Computational Prototyping

RLE Groups
Computational Prototyping Group, Biological Microtechnology and BioMEMS Group, Micro / Nanofluidic BioMEMS Group

Academic and Research Staff
L. Daniel, EECS and RLE, J. Peraire, EECS and RLE, J. Voldman, EECS and RLE, J. Han, EECS, Bioengineering Division, and RLE, A. Megretski, EECS and LIDS, K. Willcox, Aero-Astro, B. Tidor, EECS, Bioengineering Division, and CSAIL, J. White. EECS and RLE

Graduate Students
J. Bardhan, Research Assistant, EECS, B. Bond, Research Assistant, EECS, C. Coelho, Research Assistant, EECS, X. Hu, Research Assistant, EECS, T. Klemas (Graduated), Research Assistant, EECS, S. Kuo, Research Assistant, EECS, J.H. Lee, H. Reid, Research Assistant, EECS, K. C. Sou, Research Assistant, EECS, Research Assistant, EECS, D. Vasilyev, Research Assistant, EECS, A. Vithayathil, Research Assistant, EECS (Graduated), D. Willis, Research Assistant, Aero-Astro, Z. Zhu, Research Assistant, EECS (Graduated)

Support Staff
C. Collins, Administrative Assistant

1. Numerical Techniques in Biomolecule Design and Systems Biology

Sponsors
National Institutes of Health, The Singapore-MIT Alliance, and the National Science Foundation

Project Staff
Dmitry Vasilyev, Jay Bardhan, Michael Altman, Shihhsien Kuo, Patricio Ramirez,Paul Barton, Bruce Tidor, and Jacob White

In order to design an effective drug or a biochemically-based sensor, it is necessary to develop ligand molecules that bind readily and selectively to receptors of interest. Electrostatic forces play an important role in the design of ligands, but the complicated three-dimensional geometry of the problem makes it difficult to assess the electrostatic fields and then optimize the ligand. We have been developing fast methods for the electrostatic analysis, and have been focused on three aspects. First, we have developed a fast analysis program based using a discretized integral equation formulations plus sparsification-accelerated iterative techniques. Second, we have coupled the electrostatic analysis with the ligand charge optimization problem using a Hession-implicit approach[1]. Finally, we have been developing improved discretizations of the molecular surface geometry using curved panels, and have developed approaches for computing integrals over curved panels[2].

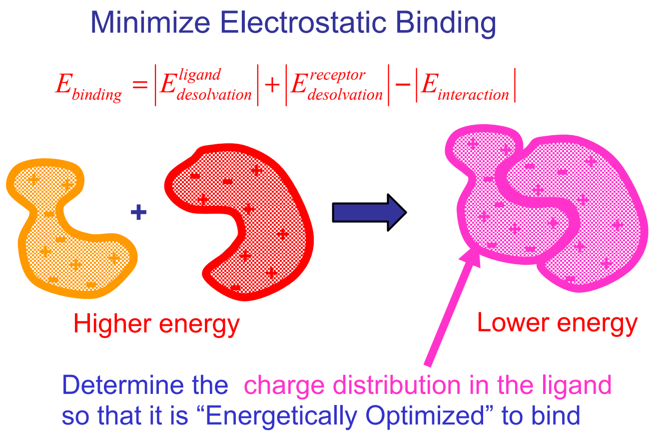

Figure 1: Electrostatic design problem

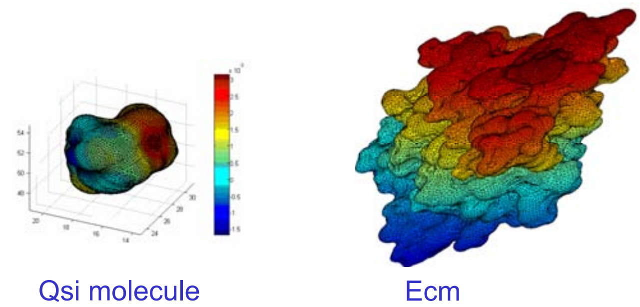

Figure 2: Molecular Surfaces for two proteins

2. Techniques for Coupled Optimization and Simulation

Sponsors
MARCO Interconnect Design Focus Centers, Singapore-MIT Alliance, DARPA

Project Staff
K.C. Sou, J.H. Lee, J. Bardhan, L. Daniel, A. Megretski, Y. Avniel, S. Johnson, and J. White

The enormous advances in both interior-point-based, convex optimization and fast methods for three-dimensional simulation are making development of design tools that perform automatic structural optimization much more feasible. We are developing strategies for coupling fast simulation and interior-point optimization for applications such as biomolecule design, nanophotonics, and optical semiconductor process inspection. Our approaches include using Hession-implicit methods in which the simulation and optimization occur in parallel [3] and strategies in which a detailed simulation model is used to generate a parameterized reduced order model [4,5,6]

3. Tools for Photonics in Integrated Circuit Design and Manufacturing

Sponsors
Marco Interconnect Focus Center, DARPA, NSF

Project Staff
J.H. Lee, Y. Avniel, S. Johnson, and J. White

Optical inspection, now the non-destructive, semiconductor process monitoring technique of choice, requires the solution of an inverse scattering problem to infer geometry from measured light. We have developed a new approach to accelerating this inverse scattering problem based on using parameterized model reduction [7]. The problem of analyzing optical effects in wavelength-sized structures also arises for developers of integrated nanophotonics, which is emerging as an important new technology. Nanophotonic designers have very few available tools, and we are beginning a project to improve the situation. We are developing approaches that can be used to extract circuit-level models of photonic devices [8,9] and are also developing new techniques for assessing the impact of roughness on the loss in photonic channels[10].

4. Numerical Techniques for Integral Equations

Sponsors
MARCO Interconnect Design Focus Centers, National Science Foundation, Semiconductor Research Corporation, Singapore-MIT Alliance, National Institutes of Health

Project Staff
M. Altman, J. Bardhan, X. Hu, S. Kuo, D. Willis, L. Daniel, J. Peraire, B. Tidor, J. White

Finding computationally efficient numerical techniques for simulation of three-dimensional structures has been an important research topic in almost every engineering domain. Surprisingly, the most numerically intractable problem across these various disciplines can be reduced to the problem of solving a three-dimensional potential problem with a problem-specific Greens function. Application examples include electrostatic analysis of sensors and actuators; electromagnetic analyses of integrated circuit interconnect and packaging; detailed analysis of frequency response and loss in photonic devices; drag force analysis of micromachined structures; and potential flow based aircraft analysis. Over the last fifteen years, we have been developing fast methods for solving these problems and have developed widely used programs such as FastCap (capacitance), FastHenry(magnetoquasistatics), FastLap (general potential problems), FastImp (full wave impedence extraction),and FastStokes (fast fluid analysis). Our most recent work is in developing higher order methods[11], methods that efficiently discretize curved geometries[12], methods that are more efficient for substrate problems [13], and methods for analyzing rough surfaces [14].

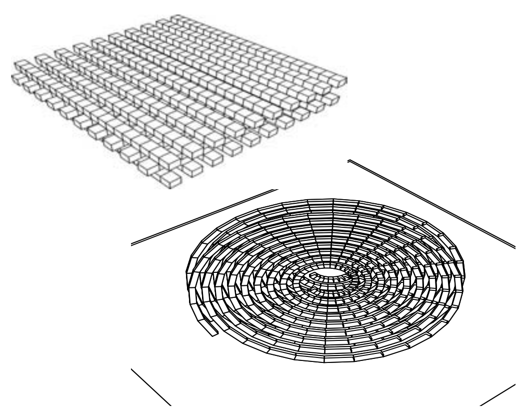

Figure 1: A buss crossing structure and a spiral Inductor over a substrate. Analyzed by FastImp in minutes.

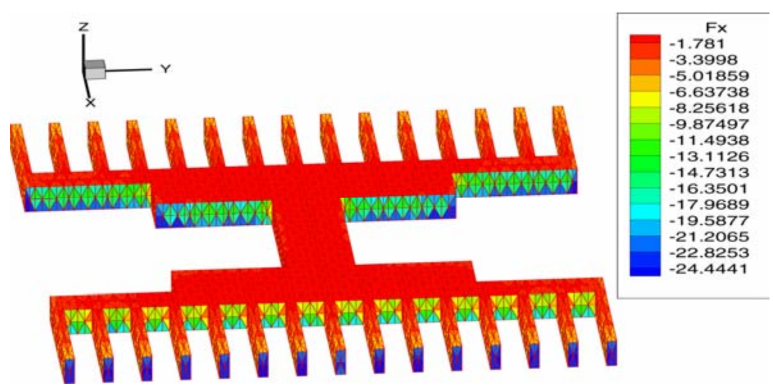

Figure 2: The fluid drag force distribution for a micromachined comb, computed using FastStokes in under five minutes.

5. Design Tools for Bio-Micromachined Device Design

Sponsors
Singapore-MIT Alliance, National Science Foundation

Project Staff
C. Coelho, N. Ngoc Son, D. Vasilyev, J. Han, J. Peraire, N. Hadjiconstantinou, J. Voldman and J. White

Using micromachining for biological applications requires complicated structures such as mixers, separators, preconcentrators, filters, and pumps, and these elements are used to process biomolecules or biological cells. To accelerate the design of these complicated devices, new tools are needed that can efficiently simulate mixing and particle or cell motion in complicated three-dimensional flows. In addition, for microfluidic devices intended for use in molecular separation, the length scales are such that noncontinuum fluid effects must be considered, and therefore hybrid approaches that combine molecular and continuum models must be developed. Finally, the wide variety of structures being developed implies that generating models for system-level simulation will require efficient simulation combined with automated model extraction [15]. Our recent work in addressing these problems includes the development of efficient time integration techniques for cells in flow [16], techniques for accurately extracting diffusion constants from measurements[17], and efficient techniques for extracting models from detailed simulations [18].

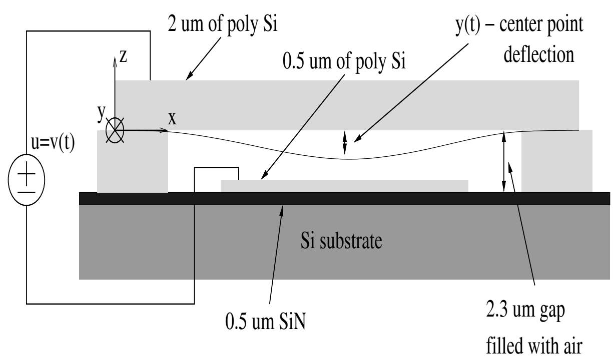

Figure 1: Micromachined clamped-clamped beam example. The input is the applied voltage, the output is the center deflection.

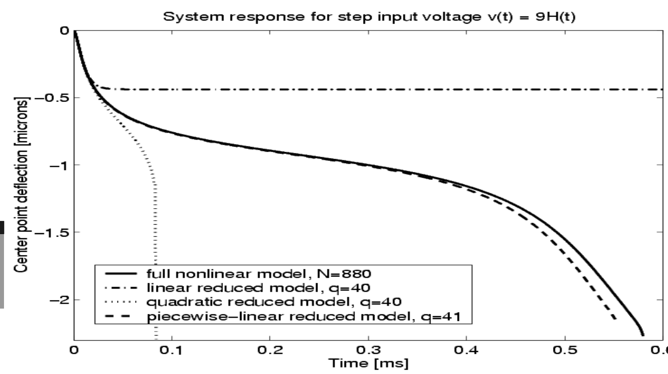

Figure 2: The Trajectory PWL extracted model (dashed line) agrees with the discretized PDE model of the device.

6. Modeling and Synthesis Tools for Analog Circuit Design

Sponsors

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

Project Staff

B. Bond, K. C. Sou, J. White, A. Megretski, and L. Daniel

The presence of several nonlinear analog circuits and Micro-Electro-Mechanical MEM components in modern mixed signal System-on-Chips (SoC) makes the fully automatic synthesis and optimization of such systems a task extremely challenging. In order to address the problem we are developing a Platform Based Design Methodology for Analog RF and Mixed-Signal systems. An Analog Platform consists of a library of pre-characterized analog components that can be instantiated, interconnected and optimally sized to realize a given functional specification at the system level. In order to enable the large scale adoption of our methodology supporting tools are needed for both characterizing the libraries of analog components, and for instantiating and optimizing each component to realize a given functionality. Our initial efforts in this research activity focus on the library characterization by developing tools for the automatic generation, of "field solver accurate", and geometrically parameterized dynamical models of analog linear and nonlinear components. Specific contributions include parameterized modeling of interconnect bus structures [19, 20], RF inductors including displacement currents, skin and proximity effects [21], substrate, fullwave and distributed effects [4, 6, 22, 23], nonlinear circuits and MEMS [24].

References

1. J.P. Bardhan, J.H. Lee, M.D. Altman, S. Leyffer, S. Benson, B. Tidor and J.K. White, “Biomolecule Electrostatic Optimization with an Implicit Hessian,” *Proc. of Modeling and Simulation of Microsystems*, March, 2004

2. J. Bardhan, M. D. Altman, S. M. Lippow, B. Tidor, and J. K. White, “A Curved Panel Integration Technique for Molecular Surfaces”, In *Proc. of Modeling and Simulation of Microsystems*, May 2005

3. J.P. Bardhan, J.H. Lee, M.D. Altman, S. Leyffer, S. Benson, B. Tidor, and J.K. White, “Biomolecule electrostatic optimization with an implicit Hessian,” *Proceedings of Modeling and Simulation of Microsystems*, pp. 164 -167, March, 2004.

4. L. Daniel and J. White, “Numerical techniques for extracting geometrically parameterized reduced order interconnect models from full-wave electromagnetic analysis,” *Proceedings of the IEEE AP-S International Symposium and USNC / URSI National Radio Science Meeting*, June, 2004.

5. J. H. Lee, D. Vasilyev, A. Vithayathil, L. Daniel, and J. White, “Accelerated optical topography inspection using parameterized model order reduction,” forthcoming, *Proceedings of the IEEE International Microwave Symposium*, June, 2005.

6. T. Klemas, L. Daniel, and J. White, “Segregation by primary phase factors: A full-wave algorithm for model order reduction,” *Proceedings of the Design Automation Conference*, Anaheim, CA, 2005.

7. J. H. Lee, D. Vasilyev, A. Vithayathil, L. Daniel, and J. White, “Accelerated optical topography inspection using parameterized model-order reduction,” forthcoming, *Proceedings of the IEEE International Microwave Symposium*, June, 2005.

8. T. Klemas, L. Daniel, and J. White, “Segregation by primary phase factors: A full-wave algorithm for model-order reduction” *Proceedings of the Design Automation Conference*, Anaheim, CA, 2005.

9. T. Klemas, L. Daniel, and J. White, “A fast full-wave algorithm to generate low-order electromagnetic scattering models," forthcoming International Symposium on Antennas and Propagation and USNC/URSI National Radio Science Meeting, Washington, DC, July, 2005.

10. Z. Zhu, A. Demir, and J. White, “A stochastic integral equation method for modeling the rough surface effect on” *Proceedings of the IEEE Conference on Computer-Aided Design*, San Jose, November 2004.

11. D.J. Willis, J.K. White and J. Peraire “A pFFT Accelerated Linear Strength BEM Potential Solver,” *Proc. of Modeling and Simulation of Microsystems*, March, 2004.

12. J. Bardhan, M. D. Altman, S. M. Lippow, B. Tidor, and J. K. White, "A Curved Panel Integration Technique for Molecular Surfaces", In *Proc. of Modeling and Simulation of Microsystems*, May 2005.

13. X. Hu, J. White, and L. Daniel “Analysis of Conductor Impedance Over Substrate using Novel Integration Techniques,” *Proceedings of the Design Automation Conference*, Anaheim, CA, 2005.

14. Z. Zhu, A. Demir, and J. White, “A Stochastic Integral Equation Method for Modeling the Rough Surface Effect On Interconnect Capacitance,” *Proceedings of the IEEE Conference on Computer-Aided Design*, San Jose, November 2004.

15. J. White, “CAD Challenges in BioMEMS Design,” *Proceedings of the Design Automation Conference*, June, 2004, pp. 629-632.

16. C.P. Coelho, J.K. White and L.M. Silveira, “Dealing with Stiffness in Time-Domain Stokes Flow Simulation,” *Proc. of Modeling and Simulation of Microsystems*, March, 2004.

17. C. Coelho, S. Desai, D. Freeman, and J. White, "A Robust Approach for Estimating Diffusion Constants from Concentration Data in Microchannel Mixers," *Proc. of Modeling and Simulation of Microsystems*, May 2005.

18. D. Vasilyev, M. Rewienski and J.K. White, "Perturbation Analysis of TBR Model Reduction in Application to Trajectory-Piecewise Linear Algorithm for MEMS Structures," *Proc. of Modeling and Simulation of Microsystems*, March, 2004.

19. L. Daniel, J. White. "A Model Reduction Approach to Generating Geometrically Parameterized Spiral Inductor Models." *IEEE International Behavioral Modeling and Simulation Conference*, San Jose Oct 2003.

20. L. Daniel, O.C. Siong, L.S. Chay, K.H. Lee, J. White. "A Multiparameter Moment Matching Model Reduction Approach for Generating Geometrically Parameterized Interconnect Performance Models." *IEEE Trans. on Computer-Aided Design of Integrated Circuits and Systems*, v 23, n 5, p 678-93, May 2004.

21. L. Daniel, J. White. "Automatic generation of geometrically parameterized reduced order models for integrated spiral RF-inductors", *Proceedings of the IEEE International Workshop on Behavioral Modeling and Simulation*, San Jose, CA p 18-23.

22. X. Hu, J. H. Lee, J White, L. Daniel. "Analysis of Full-Wave Conductor System Impedance over Substrate Using Novel Integration Techniques", *IEEE/ACM Design Automation Conference*, June 2005. USA.

23. K. C. Sou, A. Megretski, L. Daniel. "A Quasi-Convex Optimization Approach to Parameterized Model-Order Reduction", *IEEE/ACM Design Automation Conference*, June 2005. USA.

24. B. Bond, L. Daniel. "Parameterized Model Order Reduction of Nonlinear Dynamical Systems." Accepted f or publication in the *IEEE/ACM International Conference on Computer Aided Design*, San Jose, Nov 2006.

Publications

Journal Articles, Published

W. Ye, X. Wang, W. Hemmert, D. M. Freeman, and J. White, "Air damping in laterally oscillating microresonator: a numerical and experimental study," *IEEE Journal of Microelectromechanical Systems*, vol. 12, no. 5, pp. 557-566, 2003.

L. Daniel, O. C. Siong, L. S. Chay, K. H. Lee, and J. White, "A multiparameter moment matching model reduction approach for generating geometrically parameterized interconnect performance models," *IEEE Transactions on Computer-Aided Design of Integrated Circuits and Systems*, vol. 23, no. 5, May, pp. 678-693, 2004.

N. Marques, M. Kamon, L. M. Silveira, and J. White, "Generating compact, guaranteed passive, reduced-order models of 3D RLC interconnects," *IEEE Transactions on Advanced Packaging*, vol. 27, no. 4, Nov., pp. 569-580, 2004.

J. Li and J. White, "Low-rank solution of lyapunov equations," Selected for Republication in *SIAM Review*, vol. 46, no. 4, p. 693-713, 2004.

Meeting Papers, Published

D. Vasilyev, M. Rewienski, and J. K. White, "Perturbation analysis of TBR model reduction in application to trajectory-piecewise linear algorithm for MEMS structures," In *Proc. of Modeling and Simulation of Microsystems*, March, 2004

D. J. Willis, J. K. White, and J. Peraire, "A pFFT accelerated linear strength BEM potential solver," In *Proc. of Modeling and Simulation of Microsystems*, March, 2004.

C. P. Coelho, J. K. White, and L. M. Silveira, "Dealing with stiffness in time-domain stokes flow simulation," In

Proc. of Modeling and Simulation of Microsystems, March, 2004.

L. Daniel and J. White, "Numerical techniques for extracting geometrically parameterized reduced order interconnect models from full-wave electromagnetic analysis," In *Proceedings of the IEEE AP-S International Symposium and USNC / URSI National Radio Science Meeting*, 2004.

J. White, "CAD challenges in bioMEMS design," In *Proceedings of the Design Automation Conference*, 2004, pp. 629-632.

Z. Zhu, A. Demir, and J. White, "A stochastic integral equation method for modeling the rough surface effect on interconnect capacitance," In *Proceedings of the IEEE Conference on Computer-Aided Design*, 2004.

J. Bardhan, M. D. Altman, S. M. Lippow, B. Tidor, and J. K. White, "A curved panel integration technique for molecular surfaces," In *Proceedings of Modeling and Simulation of Microsystems*, 2005.

C. Coelho, S. Desai, D. Freeman, and J. White, "A robust approach for estimating diffusion constants from concentration data in microchannel mixers," In *Proceedings of Modeling and Simulation of Microsystems*, 2005.

J. H. Lee, D. Vasilyev, A. Vithayathil, L. Daniel, and J. White, "Accelerated optical topography inspection using parameterized model order reduction," In *Proceedings of the IEEE International Microwave Symposium*, 2005.

X. Hu, J. White, and L. Daniel "Analysis of conductor impedance over substrate using novel integration techniques," To appear il *Proceedings of the Design Automation Conference*, 2005.

T. Klemas, L. Daniel, and J. White, "Segregation by primary phase factors: a full-wave algorithm for model order reduction," In *Proceedings of the Design Automation Conference*, 2005.

T. Klemas, L. Daniel, and J. White, "A fast full-wave algorithm to generate low order electromagnetic scattering models," In *International Symposium on Antennas and Propagation and USNC/URSI National Radio Science Meeting*, 2005.