# The Future of Electronic Device Design

***Device and process simulation find intelligence on the World Wide Web***

**Bryan A. Biegel**

From digital cell phones to automatic teller machines to personal computers, information technology (IT) has become pervasive in our society. There are two simple reasons for this: the cost of sophisticated IT is decreasing rapidly, and its capabilities are increasing equally rapidly. IT now provides us with empowering technological innovations, enables us to address new challenges in our world (such as global warming or ozone depletion), and allows us to tackle increasingly complex questions about our universe (such as how and when it came to be).

How has this rapid advancement in IT been accomplished? Over the past several decades, the most wildly successful strategy has been to miniaturize the thousands or millions of electronic devices (such as transistors) that give intelligence to the technology. Down-scaling of electronics produces faster devices and allows more of them to be integrated on each semiconductor chip, doubly increasing functionality.

Unfortunately, as electronic devices get smaller, further down-scaling becomes more challenging. To maintain the rapid advancement of IT, technologists have increasingly turned to computer-based simulation of the fabrication and operation of electronic devices and integrated circuits (collectively called TCAD, or technology computer aided design) to determine how to continue down-scaling. In this article, I will discuss the challenges and opportunities for the future of TCAD.

## History of TCAD

Predicting the future of TCAD requires us to first analyze its (relatively short) history. Before the 1980s, numerical simulation was not a fundamental part of electronic device development (although it was used in device research). Instead, to design the next generation device, the current generation device structure and fabrication steps were modified according to a set of simple scaling laws.

Scaling laws have been particularly effective in improving the MOSFET (metal-oxide-semiconductor field effect transistor - Figure 1), which thereby became the dominant transistor technology in the early 1980s. The MOSFET's most critical feature, the channel length, has decreased from about 50 µm in 1960 to 1 µm in 1990 to 0.18 µm by 2000.

At a channel length of about 1 µm, scaling laws no longer accurately predicted the operation of real devices, due to increasing structural complexity and second-order small-geometry effects on operation. At the same time, increasingly powerful computers and TCAD software had made possible accurate multi-dimensional simulation of realistic device structures and physics. As a result, TCAD has replaced scaling laws in the central role of guiding electronics development in the 1990s. With the employment of TCAD, the current electronics advancement process is as depicted in Figure 2.

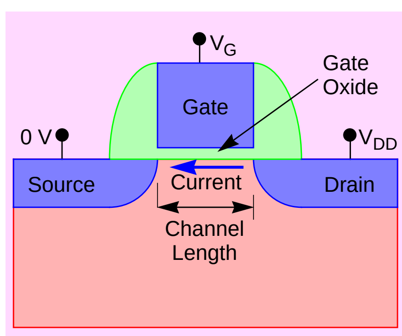



***Fig. 1*** ***Basic MOSFET structure (vertical cross-section). Blue regions are silicon with electron donating dopants, red is silicon with electron acceptor dopants, and green is silicon dioxide (an electrical insulator). Gate voltage $V_G$ controls electron flow (current) in the channel between source and drain.***

We emphasize that TCAD does more than simply improve on scaling laws - it has actually replaced some of the expensive and slow fabricate-test-redesign experimental development process. Simulation allows one to start designing devices several generations ahead of production, without requiring the development or purchase of expensive new fabrication equipment. As a result, since about 1994, the time between introduction of new electronics technology generations has decreased to two years from a historic average of three years.

The electronics technology cycle is predicted to slow to three years again after the current (0.18 µm) generation, due to increasing challenges of

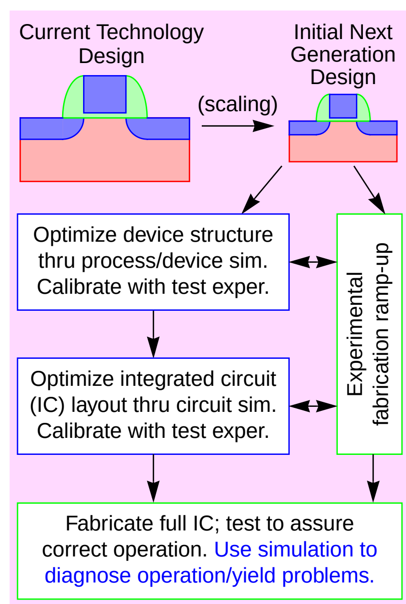



***Fig. 2*** ***Current electronics technology advancement process. Simulation (indicated by blue) now plays a significant role throughout the process.***

miniaturization. TCAD faces related challenges as it struggles to keep pace with the technology, and simultaneously assist in its advancement. We now detail the challenges and opportunities for the future of TCAD.

## Challenge 1: New Process and Device Physics

As technologists attempt to expand the role of TCAD in electronics development, the first challenge is the tremendous range of process and device physics that must be modeled. In fact, both process and device physics are rapidly getting *more* complicated in state-of-the-art products.

### Process Modeling & Simulation

For process modeling, the industry is incorporating major process and material changes into their production lines, such as the addition of copper interconnects, silicon-germanium layers, silicon-on-insulator technology, low-permittivity dielectrics, new photoresists, and many more. Accurately simulating each significantly new process requires one or more models to be developed, tuned using experimental measurements, and programed into process modeling tools. This suggests the need for a coordinated and ongoing experimental, model development, and code development effort.

A more fundamental challenge for future process modeling is that device features are shrinking to a size at which we can no longer pretend that all materials and reactants are smoothly varying. For example, dopant atoms in the channel region may soon need to be treated individually as their numbers drop with reduced device area, polycrystalline silicon regions may have dimensions similar to their grain size, gate oxides are approaching just a few atomic layers in thickness, and impurity clusters and material defects approach the size of device features. To accurately model the device fabrication and properties in these cases, process modeling tools will need a hierarchy of atomistic, molecular, atomic layer, and polycrystal models as well as bulk models.

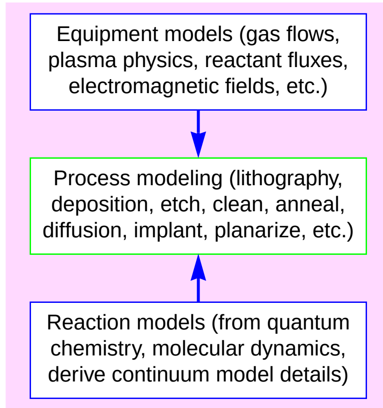



***Fig. 3** Ultimately, we will be able to derive new process models from equipment models and "first principles" reaction models. Currently, every new fabrication process and reactor must be painstakingly characterized from experimental measurements.*

A final challenge and grand opportunity for future process modeling is the incorporation of accurate atomic-scale reaction models (reaction energies, rates, and products) and process equipment models (gas flows, reactant concentrations, and temperatures versus equipment settings). With this capability, the hierarchy of models and the recent processes changes listed above could be *derived by* (rather than *specified to*) the process modeling tool, as depicted in Figure 3. Developing new process models from theory, rather than experiment, would be a major advancement.

### Device Modeling & Simulation

For device simulation, the challenge to maintain accuracy as devices shrink is at least as great as for process modeling. State-of-the-art devices show increasing small-geometry effects, including hot electron transport, punch-through, avalanche multiplication, drain-induced barrier lowering, oxide and junction breakdown, leakage currents, grain-size effects, and discrete dopant effects. As clock frequencies rise to 1 GHz and above in the next few years, we will see increased microwave interference from external sources.

Devices are also starting to exhibit significant quantum effects, including gate oxide and bandgap tunneling, inversion layer quantization, quantum transport, and carrier density smoothing. Eventually, as electronic devices approach limits to their improvement, they will be assisted, and in some cases replaced, by quantum, optoelectronic, and photonic devices. Thus, future full-function device modeling tools must contain a comprehensive set of models that span this technology range as well.

In spite of these electronic device physics changes, the relatively simple drift-diffusion model has remained dominant for high-volume device simulation for the past 30 years. However, accurate treatment of emerging device physics demands that we employ more accurate device physics models in the near future. Table 1 summarizes the set of device models that are needed.

Some commercial TCAD tools do implement a few device models in addition to drift-diffusion. However, the continued dominance of the drift-diffusion model in the electronics development cycle indicates that more accurate models are too computationally expensive, not sufficiently robust, and/or do not provide the required

| Complexity, Computational Cost | Classical Models | Quantum-Corrected Models | Full Quantum Models |
|---|---|---|---|
| Low | Drift-diffusion | Density-gradient | Schrödinger, Transfer matrix |
| Moderate | Energy balance (EB), Hydrodynamic (HD) | Quantum EB, Quantum HD | Density matrix, Wigner function |
| High | Boltzmann transport equation | Quantum Boltzmann equation | Green's functions |
| Microwave | Substitute Maxwell's equations for Poisson equation in above | | |
| Optoelectronic | Add semiconductor Bloch equations | | |

***Tab. 1** Full range of PDE-based classical and quantum, electronic and optoelectronic semiconductor device models. Full-function TCAD software should implement all of these models, and allow them to interoperate in appropriate regions of the same device in a single simulation.*

features. Our first device modeling challenge is to correct this.

Another challenge for device modeling is that the relevant length, time, and energy-scales, as well as the physics, change dramatically with position in the device (e.g., quantum effects being significant only in the channel of a MOSFET). Efficient simulation dictates that the simplest model which provides adequate accuracy should be used in each region of the device.

To summarize the device modeling challenge, device modeling physics is getting much more complicated, and a comprehensive set of device models need to be implemented and available for use in any combination and configuration in future device simulation tools. It is completely impractical for a TCAD company to use the traditional approach of developing single-model device simulation codes to implement a full set of interactive models. Further, this approach does not give the TCAD user the flexibility to modify models according to their needs.

Here again we find both a challenge and a grand opportunity for future TCAD. The solution is to abandon the development of innumerable single-model simulation tools in favor of creating a single, general-purpose partial differential equation (PDE) solver. Using a PDE-solver, a full set of PDE models (Table 1) and an unlimited number of variations can be rapidly implemented by the user with little or no additional programming. The PDE-solver could also enable these models to interact within a single device.

Figure 4 shows how TCAD model developers can proceed directly from developing their model as a system of PDEs to running simulations. First-generation PDE-solver device modeling tools exist, such as PROPHET by Lucent Technologies and Taurus by Avant!.

Admittedly, there may be some overhead in computation time when using a general-purpose PDE solver. However, computation time is measured in minutes or hours, while TCAD software development time is measured in months or years. This disparity will increase as computers get faster and software gets more complex. Clearly, it makes sense to leverage the very computational technologies TCAD is helping to create in the effort to meet TCAD's challenges.

### Virtual Fab

Given the increasing complexity of real device structures, we must run an accurate *process* simulation to get a device structure for meaningful device simulation. Similarly, accurate circuit simulations require device models derived from accurate device simulations. In fact, the ultimate platform for TCAD would be a "Virtual Fab", in which all aspects of electronics system production are simulated before the fabrication plant comes on line. This should speed development, reduce development cost, and assure that all aspects of production, as well as the final product itself, will work properly. Figure 5 depicts the major functional elements of a Virtual Fab.

## Challenge 2: New TCAD Software

As indicated above, much new TCAD software is needed to maintain the accelerated electronics technology cycle. TCAD users need simulation software with more accurate models, capability to run bigger computations, more flexibility and functionality, and better ease of use (e.g., interactive graphical input and output, more automation). Thus, the second challenge to the increased use of TCAD tools in guiding electronics development is simply the difficulty of writing the necessary TCAD software in time.

Current practice is that every TCAD researcher, group, or company must develop their own set of TCAD tools to investigate any TCAD functionality. This development approach (Figure 5a) has led to a huge duplication of effort, poor specialization, and relatively slow advancement of TCAD software.

The software challenge suggests an opportunity to revolutionize the TCAD software development process. Developers need to work together to develop a single, extensible TCAD platform with all of the essential capabilities. Advanced features are implemented in a modular fashion, just as with TCAD model development using the PDE-solver approach.

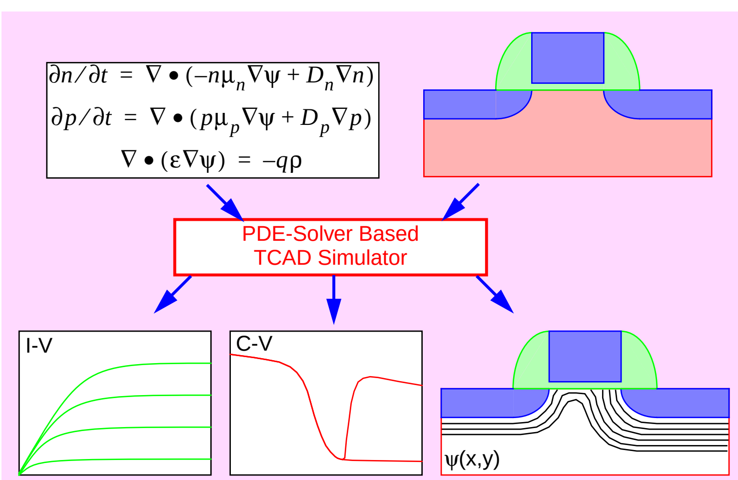



***Fig. 4** PDE solver approach to implementing new TCAD models. The model developer can go directly from specifying the model to running simulations. This is dramatically quicker than the traditional approach of having to write an entire new TCAD program for each significantly new model.*

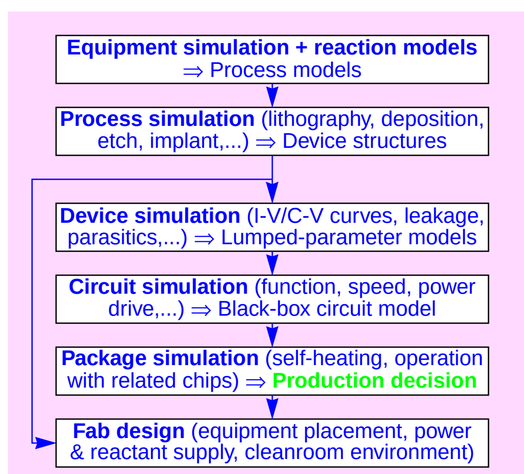
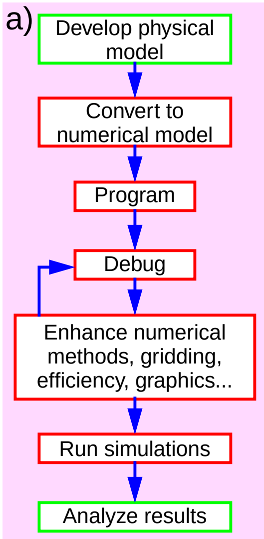



***Fig. 5** Virtual Fab software functional elements. In a virtual fab, all aspects of electronics system production can be simulated and debugged before production starts, or even before the fabrication plant comes online.*



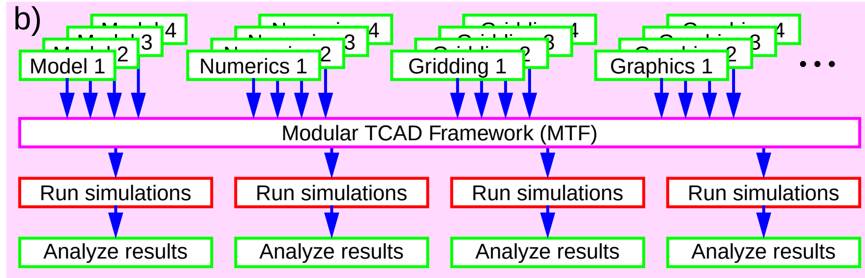




***Fig. 6*** ***TCAD tool development processes. a) The conventional development process, where a developer or group develops a new code from the ground up - a long and wasteful process. b) The proposed modular TCAD Framework (MTF) approach, where each developer is able to contribute their specific expertise, take advantage of the expertise of others, and quickly test new capabilities in simulations.***

### Modular TCAD Framework

This modular TCAD framework (MTF) would be a kind of TCAD "operating system", where software developers would install modules of TCAD functionality developed in their area of expertise. Such functionality includes model definition and code for numerical computation, gridding, graphics, non-linear and linear system solvers, graphical interfaces, and so on.

The MTF must provide a foundation for the independently-developed modules to function and interact properly. It would provide database access (for storage and retrieval of functional modules, material data, physical constants, TCAD models, etc.), memory management, file I/O, facilities for tool interaction, and a basic user interface. The MTF would also provide a standard language for describing physical quantities, physical structures, materials, activities performed (e.g., process steps or device simulations), and so on.

The MTF would enable the much more efficient TCAD development process shown in Figure 5b, where each developer can easily contribute their expertise, and each user can utilize the expertise of every specialist. The MTF enables and encourages collaboration and competition in the development of high-quality and high-functionality TCAD software. This seems essential if TCAD is to remain viable in the face of the challenges it faces in the near future.

In spite of its advantages, realization of the MTF will require a significant mind-set change for some (especially commercial) developers to accept the concept of collaborative R&D. Thus, when some of the technologies needed for a MTF were proposed several years ago by the TCAD group at Stanford University, gaining industry-wide consensus and support was problematic.

However, as commercial tools fall behind the technology curve in the near future, for reasons discussed above, the motivation for an MTF will become irresistible, and hopefully not too late. Even with the MTF, commercial TCAD vendors will still be able to charge for access to advanced TCAD features in the MTF, such as sophisticated graphics and "intelligence".

### Intelligent TCAD

A brief consideration can convince us that current TCAD tools are not very smart. They don't learn from experience, even after thousands of simulations, how to produce a result in less time, with more accuracy, or a device with better performance. They often require the user to baby-sit the simulation to make sure it completes, and to perform tedious work to derive desired information from simulations.

Intelligent TCAD software could:

· estimate the device technology, structure, and fabrication steps based on performance requirements,

· optimize device fabrication and operation for a given application,

· use self-adaptive device models (versus position and operation) to meet accuracy requirements,

· use adaptive computations (gridding, numerics, and algorithms) to optimize efficiency versus accuracy,

· estimate computational resources and time for simulations,

· have automated fault (non-convergence) detection and correction (i.e., "self-healing" software),

· derive process models from quantum chemistry and reactor models,

· automatically calibrate models (reactor, process, device) using experimental measurements,

· have intelligent user interfaces (speech, gesture, natural language, and math expression recognition; immersive environments), and

· allow real-time simulation steering.

Past parochial TCAD development efforts have apparently prevented us from collectively implementing such intelligent features that would vastly multiply the utility of TCAD tools.

## Challenge 3: New Computation Paradigm

Even if current TCAD models and software were replaced with more sophisticated versions, TCAD still could not realize its potential, due to a third challenge: that sufficiently powerful computation hardware for handling these complex models and simulation tasks is too expensive for the typical TCAD user, or perhaps *any* user. Indeed, huge computational resources (computation, memory, software, and data storage) are often an essential feature of the "intelligent" TCAD features listed in the previous section.

The challenge of insufficient computation power for TCAD again suggests an opportunity. That is to provide access to thousands or millions of otherwise idle computers around the world by linking them together into an immense virtual supercomputer, or computational grid. Many organizations, such as the National Science Foundation (NSF) supercomputer centers, are now working together to develop a computational grid infrastructure, and a few prototypes have been demonstrated. The key objectives of the Grid effort (see Figure 6) are:

· to enable distributed (e.g., Web-based) access to compute resources,

· to provide aggregate computing power vastly greater than that of any single machine,

· to enable immersive collaboration-at-a-distance, and

· to link this infrastructure to high-value experimental equipment.

The benefits of accomplishing these goals will be far-reaching:

· high performance computing would be accessible to anyone,

· temporally and spatially variable computational needs could be handled,

· the cost of computation would drop precipitously with direct competition to provide Grid resources, and

· users would not have to install or troubleshoot huge application codes on heterogeneous machines.

Based on these goals and benefits, the MTF would be a perfect application for the Grid. In fact, the Purdue University Network Computing Hubs (PUNCH), demonstrates very well some of the possibilities of distributed TCAD. PUNCH provides Web-based access to several TCAD tools, runs them on a small, distributed compute cluster, and allows users to create TCAD input files and access simulation output via the Web. The Grid will allow us to enhance and scale this concept to the size of the world-wide Web.

## Summary

We are on the path to meet the major challenges ahead for TCAD. The emerging computational grid will ultimately solve the challenge of limited computational power. The Modular TCAD Framework will solve the TCAD software challenge once TCAD software developers realize that there is no other way to meet industry's needs. The MTF also provides the ideal platform for solving the TCAD model challenge by rapid implementation of models in a partial differential solver.

## Read more about it

· For information about future semiconductor technology (predictions and challenges), see *The International Technology Roadmap for Semiconductors* at www.itrs.net/ntrs/publntrs.nsf.

· The future of TCAD is discussed in the above *ITRS*, with a longer discussion at www.sematech.org/public/docubase/abstract/2696atr.htm.

· Two vendors of state-of-the-art TCAD software are Avant! (www.avanticorp.com) and Silvaco (www.silvaco.com).

· A primer on several emerging semiconductor technologies (copper interconnects, silicon-germanium, and silicon-on-insulator) recently commercialized by IBM is at www.chips.ibm.com:80/bluelogic/showcase.

· For information about past work on TCAD frameworks, see the Stanford University TCAD group's web site: www-tcad.stanford.edu/tcad/pubs/framework.html.

· Information about the computational grid under development can be found at the NSF Supercomputing Centers: NCSA (www.ncsa.uiuc.edu) and SDSC (www.sdsc.edu), NASA Ames Research Center (www.nas.nasa.gov/Groups/Tools/IPG), and others.

· The Purdue University Network Computing Hubs (PUNCH) is at punch.ecn.purdue.edu:8000/.

## About the author

Bryan A. Biegel received his Ph.D. in electrical engineering from Stanford University in 1997, where he developed software for numerical simulation of quantum electronic devices. He is now a member and the manager of the Science and Technology Group (www. nas.nasa.gov/Groups/SciTech) in the Numerical Aerospace Simulation Division at NASA Ames Research Center. His current work focuses on the use of the PROPHET PDE solver (by Lucent Technologies) to implement the density-gradient model, which adds quantum effects to the drift-diffusion model. He is also investigating silicon-on-insulator electronics for radiation-resistant space-based applications.

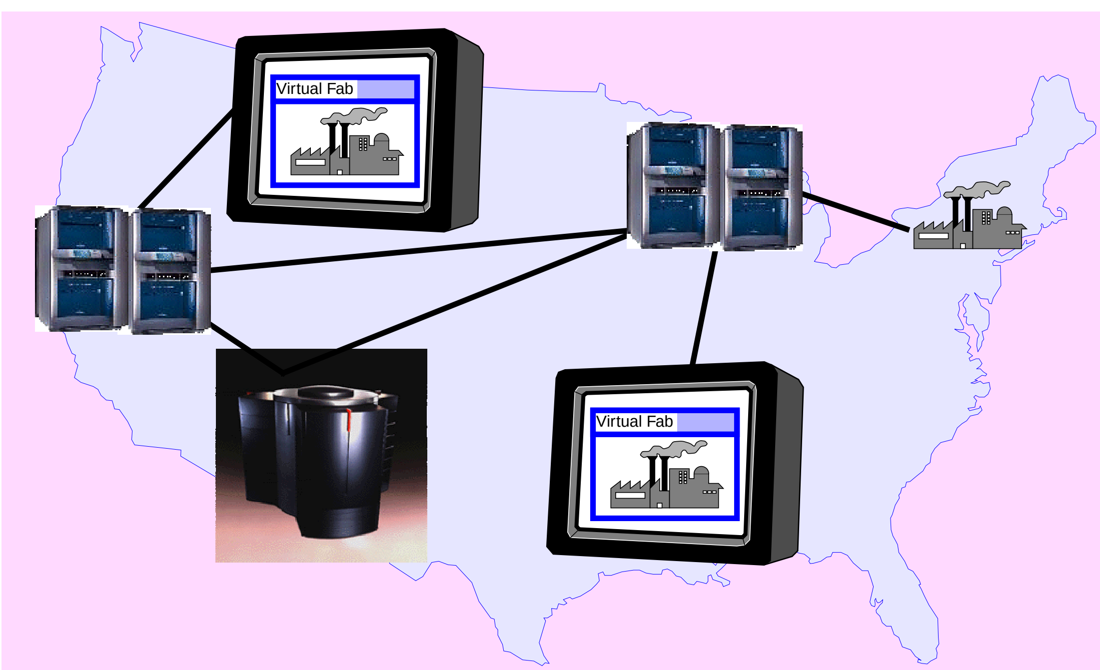



***Fig. 6 The computational grid will provide web-access to distributed supercomputer hardware, TCAD software, collaboration environments, and "instruments" (e.g., an automated fabrication facility).***