

Design Tools for Emerging Technologies

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Abstract—The rapidly expanding diversity of technology available at the nanoscale is disrupting the existing transistor-centric microelectronics design paradigm, resulting in nearly decade-long delays between prototype demonstration and technology deployment. The key to reducing these innovation-inhibiting delays is to develop algorithmic approaches that can start with first principles based descriptions of novel nanotechnology and rapidly and reliably synthesize manufacturable designs. Design tools are evolving this direction, with new extremely efficient yet customizable physical simulators, automatic parameterized low-order model extraction, and ever improving algorithms for *robust optimization*—new techniques that generate manufacturable designs by optimizing *both* system performance *and* robustness to manufacturing variations. In this paper we give a few examples of the coupling of such approaches, but mostly offer pointers to literature for researchers interested in contributed to this rapidly growing field of coupled simulation and robust optimization.

Keywords—*optimization, simulation, nanotechnology, computer-aided design*

I. INTRODUCTION (HEADING 1)

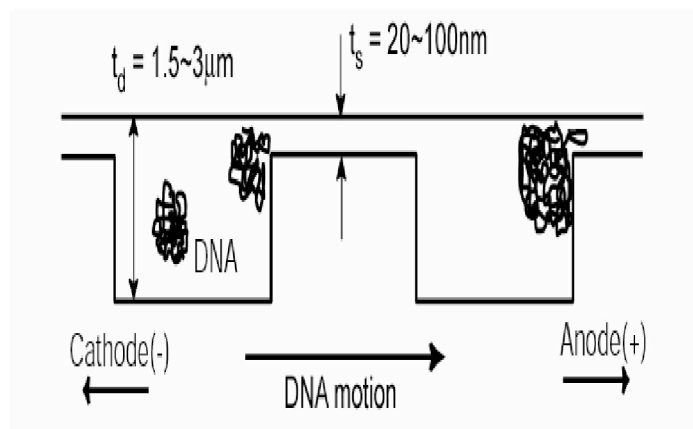


Figure 1. Nanofluidic DNA filter [2].

The diversity of technological options being generated by recent developments in micromachining, nanophotonics, carbon nanotubes, quantum wells, and molecular electronics (Figs. 1–4) is causing a major disruption to a decade's old microelectronics design paradigm; one that is based on a few technological alternatives focused solely on generating semiconducting transistors. The major ramification of this disruption is an enormous delay between prototype proof of concept and deployable technology, as is evidenced by the near decade-long product development cycle associated with the

micromachining, or MEMS, industry. Failure to address product development cycle delays as technology diversifies at the nanoscale will effectively halt progress, because the delays will cascade. Without a previous generation's technology in useable form, it is unlikely that the next generation technological investigation can thoroughly begin.

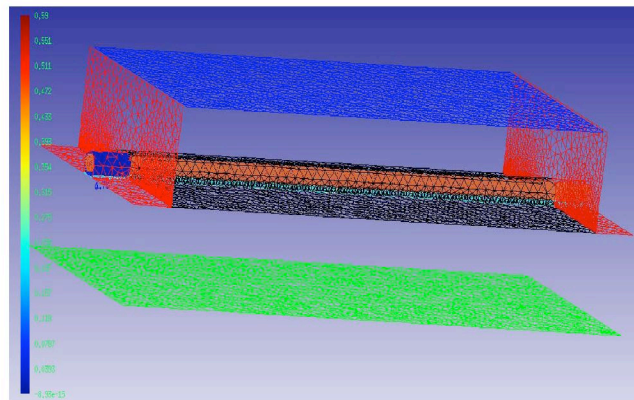


Figure 2. Carbon nanotube transistor electrostatics[2]

It is easy to suggest that one simply apply the very rapidly improving optimization software to the problem of optimizing nanoscale devices, but there are three key problems that must be addressed. The first problem is that classic optimization approaches can often find a theoretical “optimum” that is impractical, because this optimum is too rapidly degraded by manufacturing imperfections. To address this problem, we can exploit emerging “Robust optimization” approaches. Robust optimization refers to a new class of optimization techniques [1] that optimize not only the performance of a system, but also its robustness in the face of inevitable deviations of the design parameters. A second problem is to determine how best to *convexify* the problem formulations and robustness constraints so as to insure efficient and reliable optimization. The third issue is that for devices in leading-edge technologies, the only model may be a three-dimensional physics-based simulation. The optimization approach will need to be somehow combined with simulation without making the problem computationally intractable. Although these are daunting challenges, we see developing this kind of robust optimization based synthesis of manufacturable devices as the most promising approach to

cracking the diverse technology product development problem.

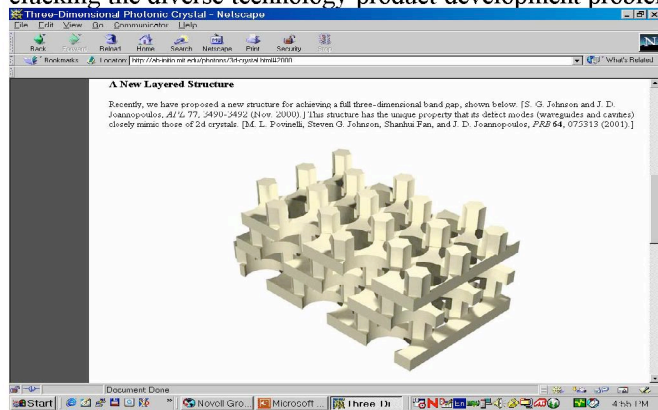


Figure 2. 3d photonic crystal [4].

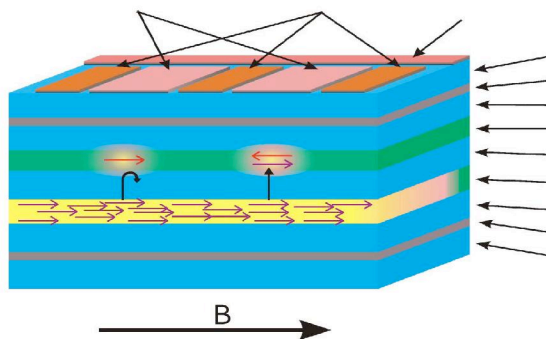


Figure 4: Quantum-well Q-bit [5].

II. ROBUST OPTIMIZATION

The idea of applying numerical optimization techniques to engineering design problems has a long history, but recently this idea has been augmented by new methods of “robust optimization,” whose importance and general ideas we summarize below.

In principle, optimization can be applied as soon as a tractable forward model, *i.e.*, a simulator, has been developed. In the simplest approach, an optimization routine adjusts the design variables, then carries out an analysis (using the forward model), and repeats this process. For a design problem with just a modest number of design variables, and a forward model that can be evaluated reasonably quickly, including gradients (perhaps by an adjoint method), this approach can work well. Two traditional pitfalls in applying optimization technology, however, are parameter variations (that occur in manufacturing or operation) and model errors (both intentional and unintentional). In either case, the performance of the system (as built or manufactured) deviates from that predicted by the model. Sometimes, the design is not too sensitive to these deviations, but in other cases the “optimized” design is notoriously sensitive to the mismatch between the real system and the model. This results in real performance that is far inferior to that predicted by the model. There are many ways to

deal with this basic problem. One is to limit the number of design variables to a small handful, carefully chosen so that none of the possible designs is too sensitive. Another standard technique is based on posterior sensitivity analysis, in which the design is at least checked for sensitivity to parameter variations or model uncertainty.

Another basic method is to add a simple regularization term to the objective that penalizes sensitive designs. The extra term penalizes designs that are sensitive to variation in the parameter, and thus avoids fragile, nonrobust designs. This basic regularization method is readily extended to far more complex situations, with many parameters, and sophisticated models for the expected variations, such as multivariable stochastic models or ellipsoidal bounding models. Unfortunately, this approach often leads to very difficult optimization problems, with nondifferentiable objectives.

A relatively recent approach is robust optimization, whose development was begun around 1995 by Nemirovski, Ben-Tal, El Ghaoui, and others. In robust optimization, the parameter variations and model mismatch are explicitly taken into account, using models for the variation that are stochastic, or, more often, unknown but bounded. Thus, for example, a set of model parameters might be known to be in a given uncertainty ellipsoid or a given uncertainty polyhedron. The constraints are required to hold for all possible values of the parameters, and the objective for the robust optimization problem is taken to be the maximum value of the objective, over all possible values of the parameters. This results in minimax optimization problems, which can be very difficult to solve. The surprising new results are that for certain specific classes of problems, including classic least-squares, linear programming, and quadratic programming, such problems can be solved exactly efficiently, using new algorithms for more general convex optimization. To give one specific example, the problem of solving a robust linear program, with the constraint that the coefficients lie in given ellipsoids, reduces to a so-called second order cone program (SOCP), and can be solved exactly, and very efficiently. (A sparse SOCP with 10^5 variables and 10^6 constraints can be solved in minutes on a desktop PC.) A decade ago, no one would have considered such a problem tractable, let alone routinely solvable.

Robust optimization is described in Ben-Tal and Nemirovski [1], as well as in Boyd and Vandenberghe [6]. The results so far are for convex problems, and mostly basic ones. But there is enough known that the methods can be useful in other problems. For example, a standard sequential quadratic programming (SQP) method, for general nonlinear problems, can be adapted to handle robustness by replacing the QP with a robust QP.

III. COUPLING OPTIMIZATION TO SIMULATION

As mentioned above, robust optimization will be most useful for nanotechnology exploration if the optimization can be combined with a detailed simulation model of the device. There are three approaches for combining optimization algorithms with simulation: combining Hessian-free optimization algorithms with efficient adjoint-based gradient computation; simultaneously optimizing and simulating the

model by only implicitly constructing the Hessian; and generating parameterized reduced-order models of the device from simulation and then using the parameterized reduced-order model in the optimization. Below we describe the latter two strategies as there have been recent promising results.

A. Simultaneous Optimization and simulation using an Implicit Hessian

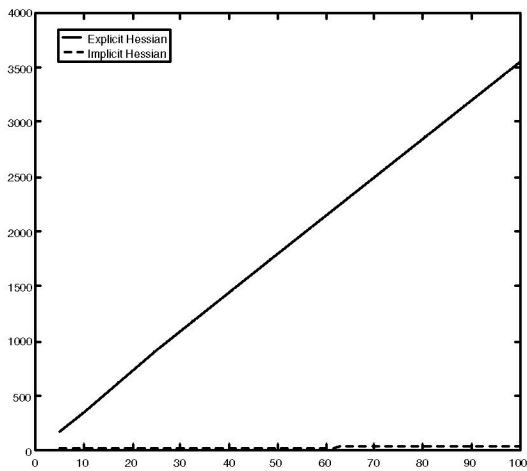


Figure 5. Optimization time vs. # parameters for implicit and explicit Hessians [7].

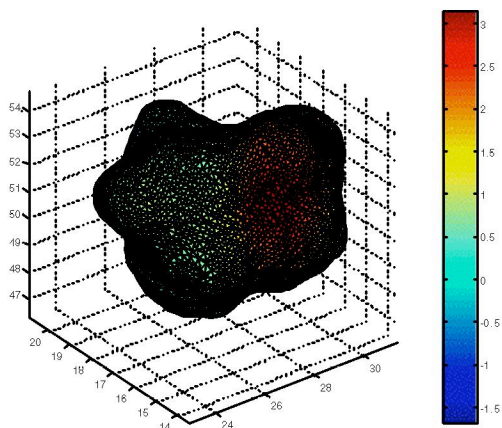


Figure 6. E. Coli Inhibitor Chorismate mutase [7].

When using the now-pervasive Primal-Dual interior point methods for convex optimization, the computation of each optimization step involves solving a large linear system that includes a Hessian associated with cost function and the constraints. For large problems, this linear system can be solved iteratively, typically using a preconditioned Krylov subspace method. Fast integral equation methods for electromagnetic analysis (useful for photonic device analysis) or finite-element based multiphysics simulators (used for a variety of nanotechnology device analyses) also form large linear systems of equations that are typically solved iteratively.

When combining an interior point based optimization technique with a fast solver or finite-element based device simulator, it is possible to avoid the expensive process of extracting the Hessian from the simulator for use in the optimizer. For example, it was recently shown for a problem in biomolecule electrostatic optimization that combining a fast 3-D electrostatic solver with a primal-dual optimization algorithm, effectively implicitly computing the Hessian, reduced the optimization time by orders of magnitude over the use of an explicit Hessian [7].

There are a number of advantages to combining the simulation and the optimization when using robust optimization methods. There are the obvious computational efficiencies, as demonstrated above in the biomolecule optimization problem. In addition, the detailed simulator discretization equations are available in the optimization algorithm, and these discretization equations typically contain the smoothest relation between design parameters and equations. This smooth relation can then be fit with first order variations, yielding the kind of explicit relation between constraints and design parameter variations needed to take advantage of recent developments in robust optimization.

B. Parameterized Reduced Order Models (PROM)

Recent developments in techniques for generating geometrically parameterized reduced order models (PROMs) from detailed physical simulation [8] are another alternative to coupling robust optimization to simulation. For example, we have used this technique to develop improved optical inspection methods for the semiconductor industry [9]. Currently, optical scattering measurements are made from a device under inspection and the geometry is determined by expensive three-dimensional electromagnetic simulation of geometrically parameterized candidate structures. In order to accelerate the approach, we developed a projection-based method for automatically extracting a PROM from the electromagnetic simulation, and then used the PROM with an optimization algorithm to determine the parameter values. As can be seen from Figure 7, a simple rectangular parallelepiped example, we were able to accurately predict structure.

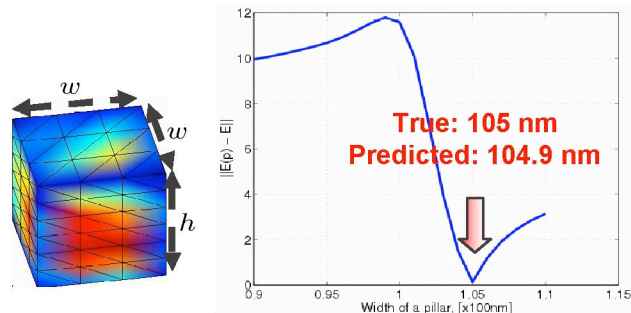


Figure 7. Optimization on 50-state parameterized reduced-order model predicts shape [9].

Although the above preliminary results demonstrate a proof of concept, there are a number of challenges to extending the PROM strategy to more realistic robust optimization problems. The first issue to consider is that the model is to be used for

optimization, and therefore the parameterized reduction strategy should not just focus on the traditional issues of fidelity and reduced model computational complexity, but must also consider the issue of maintaining convexity so that the model is easily optimized. A second critical difficulty is the rapid increase in reduced model cost with number of design parameters. To address this problem, one can pursue a strategy in which a kind of singular value decomposition is used to reparameterize the design to a much smaller set of more mutually independent, and more critical, design parameters. Then, the reparameterized design can be optimized, and the physical problem then inferred. Such reparameterization is likely to improve the conditioning of the subsequent optimization, but the exact approach to reparameterization can also ease the robustness constraints just by selecting reparameterizations that are less sensitive to process variations.

IV. CONCLUSIONS

In this brief paper, the authors attempted to expose the reader to some of the issues associated with developing products with emerging nanotechnology, and provide some insight into the authors' view of how design tools must evolve to meet the challenge of reducing "time-to-market" for products based on this emerging technology. We hope to encourage more researchers to join this exciting field.

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REFERENCES

- [1] A. Ben-Tal and A. Nemirovski, *Lectures on Modern Convex Optimization* (SIAM, 2001).
- [2] H. Reid and J. White, Manuscript under development.
- [3] J. Han and H. G. Craighead, "Separation of Long DNA Molecules in a Microfabricated Entropic Trap Array," *Science* **288**, 1026 (2000).
- [4] S. G. Johnson and J. D. Joannopoulos, "Three-dimensionally periodic dielectric layered structure with omnidirectional photonic band gap," *Appl. Phys. Lett.* **77**, 3490 (2000).
- [5] R. Caflisch, <http://www.math.ucla.edu/~material/presentations/USCApplMath.ppt>
- [6] Stephen Boyd and Lieven Vandenberge, *Convex Optimization* (Cambridge Univ., 2004).
- [7] J. Bardhan *et al.*, "Fast methods for biomolecule charge optimization," *Intl. Conf. on Modeling and Simulation of Microsystems* (San Juan, April 2002).
- [8] L. Daniel *et al.*, "A multiparameter moment matching model reduction approach for generating geometrically parameterized interconnect performance models," *IEEE Trans. Computer-Aided Design Integ. Circuits Syst.* **23** (5), 678–693 (2004).
- [9] J. Lee *et al.*, "Accelerated optical topography inspection using parameterized model order reduction," to appear in *Microwave Theory Tech. Symp.* (June 2005).