

Chapter 2. Computational Prototyping Tools and Techniques

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2.1 Free-Surface Hydrodynamics for Offshore Structure Analysis

Sponsors

Industry Consortium (Mobil, Statoil, DNV Software, Shell, OTRC, Petrobras, NorskHydro, Exxon, Chevron, SAGA, NSWC)

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The free-surface hydrodynamics subgroup of our research group invents and implements algorithms used in boundary-element prototyping tools used in offshore engineering.¹ Work is done on linear and nonlinear approaches in the time and frequency domains. Our current focus is on the advancement of higher-order element techniques² and the acceleration of solutions by sparsification. The higher-order boundary element algorithms offer a continuous representation of the solution and gains in efficiency over the low-order approach. The sparsification algorithms (both multipole acceleration and pre-corrected

FFT acceleration) reduce the computational complexity of the solution while preserving the accuracy within an *a priori* tolerance.

The group has had considerable recent success in both of these areas, and the present goal is to combine them to achieve unprecedented efficiency in the hydrodynamic analysis of offshore structures. Current areas of research are: (1) stability issues in the rankine-element time-domain simulation of body and gravity wave interaction, (2) large-amplitude motions of multiple bodies forced by gravity waves using a free-surface Green function formulation, (3) resolution of corner flow singularities by graded higher-order meshes, application of higher-order elements to the second-order frequency domain problem, and (4) pre-corrected FFT and other circulant-based acceleration algorithms for very large hydrodynamic problems.

2.2 Simulation Tools for Micromachined Device Design

Sponsors

Analog Devices

Defense Advanced Research Projects Agency
Contract J-FBI-95-215

1 F.T. Korsmeyer and H.B. Bingham, "The Forward Speed Diffraction Problem," *J. Ship Res.*, forthcoming 1998.

2 C.-H. Lee, "Wave Interaction with Huge Floating Structures," Proceedings of 8th International Conference on the Behavior of Offshore Structures, Delft, The Netherlands, 1997; D. Danmeier, "Multiple-body Simulations Using a Higher-order Panel Code," The Thirteenth International Conference on Water Waves and Floating Bodies, Delft, The Netherlands, 1998.

Dr. Narayana R. Aluru, Dr. Ali Beskok, Professor Martin A. Schmidt, Professor Stephen D. Senturia, Deepak Ramaswamy, Junfeng Wang, Professor Jacob K. White

Micromachining technology has enabled fabrication of several novel microsensors and microactuators. Because of the specialized processing involved, the cost of prototyping even simple microsensors, microvalves, and microactuators is enormous. In order to reduce the number of prototype failures, designers of these devices need to make frequent use of simulation tools. To efficiently predict the performance of micro-electro-mechanical systems, these simulation tools need to account for the interaction between electrical, mechanical, and fluidic forces. Simulating this coupled problem is made more difficult by the fact that most MEMS devices are innately three-dimensional and geometrically complicated. It is possible to simulate efficiently these devices using domain-specific solvers, provided the coupling between domains can be handled effectively. In this work, we have developed several new approaches and tools for efficient computer aided design and analysis of MEMS.³

Our most recent work in this area has been to develop a matrix-free multilevel Newton method for coupled domain simulation.⁴ The approach has much more robust convergence properties than just iterating between domain-specific analysis programs, but still allows us to treat the programs as black boxes.

Our second effort is to find fast approaches to computing geometric sensitivities of electrostatic forces for use in fast coupled-domain simulation and structural optimization.⁵ Our new approach, based on the precorrected-FFT accelerated algorithm,⁶ is hundreds of times faster than direct computation for structures with as few as two thousand discretization unknowns.

Our third effort is in accelerating coupled-domain simulation by allowing physical simplifications where appropriate. We refer to this as mixed regime simulation. For example, self-consistent coupled electromechanical simulation of MEMS devices face a bottleneck in the finite element based nonlinear elastostatic solver. Replacing a stiff structural element by a rigid body approximation which has only six variables, all variables associated with the internal and surface nodes of the element are eliminated which are now a function of the rigid body parameters. The rigid/elastic interface forces obtained from the finite element stiffness matrix contribute to the equilibrium of the rigid body. By an application of the chain rule, the contribution of the elastic "rigid" variables to the "elastic" body part of the jacobian is determined. The rigid/elastic formulation is then coupled with the electrostatic solver in a multilevel newton method. With this approximation, an entire comb drive accelerometer can be solved in less than 15 minutes compared to approximately 135 minutes for an elastic analysis.⁷

2.3 Simulation Algorithms for RF Circuits

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RF integrated circuit designers make extensive use of simulation tools which perform nonlinear periodic steady-state analysis and its extensions. However, the computational costs of these simulation tools have restricted users from examining the detailed behavior of complete RF subsystems. Recent algorithmic developments, based on matrix-implicit itera-

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- 3 S. Senturia, N. Aluru, and J. White, "Simulating the Behavior of MEMS Devices: Computational Methods and Needs," *IEEE Computat. Sci. Eng.* 4(1): 30-43 (1997).
 - 4 N. Aluru and J. White, "A Multi-level Newton Method for Static and Fundamental Frequency Analysis of Eletromechanical Systems," International Conference on Simulation of Semiconductor Processes and Devices (SISPAD), Boston, Massachusetts, September 1997, pp. 125-28.
 - 5 J.R. Phillips and J.K. White, "A Precorrected-FFT Method for Electrostatic Analysis of Complicated 3-D Structures," *IEEE Trans. on Comput.-Aided Des.*, forthcoming.
 - 6 J. Wang and J. White, "Fast Algorithms for Computing Electrostatic Geometric Sensitivities," International Conference on Simulation of Semiconductor Processes and Devices (SISPAD), Boston, Massachusetts, September 1997, pp. 121-24.
 - 7 D. Ramaswamy, "Mixed Regime Simulation for MEMS," Proceedings of the 1998 MIT Student Workshop on High Performance Computing in Science and Engineering.

tive methods, is rapidly changing this situation and providing new faster tools which can easily analyze circuits with hundreds of devices. We have investigated these new methods by describing how they can be used to accelerate finite-difference, shooting-Newton, and harmonic-balance based algorithms for periodic steady-state analysis.⁸

When simulating RF circuits, it is important to include parasitics associated with a layout. However, most layout extraction tools generate an enormous number of resistors, capacitors and inductors for a given layout, and this makes subsequent simulation expensive. There are a number of heuristic algorithms for reducing lines of resistors, capacitors and inductors, but we have recently derived an approach with a formal, but odd, optimality property. The approach is based on recasting the problem into a problem in determining the distribution, with respect to resistance, of the capacitance and inductance. Then, one can solve the reduction problem directly using optimal Gaussian-quadrature.⁹

2.4 Numerical Techniques for Integral Equations

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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; electro- and magneto-quasistatic analysis of integrated circuit interconnect and packaging; and potential flow based analysis of wave-ocean structure interaction.

Although the boundary element method is a popular tool to solve the integral formulation of many three-dimensional potential problems, the method becomes slow when a large number of elements are used. This is because boundary-element methods lead to dense matrix problems which are typically solved with some form of Gaussian elimination. This implies that the computation grows as cubically with the number of unknowns tiles needed to accurately discretize the problem. Over the last decade, algorithms which grow linearly with problem size have been developed by combining iterative methods with multipole approximations.

Our more recent work in this area has been to develop precorrected-FFT techniques which can work for general Greens functions.¹⁰ This approach uses an approximate representation of charge density by point charges lying on a uniform grid. An extension of this work showed that using dual grid (cube vertex) multipole expansions is more efficient for a given required accuracy than either point-charge or standard (cube center) multipole expansions. As is not surprising, the gain in efficiency can be as much as as a factor of eight.¹¹

After a decade of research on fast numerical schemes for potential problems, a somewhat unsatisfying picture has emerged. On one hand, some methods exploit the fact that interactions can be approximated by low order expansions if their sources are sufficiently separated in space. Algorithms that are based on that principle only give a partial solution to deal with complicated problems, in that they allow potential calculations in nearly linear time. However, it still remains unclear how to precon-

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- 8 R. Telichevesky, K. Kundert and J. White, "Fast Simulation Algorithms for RF Circuits," invited paper, Proceedings of the Custom Integrated Circuits Conference, San Diego, California, May 1996.
- 9 K. Nabors, T.-T. Fang, H.-W. Chang, K. Kundert, and J. White, "A Gaussian-Quadrature Based Algorithm for RLC-line to RLC-line Reduction," Proceedings of the 34th Design Automation Conference, Anaheim, California, June 1997; K. Nabors, T.-T. Fang, H.-W. Chang, K. Kundert, and J. White, "An RLC Line Reduction Algorithm with an Odd Optimality Property," Invited Paper, *Proceedings of Progress in Electromagnetics Research Symposium*, Cambridge, Massachusetts, July 1997.
- 10 J.R. Phillips and J.K. White, "A Precorrected-FFT Method for Electrostatic Analysis of Complicated 3-D Structures," *IEEE Trans. Comput.-Aided Des.*, forthcoming.
- 11 J. Li and J. White, "Approximation of Potentials by Multipole Grid Projections," Topical Meeting on Electrical Performance of Electronic Packaging, San Jose, California, November 1997.

dition these algorithms efficiently. On the other hand, a better method using wavelets allows nearly sparse representations of integral operators. Furthermore, the multilevel setting of wavelets allows the construction of efficient preconditioners. Since wavelets are usually constructed in a parameter space of the boundary surface, they are inefficient when the geometry is represented by a large number of parameter patches.

Rather than using vanishing moments in the parameter space, we have constructed a wavelet-like basis with vanishing multipole expansion coefficients, thus avoiding the need of a surface parameterization. We have obtained numerical results which show that integral operators are nearly sparse in this basis, even for complex, multiply connected geometries. Furthermore, the preconditioned system converges in a number of iterations that is independent of the geometry as well as the discretization fineness.¹² We have also investigated improving the condition number by developing second-kind formulations.¹³

2.5 Efficient Three-Dimensional Interconnect Analysis

Sponsors

Defense Advanced Research Projects Agency
Harris Semiconductor
IBM Corporation
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Project Staff

Igor Balk, Michael Chou, Mattan Kamon, Yehia Masoud, Joel R. Phillips, Dr. Johannes Tausch, Professor Jacob K. White

We have developed multipole-accelerated algorithms for computing capacitances and inductances of complicated 3D geometries and have implemented these algorithms in the programs FASTCAP and FASTHENRY. The methods are accelerations of the boundary-element or method-of-moments techniques for solving the integral equations associated with the multiconductor capacitance or inductance extraction problem. Boundary-element methods become slow when a large number of elements are

used because they lead to dense matrix problems which are typically solved with some form of Gaussian elimination. This implies that the computation grows as n^3 , where n is the number of panels or tiles needed to accurately discretize the conductor surface charges. Our new algorithms, which use Krylov subspace iterative algorithms with a multipole approximation to compute the iterates, reduces the complexity so that accurate multiconductor capacitance and inductance calculations grow nearly as nm where m is the number of conductors. For practical problems which require as many as 10,000 panels or filaments, FASTCAP and FASTHENRY are more than two orders of magnitude faster than standard boundary-element based programs. Manuals and source code for FASTCAP and FASTHENRY are available from MIT.

In more recent work, we have been developing an alternative to the fast-multipole approach to potential calculation. Our new approach uses an approximate representation of charge density by point charges lying on a uniform grid instead of by multipole expansions. For engineering accuracies, the grid-charge representation has been shown to be a more efficient charge representation than the multipole expansions. Numerical experiments on a variety of engineering examples arising indicate that algorithms based on the resulting "precorrected-FFT" method are comparable in computational efficiency to multipole-accelerated iterative schemes, and superior in terms of memory utilization.

The precorrected-FFT method has another significant advantage over the multipole-based schemes, in that it can be easily generalized to some other common kernels. Preliminary results indicate that the precorrected-FFT method can easily incorporate kernels arising from the problem of capacitance extraction in layered media. More importantly, problems with a Helmholtz equation kernel have been solved at moderate frequencies with only a modest increase in computational resources over the zero-frequency case. An algorithm based on the precorrected-FFT method which efficiently solves the Helmholtz equation could form the basis for a rapid yet accurate full-wave electromagnetic analysis tool.¹⁴ Our latest work has been on extending the applicability of precorrected-FFT and fast multipole schemes. We have

12 J.R. Phillips and J.K. White, "A Precorrected-FFT Method for Electrostatic Analysis of Complicated 3-D Structures," *IEEE Trans. Comput.-Aided Des.*, forthcoming.

13 J. Li and J. White, "Approximation of Potentials by Multipole Grid Projections," Topical Meeting on Electrical Performance of Electronic Packaging, San Jose, California, November 1997.

combined these fast techniques with new numerically stable integral formulations for problems in electroquasistatics (distributed RC) and for problems with high dielectric permittivity ratios.¹⁵ In addition, we have extended the algorithms in FASTHENRY to include finite substrate conductivity and used it to analyze on-chip inductance.¹⁶ We have also developed parallel versions of the precorrected-FFT algorithm, as well as preconditioners which improve the convergence of the iterative solver used in FASTHENRY.¹⁷

Reduced-order modeling techniques are now commonly used to efficiently simulate circuits combined with interconnect. Generating reduced-order models from realistic 3D structures, however, has received less attention. Recently, we have been studying an accurate approach to using the iterative method in the 3D magnetoquasistatic analysis program FASTHENRY to compute reduced-order models of frequency-dependent inductance matrices associated with complicated 3D structures.

This method, based on a Krylov-subspace technique, namely the Arnoldi iteration, reformulates the system of linear ODEs resulting from the FASTHENRY equation into a state-space form and directly produces a reduced-order model in state-space form. The key advantage of this method is that it is not more expensive than computing the inductance matrix at a single frequency.

The method compares well with the standard Pade approaches and may present some advantages. In the Arnoldi-based algorithm, each set of iterations produces an entire column of the inductance matrix rather than a single entry; if matrix-vector product costs dominate, then the Arnoldi-based algorithm

produces a better approximation for a given amount of work. Finally, we have shown that the Arnoldi method generates guaranteed stable reduced order models even for RLC problems.¹⁸

Our recent work has focused on fast techniques of model reduction which *automatically* generate low order models of the interconnect directly from the discretized Maxwell's equations under the quasistatic assumption. When combined with fast potential solvers, the overall algorithm efficiently generates accurate models suitable for coupled circuit-interconnect simulation.¹⁹

The design of single-chip, mixed-signal systems, which combine both analog and digital functional blocks on a common substrate, is now an active area of research, driven by the relentless quest for high-level integration and cost reduction. A major challenge for mixed-signal design tools is the accurate modeling of the parasitic noise coupling through the common substrate between the high-speed digital and high-precision analog components.

We are working on a sparsification method which, based on eigendecomposition, handles edge effects more accurately than previously applied multipole expansion techniques. Then we combine the sparsification approach with a multigrid iterative method that converges more rapidly than previously applied Krylov-subspace methods. Results on realistic examples demonstrate that the combined approach is up to an order of magnitude faster than the sparsification and Krylov-subspace method and orders of magnitude faster than not using sparsification.²⁰

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- 14 J. Tausch and J. White, "Precondition and Fast Summation Techniques for First-Kind Boundary Integral Equations," Third IMACS International Symposium on Iterative Methods in Scientific Computation, Jackson Hole, Wyoming, July 9-12, 1997.
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 - 16 J. Tausch and J. White, "BEM Solution of Laplace's Equation in Multi-Layered Media with High Permittivity Ratios," Numerical Treatment of Multi-Scale Problems, Third GAMM-Seminar, Kiel, Germany, January 24-26, 1998; M. Chou and J.K. White, "Efficient Formulation and Model-Order Reduction for the Transient Simulation of Three-Dimensional VLSI Interconnect," *IEEE Trans. Comput.-Aided Des. Integrat. Circ. Syst.*, forthcoming.
 - 17 M. Kamon, N. Marques, and J. White, "FastPep: A Fast Parasitic Extraction Program for Complex Three-Dimensional Geometries," Proceedings of the IEEE Conference on Computer-Aided Design, San Jose, California, November 1997; M. Kamon, N. Marques, L.M. Silveira, and J. White, "Generating Reduced Order Models via PEEC for Capturing Skin and Proximity Effects," *Proceedings of the Sixth Topical Meeting on Electrical Performance of Electronic Packaging*, San Jose, California, November 1997.
 - 18 L.M. Silveira, I. Elfadel, M. Kamon, and J. White, "Coupled Circuit-Interconnect Analysis Using Stable Arnoldi-Based Model-Order Reduction," *Proceedings of Progress in Electromagnetics Research Symposium*, Cambridge, Massachusetts, July 1997.
 - 19 M. Kamon, N. Marques, and J. White, "FastPep: A Fast Parasitic Extraction Program for Complex Three-Dimensional Geometries," Proceedings of the IEEE Conference on Computer-Aided Design, San Jose, California, November 1997; M. Kamon, N. Marques, L.M. Silveira, and J. White, "Generating Reduced Order Models via PEEC for Capturing Skin and Proximity Effects," *Proceedings of the Sixth Topical Meeting on Electrical Performance of Electronic Packaging*, San Jose, California, November 1997.

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- Aluru, N., and J. White. "A Multi-level Newton Method for Static and Fundamental Frequency Analysis of Electromechanical Systems." *International Conference on Simulation of Semiconductor Processes and Devices (SISPAD)*, Boston, Massachusetts, September 1997, pp. 125-28.
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- Costa, J.P., M. Chou, and L.M. Silveira. "Efficient Techniques for Accurate Modeling and Simulation of Substrate Coupling in Mixed-Signal ICs." Design, Automation and Test in Europe, Exhibition and Conference (DATE '98), Paris, France, February 1998.
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