeling biomolecular filters using continuum models of ion transport in fluid. In particular, we are developing efficient numerical techniques for solving the three-dimensional Poisson-Nernst-Planck (or Poisson-Drift-Diffusion) equations combined the Navier-Stokes equation, and then investigating how well the computed solutions predict the behavior of fabricated devices.

3. Efficient Simulation of Micro-fluidic Devices for processing Biological Cells

Sponsors
Singapore-MIT Alliance (SMA)

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

In an ever-widening variety of biological research and medical diagnostic applications, micro-fluidic devices are being used to sort, collect, stimulate, examine, and lyse cells. Optimizing the design of these micro-fluidic devices is proving problematic, as there are few simulation tools capable of quickly analyzing the motion of cells in complicated three-dimensional device geometries.

We have developed a precorrected-FFT based integral equation method for simulating cells in Stokes flow, as Stokes flow is a reasonable model for the fluids at the microscale. Our method uses the Green's function for Stokes flow bounded by an infinite plane, as this implicitly represents the device substrate, thus requiring a number of modifications to the pre-corrected FFT algorithm. To calculate the velocity due to force distribution on a panel near a substrate, an new 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, that even though representing the substrate implicitly has many benefits it does *not* completely decouple discretization fineness from distance to the substrate.

We have used our precorrected-FFT based fast Stokes solver to calculate the dynamic behavior of cells in micro-fluidic devices. In our approach, we modeling the cells as moving rigid bodies, and then using a stable velocity-implicit time integration scheme to compute the cell trajectories. A standard ODE library was combined with the solver to enable the simulation of systems with collisions, contacts and friction. Several techniques were developed to accelerate the time-step computations, and made it possible to simulate candidate cell trap designs (see figure below).

We also developed a second approach to simulating cells in flow, one that can model the fluid with the full incompressible Navier-Stokes equation and can model the deformation of the cell as it moves through the fluid. This second approach uses an efficient immersed boundary that is a combination of an implicit time-integration method with a Jacobian-free Newton-Krylov method (JFNK) to solve the implicit equations at each time-step. The combination is efficient; the implicit time integration method can use larger, and therefore many fewer, time-steps than standard explicit methods, and the Jacobian-free approach avoids the difficulties associated with forming and storing the true Jacobian. Our new approach was validated using an oscillating membrane placed in a still fluid, and then the approach was used to examine both the behavior of capsule membranes in shear flow as well as the large deformation of red blood cells subjected to hydrodynamic stretching forces.

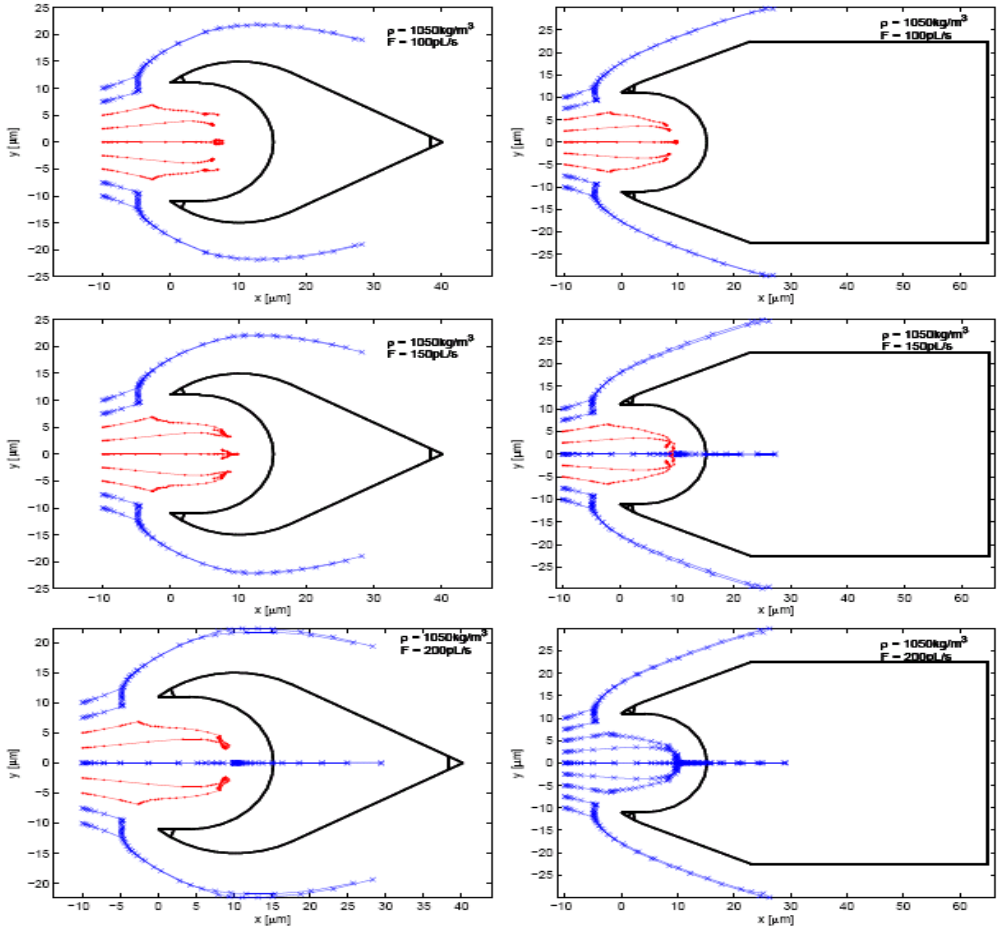


Figure: Characterization of the trapping region for pachinko trap model 1, on the left, and pachinko trap model 4, on the right. The curves in red, with the dot marker, represent situations where the bead was trapped; the curves in blue, with the cross marker, represent situations where the bead was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

4. Fast Methods for Computing Casimir Forces in Complicated 3-D Geometries

Sponsors
Singapore-MIT Alliance, MARCO Interconnect Focus Center

Project Staff
H. Reid, S. Johnson, J. White

Casimir forces, forces between nanometer separated structures due to quantum mechanical effects, were first predicted in the middle of the twentieth century; though the first experimental measurements of Casimir forces are barely a decade old. Since those first experiments, Casimir forces have been measured in wide variety of nano-scale canonical geometries including: plate-plate, sphere-plate, sphere-comb, and cylinder-cylinder configurations. Recent experiments indicate that Casimir forces may be playing a role in existing commercially fabricated micro-electro-mechanical devices (MEMS). As MEMS continue to shrink, it is certain that it will be important to accurately model Casimir forces in the complicated geometries typically associated with these devices.

We developed an efficient technique for computing Casimir energies and forces between arbitrarily complex 3D objects. In contrast to other recently developed methods, our technique easily handles non-spheroidal, non-axisymmetric objects and objects with sharp corners. Using our new technique, we obtained the first predictions of Casimir interactions in a number of experimentally relevant geometries, including crossed cylinders and tetrahedral nanoparticles (see figure below).

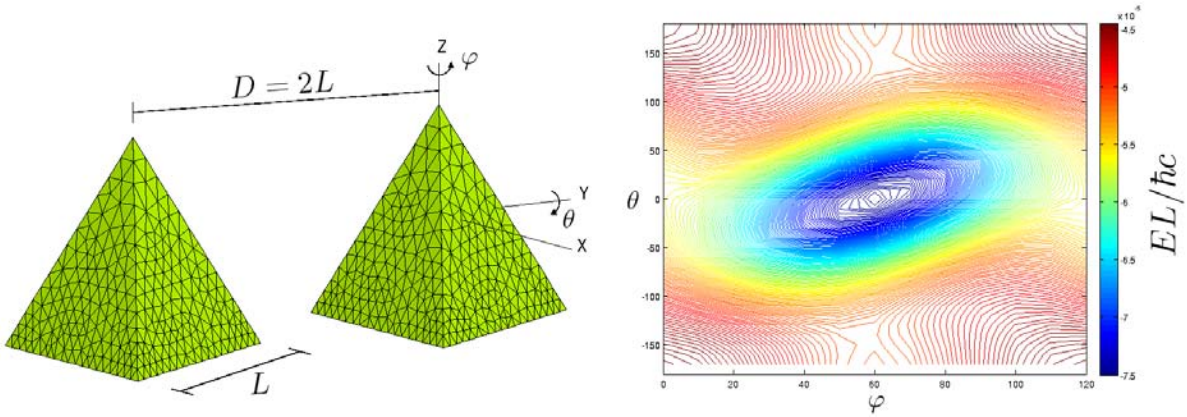


Figure: Contour plot of Casimir energy vs. orientation angles for tetrahedral nanoparticles separated by a distance D = 2L.

5. Numerical Methods for Biomolecule Electrostatic Analysis and Optimization

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

Project Staff
J. Bardhan, 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.

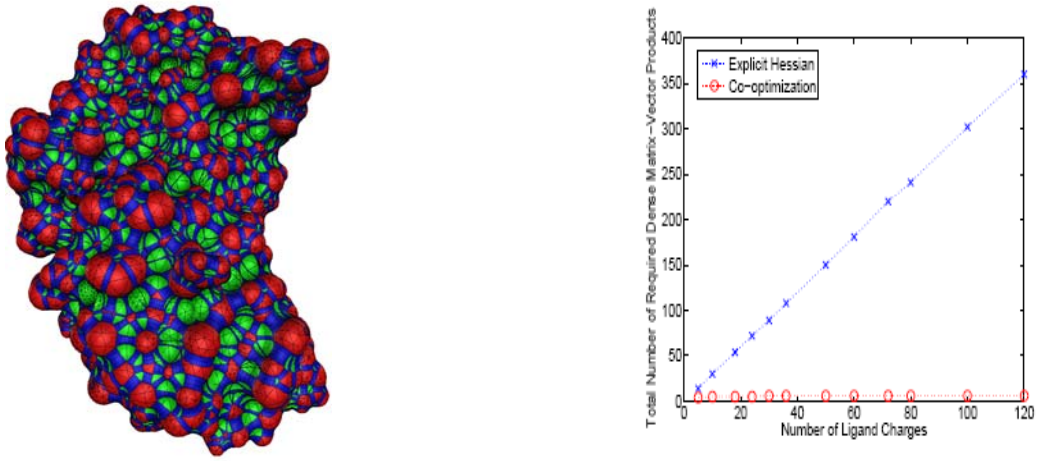


Figure: On the left is the molecular surface of the Barnase-Barstar receptor-ligand complex easily analyzed with our new fast solver, and on the right is a graph comparing the computational cost of explicit-Hessian versus our new co-optimization approach. Note that the cost of the co-optimization approach 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.

6. Mass-Action Kinetics Modeling of Biological Networks

Sponsors

NIH Integrated Cancer Biology Program, Singapore-MIT Alliance

Project Staff

B. S. Kim, J. Wang, Y. Shi, H. Li, H. Hsieu, J. Toettcher, J. Apgar, A. Castillo, B. Tidor, J. K. White

Intra- and inter-cellular biochemical signal transduction and regulation are being increasingly investigated from a system point of view, and there is an escalating demand for computational models that can assist experimentalists in understanding such systems. Developing models that assist in understanding phenomenon such as p53 oscillations in response to DNA damage, synergism between chemotherapy drugs for inducing apoptosis in tumor cells, or the impact of intracellular diffusion in liver fibrosis, require a combination of experimental and computational expertise.

In this project we have been developing mass-action kinetics (MAK) models of the above biological processes as an interdisciplinary activity requiring both biological and numerical expertise. Mass-action kinetics models are differential equations models derived from the chemical reactions that take place within the biological process (basic illustration in the figure below). Developing such models entails determining the species involved in the process of interest, and then determining the reaction rates (such as k_1 and k_2 in Figure 1) or initial conditions that lead to outputs that match experimental measurements.

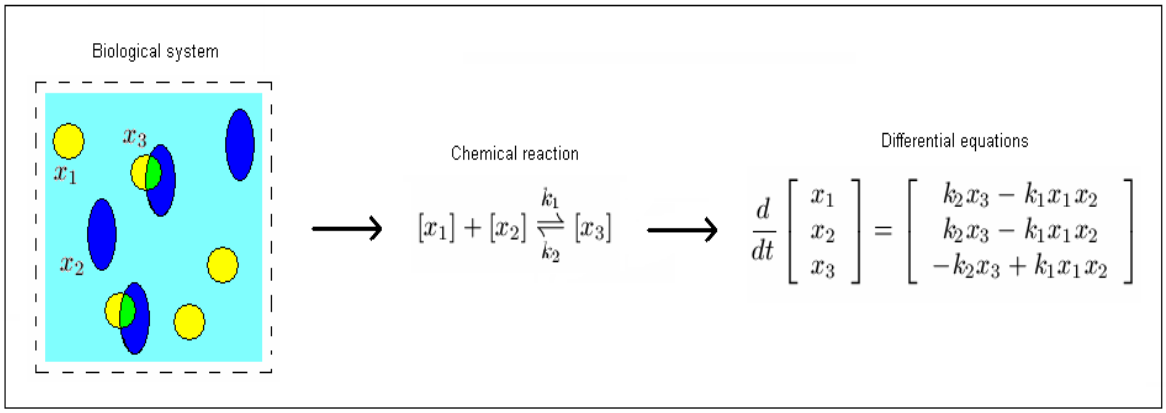


Figure: Basic illustration of modeling a biological system with differential equations.

As difficult as it is to develop MAK models of a process of interest, developing the model is only the first step. Designing experiments and algorithms to calibrate the model, and then developing the numerical techniques to extract insight from the model, are also difficult problems that require considerable numerical expertise. In order accelerate the development of these techniques, we developed an easily extendable Matlab-based software package for analyzing MAK models, Kronecker-Bio. Kronecker-Bio allows users to easily add calibration and analysis techniques, and then share those techniques with others, while still providing impressive computational performance. Using Kronecker-Bio, MAK models with even thousands of species can be analyzed in minutes on a desktop computer.

We are now using the Kronecker-Bio software in a number of applications. We are developing techniques for sensitivity analysis of biochemical oscillators, and investigating the impact of conservation laws in oscillator analysis. We are developing fast simulation techniques for computing single-cell and cell-averaged data. We are also developing approaches for analyzing the impact of extra-cellular diffusion on inter-cellular signaling. Finally, we are trying to decipher what kind of biological insights can be gained by examining species trajectories, ones that are beyond the insights associated with analyzing species steady-states.

7. Verilog-A Implementation of a Physical Semi-Empirical Short-Channel MOSFET Compact Model with Self-Consistent Terminal Currents and Charges

Sponsors
MIT UROP Office, MSD Center, IFC FRCP Center

Project Staff
O. Mysore, D. A.. Antoniadis, L. Daniel

In commercial circuit simulators, behavioral blocks can be specified using Verilog-A, a language designed for describing analog circuits. For the behavioral blocks, the relationships of the currents and voltages at the terminals and internal nodes can be specified using mathematical and logical functions. Compact dynamical models for devices and systems can be described using the mathematical and logical functions. Verilog-A provides a simple method of integrating and simulating within commercial simulators such compact dynamical models as part of complex circuits.

In this project, Verilog-A is used to implement a simple, semi-empirical, charge based, short-channel MOSFET in the commercial simulator, Spectre. The MOSFET model only relies on ten parameters, all of which are physically meaningful, so it is suitable for technology benchmarking and performance projection. To implement the model in Verilog-A, the four terminals corresponding

to the drain, gate, source, and body, plus an internal node are used. The four-terminal model is entirely symmetrical and computes the channel current based on the channel charge at the virtual source as related to the terminal voltages. The internal node was used to determine the displacement currents that flow into the other four terminals due to intrinsic charges associated with them that are calculated by quasi-static equations. Because the model is charge-based, the intrinsic terminal currents equations are automatically consistent with the current equation and the model is charge-conservative. The intrinsic charge displacement currents were determined by differentiating the charge equations in time and fixing the value of the derivative as the current from each terminal to the internal node. A ring oscillator was simulated in Spectre using the Verilog-A implementation of the model for a typical 65 nm CMOS technology. A waveform from this simulation is shown in the figure below. Comparison with a BSIM4.3 of the same technology shows excellent agreement.

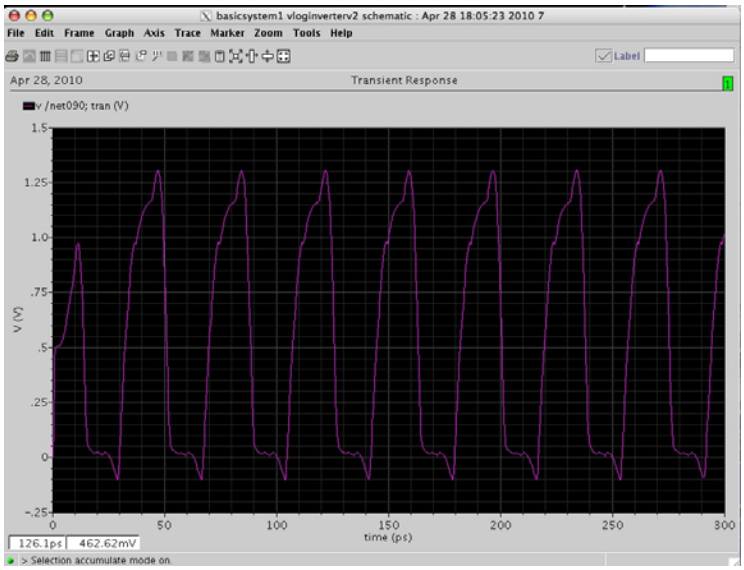


Figure: Waveform produced by the ring oscillator simulated in Spectre using the developed Verilog-A new model.

8. Fast-Caplet: an Efficient 3D Capacitance Solver for Small and Medium Scale 3D VLSI Interconnects Using Instantiable Basis Functions

Sponsors

Semiconductor Research Corporation, FCRP Interconnect Focus Center, Mentor Graphics, Advanced Micro Devices

Project Staff

Y-C. Hsiao, T. A. El-Moselhy, L. Daniel

State-of-the-art capacitance extraction methods for Integrated Circuits (IC) involve scanning 2D cross sections, and interpolating 2D capacitance values using a table lookup approach. This approach is fast and accurate for a large percentage of IC wires. It is however quite inaccurate for full 3D structures, such as crossing wires in adjacent metal layers, or for example comb capacitors. For these cases, electrostatic field solvers are required. Unfortunately standard field solvers are inherently very time-consuming, making them completely impractical in typical IC design flows. Even fast matrix-vector product approaches (e.g. fast-multipole or pre-corrected FFT) have a significant computational overhead and start to scale linearly with the number of conductors only when there are more than several hundreds of wires. In this project we are developing a new 3D extraction field solver that is extremely efficient particularly for the smaller scale extraction problem:

the full 3D structures comprised of ten to one hundred conductors that cannot be handled by the 2D scanning and table lookup approach.

Because of the highly restrictive design rules of today's sub-micro to nano-scale IC technologies, template charge distributions extracted from simple model structures can be reused to instantiate (stretch and combine) basis functions in other realistic complicated geometries, such as wire buses and metal capacitors. This "template-instantiation" strategy largely reduces the number of unknowns and computation time without additional overhead. This work verifies that only *two* fundamental templates, shown in the figure below, are required for virtually all valid IC geometries. Also, this work shows that when considering practical aspect ratios and wire spacing, the edge and corner charge singularities can be totally neglected for a target 5% capacitance accuracy. In the example in the figure below, a preliminary version of our code runs 25 times faster and requires 33 times fewer unknowns compared to using standard piece-wise constant basis functions.

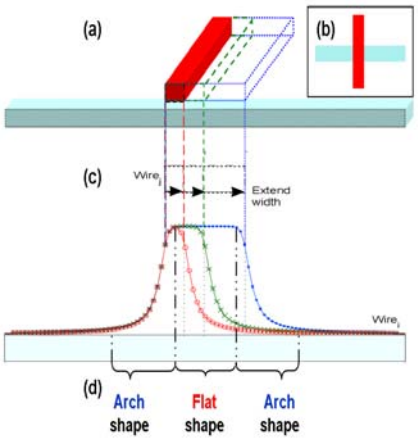


Figure: (a) The 3D view of a pair of crossing wires. The upper wire is stretched out to three different widths. (b) The top view of the geometry (c) The front view of the lower wire and the charge distribution induced by the upper wire of three different widths (d) The definition of arch and flat shapes from the widest upper wire case which can be reused in other geometries.

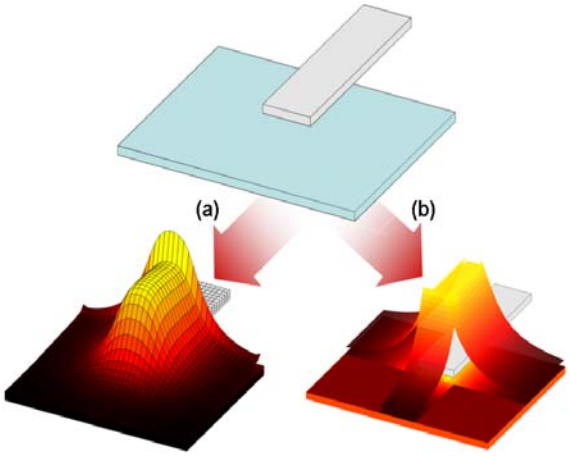


Figure: Partially overlapping wires are extracted by (a) traditional boundary element methods with piece-wise constant basis functions, using 572 unknowns, and by (b) Fast-Caplet with the instantiable basis functions, using only 17 unknowns. It takes 760 ms and 30 ms to extract for each method, respectively.

9. A Random Walk based Hierarchical Algorithm for Fabric-Aware Interconnect Extraction of Large Scale VLSI Interconnect

Sponsors
FCRP IFC, SRC, IBM, Mentor Graphics, AMD

Project Staff
T. A. El-Moselhy, Y. Zhao, H. Fernandes, I. M. Elfadel, L. Daniel

With the adoption of restricted design rules (RDR) and ultra regular fabric paradigms for controlling design printability at the 22nm node and beyond, there is an emerging need for a layout-driven, pattern-based parasitic extraction of alternative fabric layouts. Such paradigms are imposing two requirements of micro and macro regularity on the layouts. "Micro" regularity is achieved by restricting shape edges to lie on a restricted design grid that also imposes stringent directionality on shape orientation. "Macro" regularity is achieved by using a very restricted set of litho-friendly logic

cells. Such regularities have motivated using a relatively small number of optimized (litho-friendly and robust) layouts as building blocks to construct any arbitrary structure. These building blocks will be referred to subsequently as “motifs”. A designer typically examines different arrangements of the “motifs” in order to choose the “optimal” (in terms of printability, area, and electrical performance) design. Consequently, from an extraction point of view, there is a need to develop tools that are aware of topological variations.

In this project, we propose a hierarchical floating random walk (HFRW) algorithm for computing the 3D capacitances of a large number of topologically different layout configurations that are all composed of the same layout motifs. Our algorithm is not a standard hierarchical domain decomposition extension of the well established floating random walk technique, but rather a novel algorithm that employs Markov Transition Matrices (MTMs). Specifically, we first compute for each motif a MTM, representing the probability of making a transition from any point on the motif boundary to any point on the motif boundary or on a surface of the conductors inside of the motifs. Then the capacitance of the different layout configurations is extracted using the pre-computed motif MTM to form a large Markov Chain, and finally simulating such a chain using random walks. The complexity of our algorithm is primarily related to the computation of the motif MTM. Such computation needs to be performed once for each motif, independent of the number of configurations. On the other hand, the complexity of simulating the Markov Chains (computing the configuration) is almost negligible. Consequently, the main practical advantage of the proposed algorithm is its ability to compute the capacitance of a set of layout configurations in a complexity that is basically independent of the set size. For instance, in a large 3D layout example, the capacitance calculation of 120 different configurations made of similar motifs is accomplished in the time required to solve independently just 2 configurations, i.e. a 60× speedup.

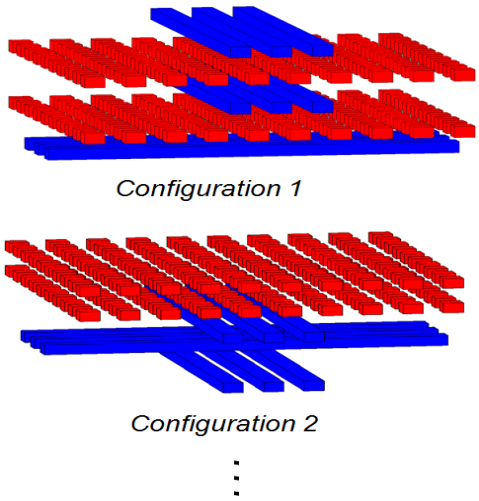


Figure: Five layer configurations. Each layer has a different dielectric constant. Different configurations are constructed by different ordering of the five layer. Each configuration is composed of 209 conductors.

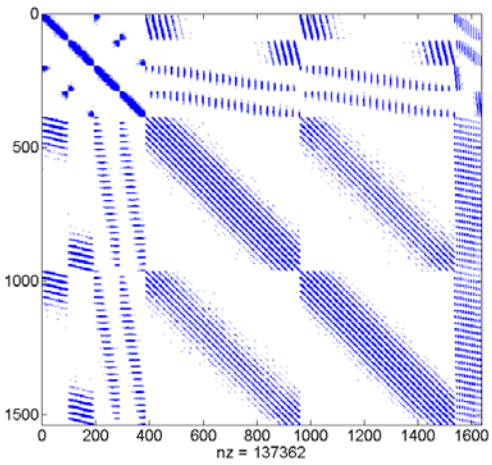


Figure: Markov Transition Probability associated with one of the layers..
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Variation-Aware Parasitic Extraction

Uncertainties in the integrated circuit manufacturing processes typically result in interconnect structures, whose dimensions and shapes deviate from the original design intent. Such geometrical variations are typically assumed random, and affect the electrical performance of the manufactured interconnect structures. Consequently, the effect of such variations on the electrical performance of the manufactured interconnects needs to be estimated and accounted for during the design phase.

To achieve such objective one needs to develop efficient variation-aware parasitic extraction tools. There are two different categories of algorithms for variation-aware extraction, namely, “intrusive” and “non-intrusive”. “Non-intrusive” algorithms are those that rely on sampling the parameter space, and then using any standard deterministic solver to compute a deterministic solution at the different sampling points. The main challenge facing such methods is the need to simultaneously and efficiently solve a very large number of linear systems corresponding to each different sample point. The term “intrusive” refers to the fact that the solution is computed using specialized stochastic algorithms, such as the stochastic Galerkin method, the Neumann expansion, or the Combined Neumann-Hermite Expansion.

10. Stochastic Dominant Singular Vectors Method for Variation-Aware Interconnect Extraction: An Intrusive Approach

Sponsors
FCRP IFC, SRC, IBM, Mentor Graphics, AMD

Project Staff
T. A. El-Moselhy, L. Daniel

In this project we present a novel intrusive stochastic algorithm. The main idea behind our algorithm is to search simultaneously for dominant basis vectors in both the spatial and stochastic spaces, which best represent the unknown solution. We formulate a simple nonlinear optimization problem which uncovers sequentially the most dominant basis vectors in the combined spatial-stochastic space. The main computational advantage of the proposed approach stems from the fact that at every step of the algorithm only two dominant basis vectors, one in the spatial space and another in the stochastic space, are simultaneously computed. The two dominant bases are computed such that the equation residual is minimized. After each step both the solution and the equation residuals are updated. The algorithm is terminated when the norm of the equation residual is sufficiently small. Consequently, meaningful error measures are provided which determine the quality of the solution. The final complexity of our algorithm scales with the sum (rather than the product) of the sizes of the spatial and stochastic spaces, hence it is orders of magnitude more efficient than many of the available state of the art techniques. Finally, we validate our algorithm on a variety of on-chip and off-chip capacitance and inductance extraction problems, ranging from moderate to very large size, not feasible using any of the available state of the art techniques.

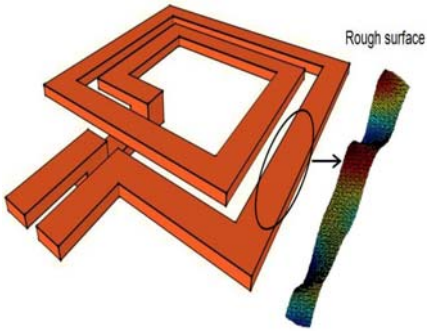

Figure 1: Geometry of a two-turn, 1mm side-length, square inductor with surface roughness. The inductor is discretized using 2.500 spatial elements. The roughness is modeled using 400 random parameters.

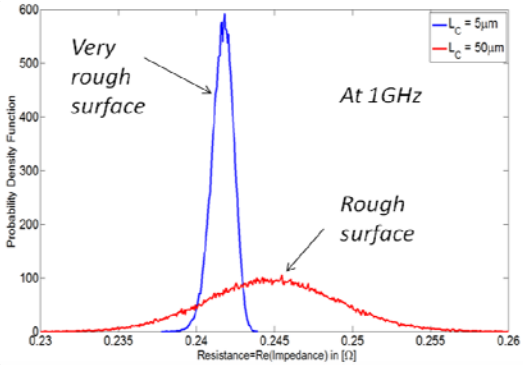

Figure 2: Probability density function of the input resistance for two different roughness profiles.

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11. Statistical-Moment-Preserving Model Order Reduction for Variation-Aware Extraction: A Non-Intrusive Approach

Sponsors
FCRP IFC, SRC, IBM, Mentor Graphics, AMD

Project Staff
T. A. El-Moselhy, L. Daniel

"Non-intrusive" sampling based methods are embarrassingly parallel and can easily exploit the state of the art "fast" solvers. Consequently, such methods are of great practical importance. However, one of the remaining computational challenges of sampling based methods is how to solve simultaneously and efficiently the large number of linear systems corresponding to each different sample point. In this project we present new non-intrusive algorithm based on a stochastic model reduction technique that exploits the similarity among the different solves to reduce the computational complexity of subsequent solves. We first propose a projection matrix such that the statistical moments and/or the coefficients of the projection of the stochastic vector on some orthogonal polynomials are preserved when computed using the reduced model. We further introduce a proximity measure, which we use to cheaply determine if the available reduced basis accurately represents the solution at a new point in the parameter space, or if instead the reduced basis needs to be expanded. Finally, in order to reduce the time required for the system assembly, we use the multivariate Hermite expansion to represent the system matrix. We verify our method by solving a variety of variation-aware capacitance extraction problems ranging from on-chip capacitance extraction in the presence of width and thickness variations, to off-chip capacitance extraction in the presence of surface roughness. We further solve very large scale problems that cannot be handled by any other state of the art technique.

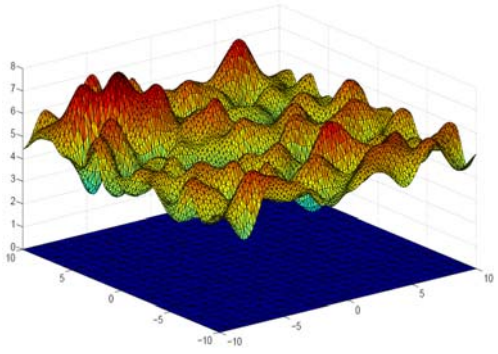

Figure 1: A parallel plate capacitor with upper rough surface, discretized using more than 20,000 spatial elements. Stochastic variation modeled using 323 independent random variables.

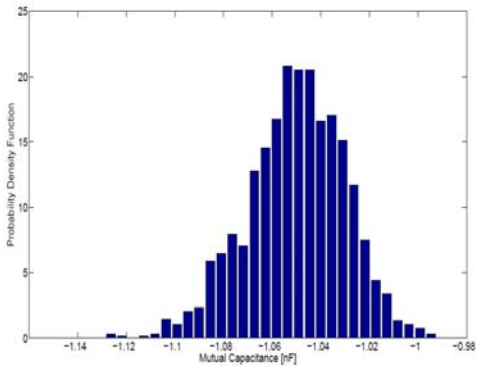

Figure 2: Probability density function of the mutual capacitance of the parallel plate conductor.

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12. Passive Compact Dynamical Modeling via Semidefinite Programming for *Multiport* Interconnect

Sponsors
SRC, FCRP IFC, AMD, Mentor Graphics, IBM, DARPA

Project Staff
Z. Mahmood, B. Bond, A. Megretski, L. Daniel

Automatic generation of accurate, compact, and passive models for multiport interconnect structures is a crucial part of the design process for circuits. Conventionally, interconnect structures

are laid out in a field solver and simulated for frequency response in the desired frequency band. Based on the frequency samples extracted by the solver, a reduced model is developed which can be incorporated into a circuit simulator for time-domain simulations of a larger system containing also nonlinear devices. A small violation of any basic property of the structure, such as passivity, can cause huge errors in the response of the overall system, and the results become completely nonphysical. Therefore, it is essential to preserve basic system properties during the model identification. To model multiport structures from given frequency response samples, the only available approach so far is to identify a stable, but non-passive, model, and then perturb the model to make it passive. However such approaches suffer from limitations if the initial non-passive model has significant passivity violations.

In this work we propose a new technique for passive modelling of *multiport* interconnect structures. Given transfer function samples, we identify a rational transfer function reduced model that minimizes the mismatch at the given frequencies subject to a global passivity constraint. After a convex relaxation, this problem is formulated as a semidefinite optimization problem, which can be solved efficiently using existing techniques. Numerical results are presented for a power distribution grid (shown in figure 1) and an array of inductors having 8 and 4 ports respectively. Figure 2 provides a comparison for accuracy between our identified passive models and given data from field solver.

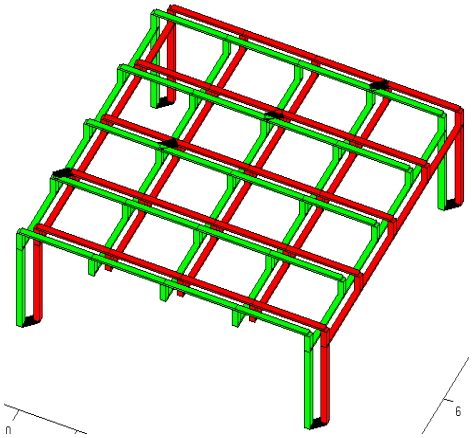

Figure 1: 3D layout of the distribution grid (not to scale) showing *Vdd* (*red or dark grey*) and *Gnd* (*green or light grey*) lines. Black strips represent location of ports.

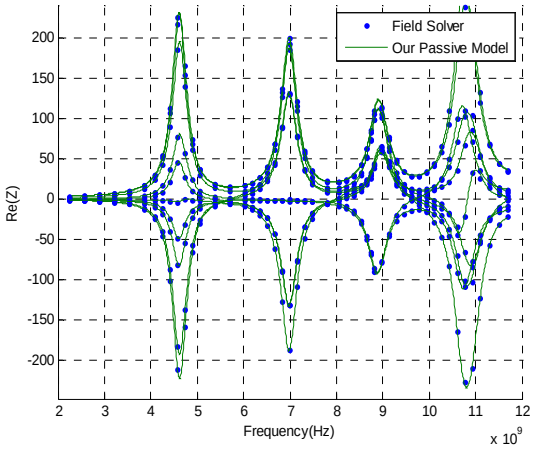

Figure 2: Comparing real part of frequency response from our passive model (solid line) and from field solver (dots). This plot demonstrates the accuracy of our identified models by showing close match with given field solver data.

13. Passive Compact Dynamical Modeling via Semidefinite Programming for *Parameterized* Interconnect

Sponsors
SRC, IFC, AMD, Mentor Graphics, IBM, DARPA

Project Staff
Z. Mahmood, B. Bond, L. Daniel

System level design optimization has recently started drawing the attention of circuit designers. A system level optimizer would search over the entire design space, defined by the parameters of interest. Such optimizers therefore require the availability of *parameterized compact dynamical models* of individual modules. The parameters may include geometrical quantifiers, such as width and spacing for an on-chip inductor, or design parameters such as center frequency or characteristic impedance in case of distributed transmission line structures. The parameterized models of individual blocks need to be compact and *stable* since the optimizer would be solving ordinary differential equations (using time domain integration or periodic steady state methods) to compute the performance metrics.

In this project we have developed a method for generating parameterized models of linear systems that the user will be able to instantiate for any parameter value. Given a collection of systems swept over design and geometrical parameters of interest, we identify a closed form parameterized dynamical model using constrained fitting. The proposed algorithm is completely independent from the type of initial non-parameterized identification procedure used for the individual systems. In other words, the individual (non parameterized) models may be generated by any stability preserving modeling scheme, such as convex optimization based approaches or vector fitting based approaches. The models are first converted into an equivalent pole-residue form. Final parameterized models are developed by polynomial or rational multivariate approximation between residue matrices, system poles and direct matrix. We have finally showed the effectiveness of the proposed approach by modeling several practical circuit blocks. Figure 1 plots the trajectory of poles in response to parameter variation. Figure 2 plots the real part of frequency response of our stable parameterized model as a function of densely sampled parameter values.

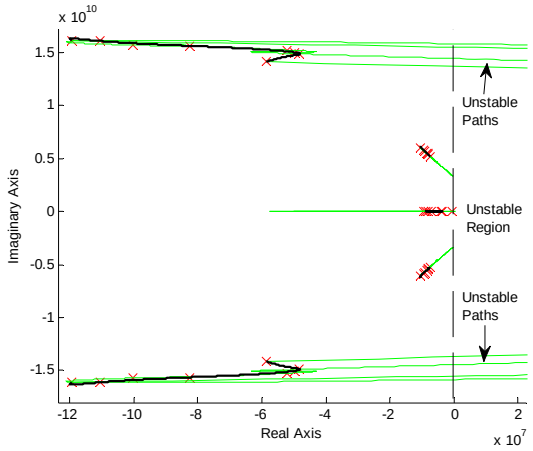

Figure 1: Plot showing the trajectory of poles with parameter variation. Thick black lines trace the poles' location from our stable parameterized model, while thin grey (or green) lines trace the poles' location from the unconstrained fit (which clearly becomes unstable as indicated by the arrows)

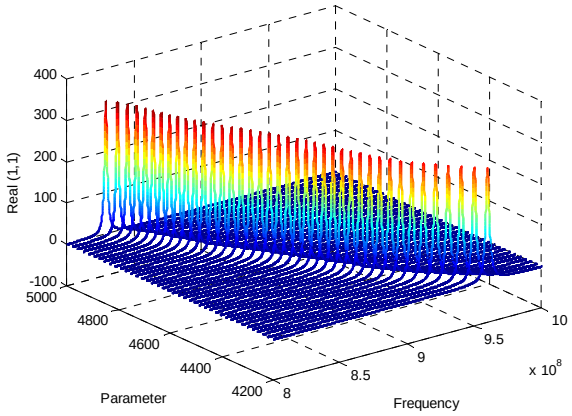

Figure 2: Surface traced by real part of the frequency response of parameterized model of patch antenna over parameter sweep

14. Compact Modeling of NON-LINEAR Analog Circuits using System Identification via Semidefinite Programming and Incremental Stability Certification

Sponsors
DARPA, SRC, FCRP IFC

Project Staff
B. Bond, Z. Mahmood, A. Megretski, V. Stojanovic, L. Daniel

During recent years, a great effort has been made by researchers of the Electronic Design Automation community to develop new techniques for automatically generating accurate compact models of NON-LINEAR system blocks. The majority of the existing methods for creating stable reduced models of nonlinear systems require knowledge of the internal structure of the system, as well as access to the exact model formulation for the original system. Unfortunately, this information may not be easily available if a designer is using a commercial design tool, or may not even exist if the system to be modeled is a physical fabricated device.

As an alternative approach to nonlinear model reduction, we have proposed a system-identification procedure. This procedure requires only data available from simulation or measurement of the original system, such as input-output data pairs. By enforcing incremental stability, it is possible to formulate a semi-definite optimization problem whose solution is a stable nonlinear model that optimally matches the given data pairs from the original system. In addition, the proposed optimization formulation allows us to specify completely the complexity of the identified reduced model through the choice of both model order and nonlinear function complexity.

Applications for the proposed modeling technique include analog circuit building blocks such as operational amplifiers and power amplifiers, MEMS devices, and individual circuit elements such as transistors. The resulting compact models may then be used in a higher-level design optimization process of a larger system. One such example of an analog circuit block is the low-noise amplifier shown in Figure 1; it contains both nonlinear and parasitic elements. For this example, input-output training data was generated from a commercial circuit-simulator and used to identify a compact nonlinear model. The output responses of the original system and the identified model are compared in Figure 2.

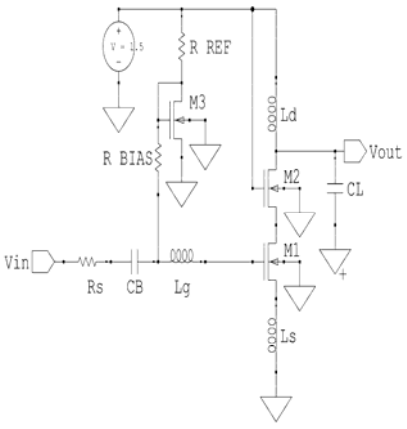

Figure 1: Application example: Low-noise amplifier designed in CMOS technology.

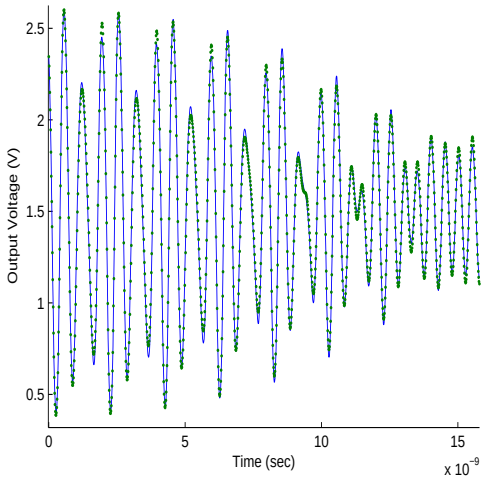

Figure 2: Comparison of the output response from a commercial circuit simulator (solid blue line) and the output response from a stable nonlinear reduced model created with the proposed approach (green dots).

15. Modeling and Simulation of Blood Flow in Arterial Networks

Project Staff
T. A. El-Moselhy, B. Bond, J. Lee, J. White and L. Daniel

Understanding certain medical conditions requires understanding certain aspects of the blood flow in the arterial network. For instance, studying atherosclerosis requires capturing detailed flow inside an arterial segment. Such study requires developing accurate solvers for the detailed equations describing both the blood flow and the elastic behavior of the arteries. On the opposite spectrum, studying hypertension requires computing pressure and averaged flow over a larger arterial network. Such analysis requires developing compact computationally inexpensive models of complex segments of the arterial network. These models relate the pressure and average flow at the terminals of the arterial segments and must be easily interconnected together to form complex and large arterial networks.

In this project we are developing a 2-D fluid-structure interaction solver to accurately simulate blood flow in arteries with bends and bifurcations. Such blood flow is mathematically modeled using the incompressible Navier-Stokes equations. The arterial wall is modeled using a linear elasticity model. Our solver is based on an enhanced immersed boundary method (IBM). As a second step we are developing system identification techniques to generate passive models for complex arterial segments such as large arteries, arterial bends and bifurcations. We have validated our IBM solver results versus reference results obtained from MERCK Research Laboratories for a straight vessel of length 10cm and diameter 2cm. Our results for pressure, flow and radius variations are within 3% of those obtained from MERCK. Furthermore, we are validating our model results by cascading different models and comparing the results of the resulting network to those predicted by the IBM solver. Our preliminary results for pressure and flow at the terminals of the models are within 10% of those obtained from the full simulator. In addition, by using the models we obtain more than 100,000 times reduction in the computational time.

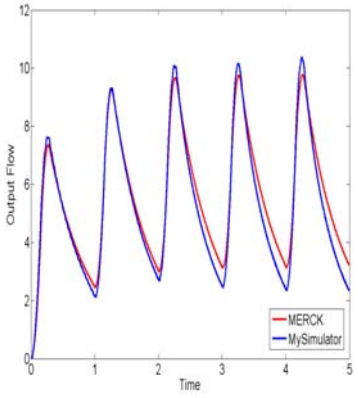

Figure 1: Output flow at the middle of a straight 10cm artery as a function of time. Simulations performed using our immersed IBM code and compared to reference results obtained from MERCK.

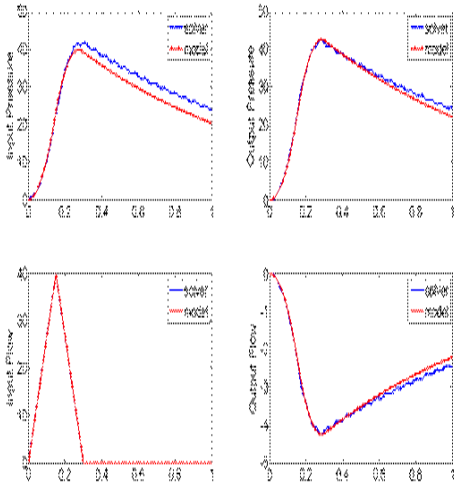

Figure 2: A 20-cm artery is constructed by cascading two models for a 10-cm artery. The model results are compared to those obtained by simulating the 20-cm using the IBM. Figure shows input/output flow and input/output pressure at the terminals of a 20 cm

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