Computational Prototyping Group

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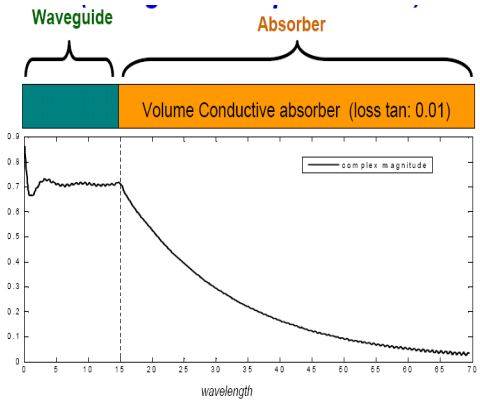
Group Summary
Our research group uses several engineering design applications to drive research in simulation and optimization algorithms and software. Recent efforts have focused in the areas of model-order reduction, fast methods for solving integral equations, and efficient algorithms for coupling 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.

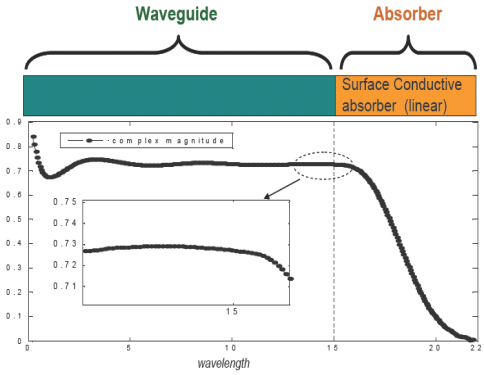
1. Fast Solver Development for 3-D Nanophotonics

Sponsors
Defense Advanced Research Projects Agency, MARCO Interconnect Focus Center, 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.

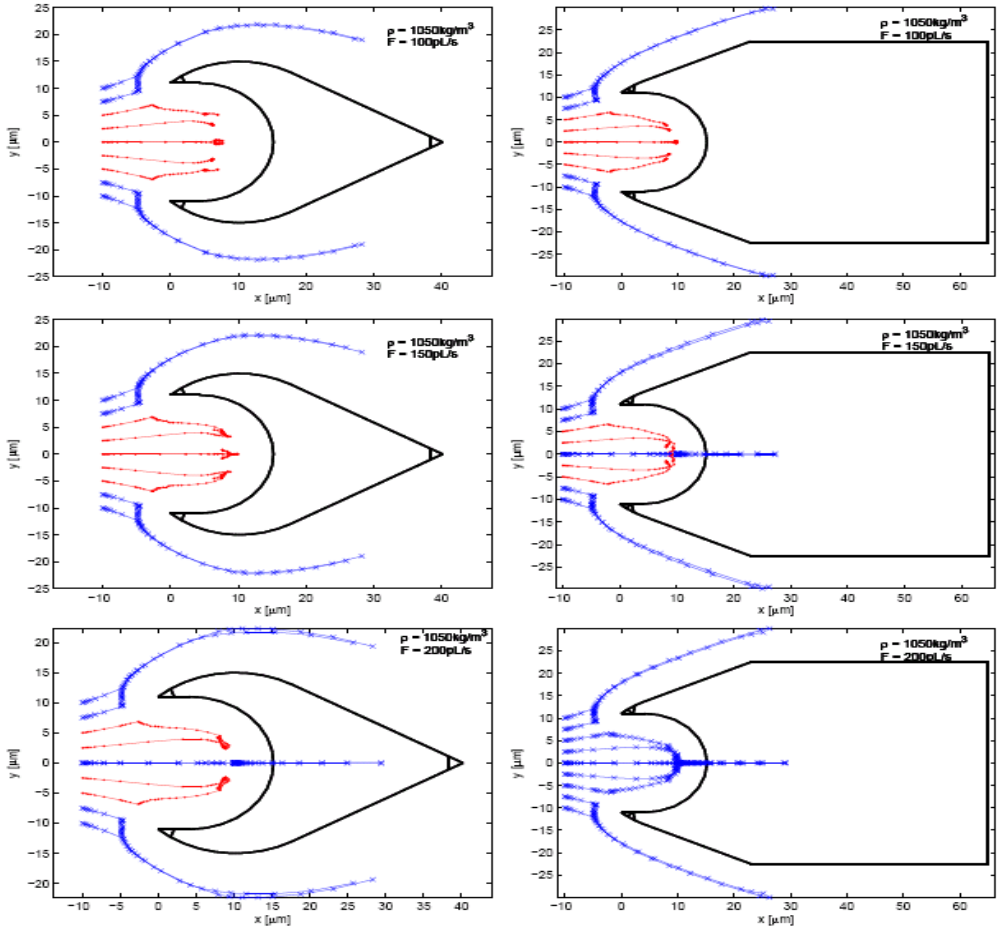


Figure: Characterization of the trapping region for pachinko trap model 1, on the left, and pachinko trap model 4, on the right. The curves in red, with the dot marker, represent situations where the bead was trapped; the curves in blue, with the cross marker, represent situations where the bead was 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).

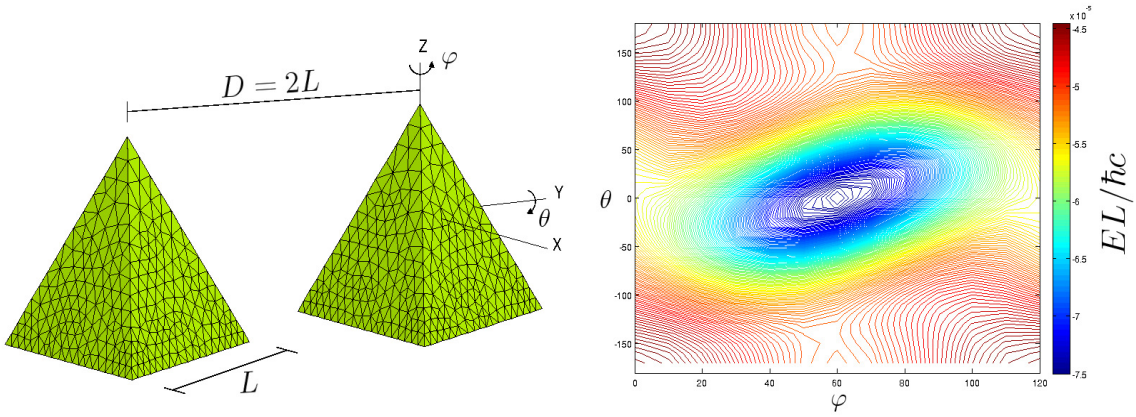


Figure: Contour plot of Casimir energy vs. orientation angles for tetrahedral nanoparticles separated by a distance D = 2L.

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.

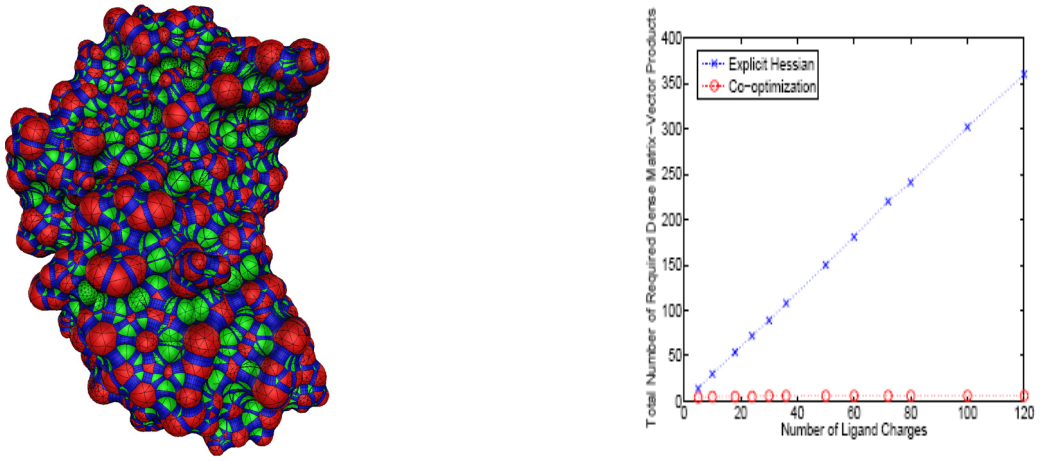


Figure: On the left is the molecular surface of the Barnase-Barstar receptor-ligand complex easily analyzed with our new fast solver, and on the right is a graph comparing the computational cost of explicit-Hessian versus our new co-optimization approach. Note that the cost of the co-optimization approach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

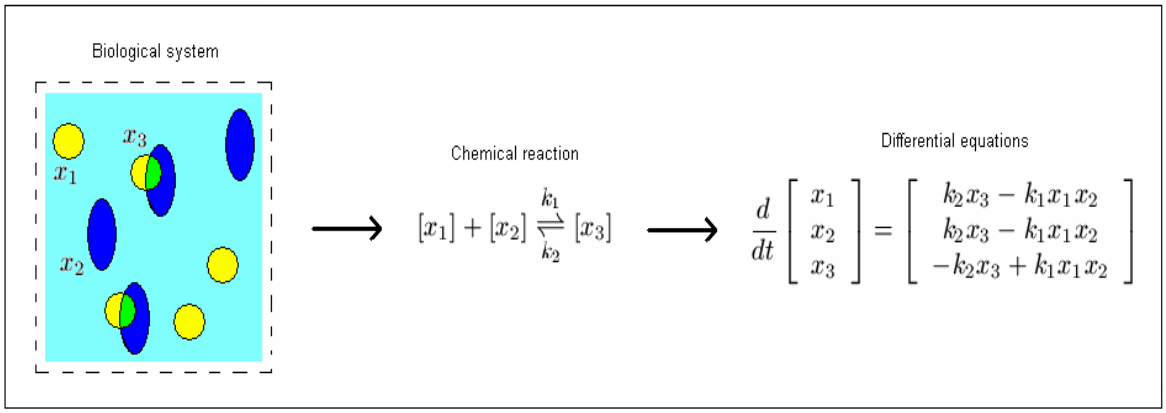


Figure: Basic illustration of modeling a biological system with differential equations.

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. Efficient Capacitance Extraction Targeted to Small to Medium Scale 3D Interconnect

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

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

Integrated circuit performance and signal integrity can be largely affected by interconnect parasitic capacitance, and require fast and accurate extraction tools. Satisfying simultaneously both constraints is however an extremely challenging task. The current state-of-the-art in efficient extraction methods involves 2D cross section scanning, determining wire adjacency, calculating 2D capacitance in a table lookup approach, and then reconstructing quasi-3D capacitance. Such approach is indeed fast, yet it is accurate only for 2D structures. Full 3D structures (e.g. crossing wires in adjacent metal layers) need the accuracy of field solvers such as FastCap, Precorrected-FFT. Such tools are based on piece-wise constant basis functions, and are accelerated by fast matrix-vector products which have a significant computational overhead, but scale almost linearly with the number of conductors. Hence they are ideal for very large scale examples. This project is target instead at efficient small-to-medium scale capacitance extraction. The key idea is to exploit

the highly restrictive design rules of the recent sub-micro to nano-scale technologies. In this scenario, a limited number of pre-computed surface charge distributions can be used as a set of fundamental template basis functions. Figure 1 shows an example of charge distribution "stretchability," enabling the instantiation of basis functions for every practical interconnect structure. Using a total of just 72 template-instantiated basis functions, the example in Figure 2 results in a worst-case relative error of 3% with respect to the total capacitance of each conductor, compared to the result extracted by FastCap in a very fine discretization with tens of thousands of unknowns. FastCap requires 732 unknowns to produce the same 3% error in a coarser discretization. Hence, for the same 3% accuracy, our algorithm requires approximately 10x fewer unknowns. In such medium size examples, the overhead of the FastCap multipole expansion makes the linear acceleration ineffective, while in our approach, analytical formulas and numerical tabulation of the Galerkin coefficients for our template basis functions can effectively limit the setup overhead, producing two orders of magnitude improvements in both simulation time and memory requirement.

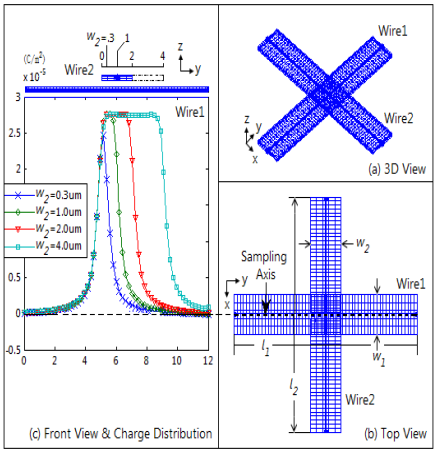


Figure 1: A pair of crossing wires: (l1, w1, l2, w2) = (12, 2, 12, 2) (um). (a) 3D View (b) Top View (x-y plane) (c) Front View (y-z plane) and charge distribution sampled along the sampling axis of Wire1shown in (b) as a broken line. Note the charge distributions are "stretchable" with w2 while preserving decaying shapes off the edge of Wire2.

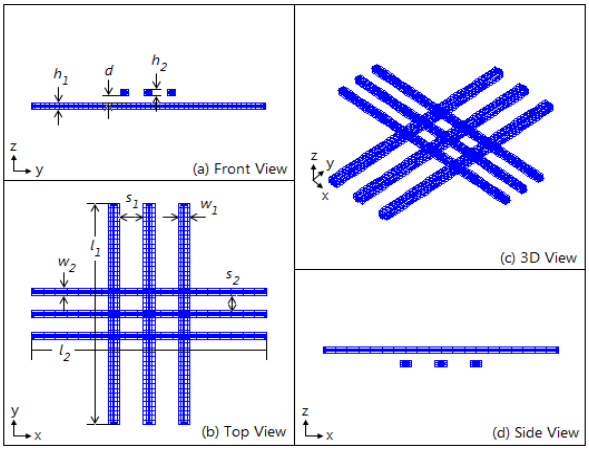


Figure 2: Six wires in two metal layers: (l1, w1, h1, s1 | l2, w2, h2, s2 | d) = (10, 0.2, 0.3, 0.2 | 10, 0.2, 0.3, 0.2 | 0.3) (um). (a) Front View (y-z plane) (b) Top View (x-y plane) (c) 3D View (d) Side View (x-z plane). The width and spacing are exaggerated for clarity.

8. Variation-Aware Parasitic Extraction

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 significantly affecting the electrical characteristics of the interconnect structures. The effect of such variations on the electrical characteristics can be efficiently extracted using the so-called variation aware parasitic extraction tools. Such solvers can be in general divided into two categories, namely, those based on deterministic algorithms and those based on stochastic algorithms.

8.1 Variation-Aware Parasitic Extraction: A Deterministic Approach

Sponsors
FCRP Interconnect Focus Center.

Project Staff
T. A. El-Moselhy, I. Elfadel (IBM), L. Daniel.

In this part of the project we are developing a new deterministic variation-aware extraction algorithms based on the well-known floating random walk algorithm (FRW). First, we have developed a new finite-difference-based sensitivity analysis within the improved FRW algorithm to efficiently compute capacitance sensitivities with respect to a large number of small parameter variations. We have demonstrated that the expected complexity of computing the nominal capacitance and all the sensitivities is less than 2 times that of computing only the nominal capacitance regardless of the number of parameters. The complexity of our sensitivity algorithm is therefore independent of the number of varying parameters (unlike standard finite difference sensitivity analysis) and independent of the number of output capacitances (unlike standard adjoint sensitivity analysis). Second, we have developed a new incremental FRW algorithm to efficiently compute the capacitances of similar geometrical configurations resulting from simultaneous large perturbations of the geometrical parameters of a common geometrical topology. The new algorithm satisfies a major objective of variation-aware parasitic extraction, namely, that the average time required to solve a single geometrical configuration within a set of similar configurations is reduced as the cardinality of the set is increased. We have observed that the average simulation time of each configuration from a set of similar configurations of cardinality 100,000 is reduced by three orders of magnitude. Consequently, we were able to solve more than 130,000 similar configurations in the time required to solve just 50 independent configurations. We believe that the latter result will naturally fit in a litho- and CMP-aware extraction flow.

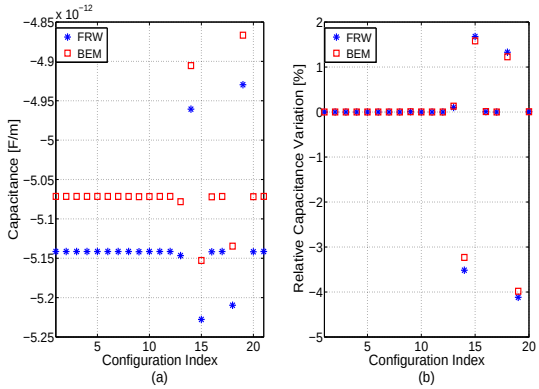


Figure 1: (a) Capacitance, (b) Relative capacitance variation, i.e. the difference between the capacitance of any configuration and that of the nominal configuration divided by the capacitance of the nominal, as computed using our FRW sensitivity algorithm and the standard boundary element method (BEM) for different geometrical configurations.

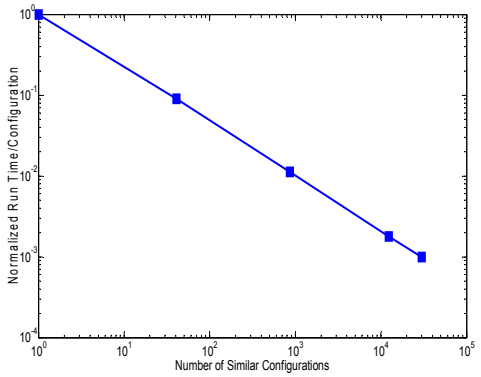


Figure 2: Normalized Average simulation time for a single geometry (configuration) in a set of similar geometries versus the total number of configurations in the set..

8.2 Variation-Aware Parasitic Extraction: A Stochastic Approach

Sponsors
FCRP Interconnect Focus Center

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

In this part of the project we are developing a new stochastic algorithms to solve large stochastic linear systems typically appearing during variation aware extraction. We have derived a new approach to help 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 approach 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 an approach 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 parallelizable 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.

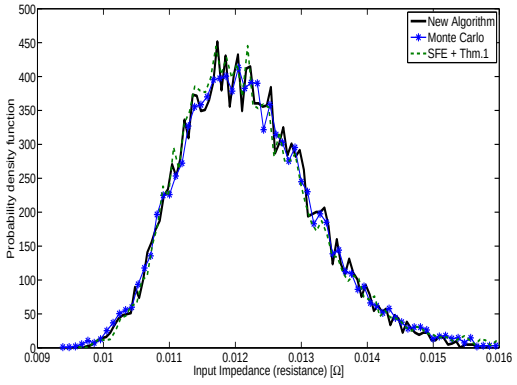


Figure 1: Comparison between the probability density function of the microstrip line obtained from our new algorithm and the reference Monte Carlo simulation.

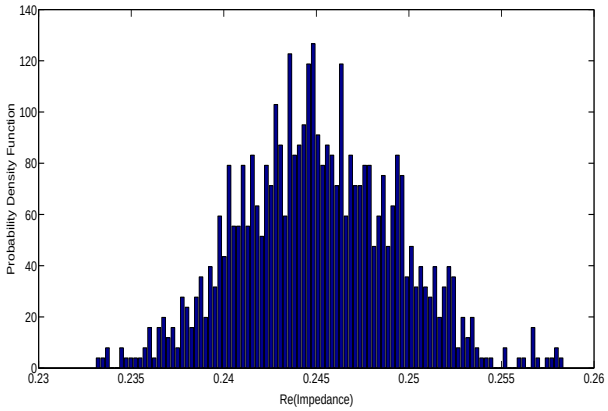


Figure 2: Probability density function of the real part of the input impedance at 1GHz for correlation length Lc = 50μm. The resistance of the non-rough surface is 11.3% smaller than the mean of the obtained distribution.

9. Stable Model Reduction: A Semi-Definite System-identification Approach for Nonlinear Systems

Sponsors
DARPA, FCRP Interconnect Focus Center

Project Staff
B. Bond, Z. Mahmood, R. Sredojevic, Y. Li, A. Megretski, V. Stojanovic, Y. Avniel, 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 nonlinear system blocks. The majority of 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 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 are developing 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 passivity 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.

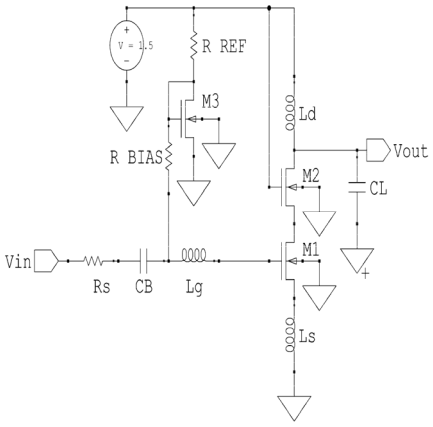


Figure 1: Application example: Low-noise amplifier designed in CMOS technology.

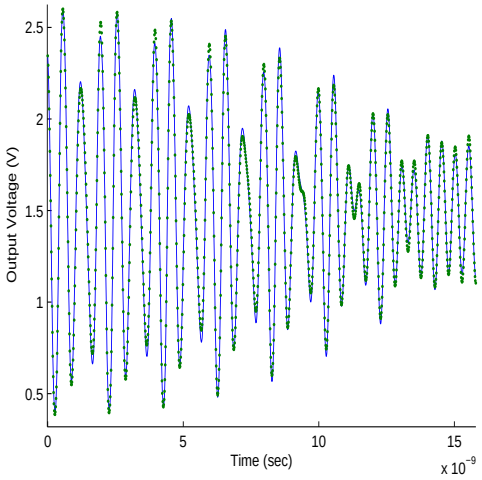
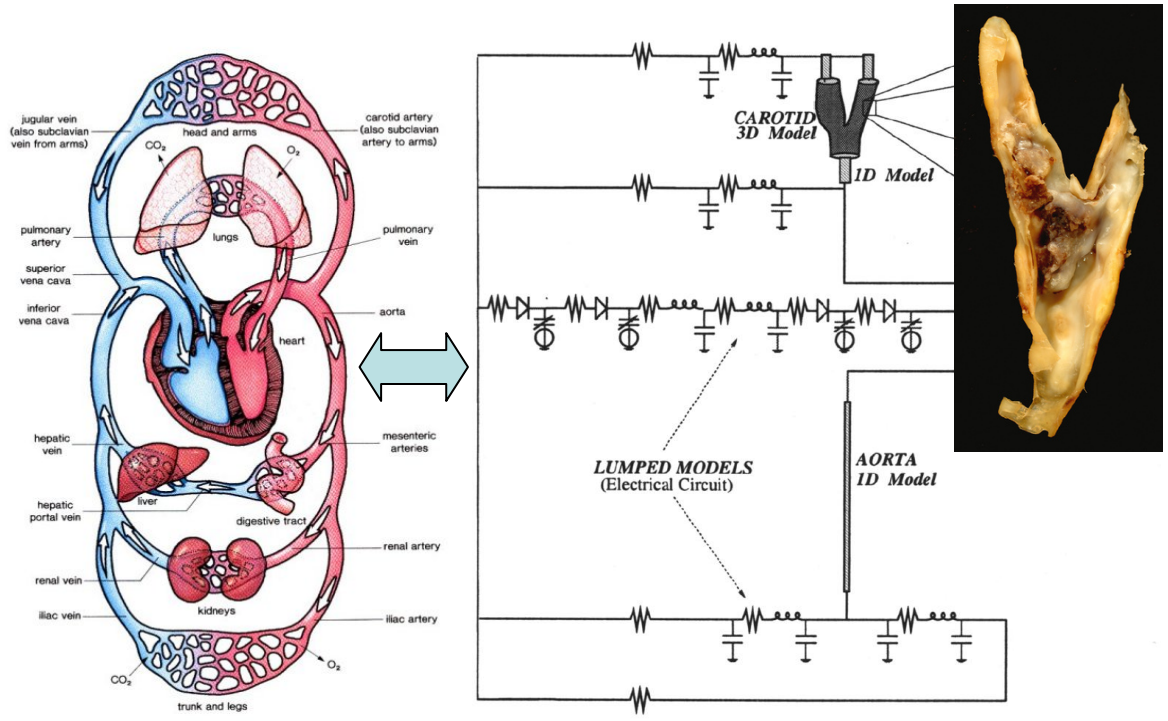


Figure 2: Comparison of the output response from a commercial circuit simulator (solid blue line) and the output response from a stable nonlinear reduced model created with the proposed approach (green dots).

10. Development of Modeling Tools for the Human Cardiovascular Circulatory System

Project Staff
T. A. El-Moselhy, B. Bond, J-H Lee (Merck), L. Daniel

Studying certain medical conditions, such as stroke risk due to arterial clogging or hypertension, requires the simulation of the whole cardiovascular system, including arteries, veins, and various organs treated as vascular beds. Such a requirement renders full 2-D or 3-D coupled fluid-structural simulation impractical due to their high demand in computational resources. The computational efficiency of lower dimensional models comes at a cost of sacrificing correctness. For instance, 1-D artery models cannot accurately model bends and bifurcations in the major arteries that significantly alter fluid flow, and 0-D vascular bed models cannot provide spatial information. One way to overcome the computational complexities associated with high dimensional models without sacrificing the accuracy is to use reduced order models for complex arterial segments, such as bends and bifurcations, to faithfully reproduce the flow and pressure at each end of such segments.



As a first step toward generating reduced order models for arterial segments, we developed 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 the immersed boundary method. The numerical accuracy of our solver stems from using a staggered grid for the spatial discretization of the incompressible Navier-Stokes equations. The computational efficiency of our method stems from using Chorin's projection method for the time stepping, coupled with the fast Fourier transform (FFT) to compute the pressure. We have validated our results versus reference results obtained from MERCK 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.

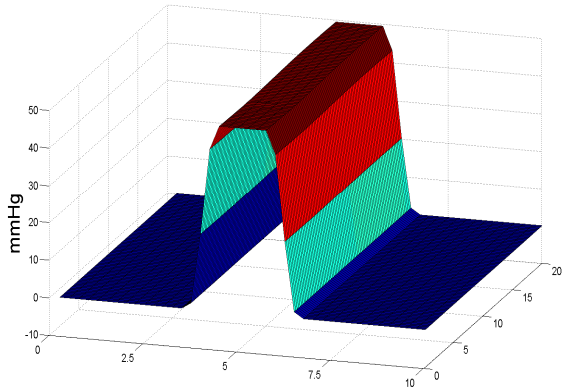


Figure 1: Pressure build-up inside of artery at time 0.165 sec. Almost uniform pressure observed inside of straight artery and almost zero pressure observed outside of the artery.

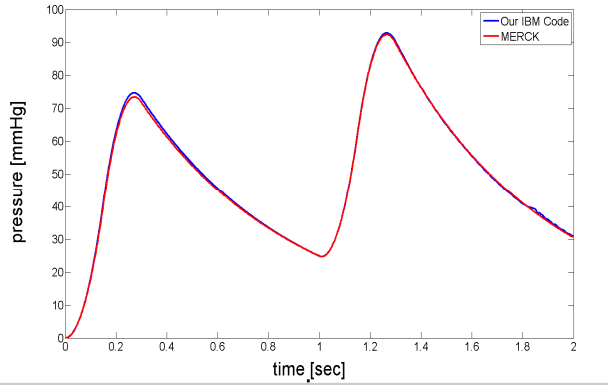


Figure 2: Pressure at the middle of a straight 10cm artery as a function of time. Simulations performed using our immersed boundary method code and compared to reference results obtained from MERCK

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