Next-Generation TCAD Tools--Supporting Rapid Prototyping of New Models and Numerics

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Abstract

With the constant scaling and broad applications for IC technology, rapid and predictive prototyping of the fabrication process is indispensable for both technological and economical development. Although there is prototyping software for IC process and device simulation, major limitations on the physical models, geometry/grid handling and computational capabilities have made simulation-based technology development practical for only limited process flows. In this paper, two major projects in the Stanford TCAD group are described, one dealing with process modeling and the other with device simulation. The SprintCAD project has made paradigm-shifting breakthroughs in the software representation and numerical techniques for 3D process simulation. A key enabling technology developed in this project, the dial-an-operator physical definition, provides flexible access to finite-element methods that robustly solve diffusive-reactive system of equations. The use of a minimalistic wafer representation with supporting geometry/grid capabilities has helped to create a computational prototyping environment ready for the challenges of IC technology into the next decade. The second project outlines a complimentary effort (joint with Lucent Technology, Bell Labs.) to support a model developer's environment that spans both the process and device domains.

1. Introduction:

The development of future generations of technology for systems application now requires new tools and approaches to deal with the growing complexity needed to achieve high-performance and low-power concurrently. Moreover, the growing need for heterogeneous technologies where microwave and opto-electronics must interface intimately with VLSI processor and memory systems pose additional challenges to the design and packaging of such systems. The use of technology computer-aided design (TCAD) has received broad acceptance among the silicon technology community owing to the demonstrated ability to reduce by half both the development time and cost for new technologies. However, with the aggressive scaling of minimal geometry features in IC fabrication, the models for the new physical effects such as defect-enhanced diffusion, geometrical and surface effects in etching/deposition, and stress-induced defects need to be rapidly implemented and predictively calibrated in 1-2-3D TCAD framework within a short cycle. An open simulation framework is essential, since not only new physical models, but also new computational methods are developed for the demands of critical design. In Figure 1 an example of open TCAD framework, SUPREM OO7, is shown. Various process simulation tools for different process steps communicate with one another through a common geometry/grid server and are controlled by a unified user interface. The framework also provides a flexible plug-and-play environment for TCAD tool builders. New utilities such as gridding, geometry modeling, numerical discretization and linear and non-linear solvers can be integrated into the environment by clearly defined application procedural interfaces (API). Within this project, simulation tools are developed from scratch or revised from an existing code to conform to the open simulation framework with 1-2-3D capabilities.

Another challenge for physical prototyping systems comes from the computational resources needed to solve large, complex 3D problems. The present environment for using TCAD commercially is dominantly based on

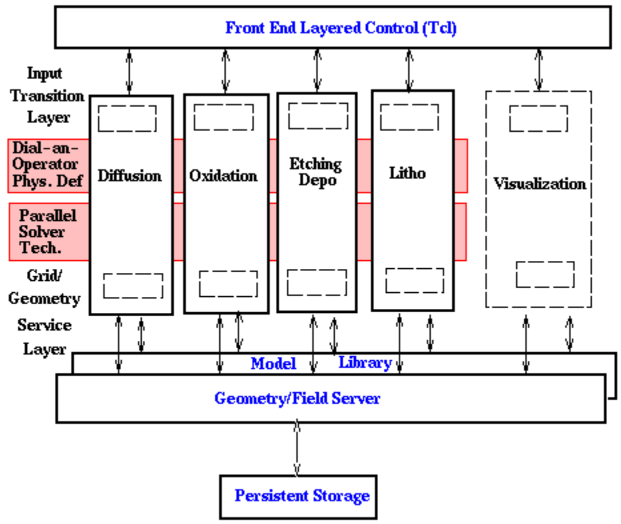

Figure 1: Schematic view of SUPREM OO7 architecture: layered control structure, server-based geometry/gridding and underlying dial-an-operator simulator development base with capabilities for parallelization (follow-on ParaSCOPE project).

engineering workstations (EWS) and is thus practically limited to two-dimensional (2D) simplifications of the actual design problems---neither the methodology nor the computer resources are in place to address the more complete problems which are inherently three-dimensional (3D) such as stress-induced defects. TCAD tools for large-domain 3D problems need to exploit the parallel computing capabilities that are generally applicable to both high performance computing (HPC) stations such as IBM/SP systems and EWS connected by efficient networking.

The SPRINT-CAD project bridges the capabilities of solid modeling, FEM-based parallel computation of fabrication processes and electrical analysis of the resulting IC structures. Under an integrated information model, an enabling "computational engine" for technology prototyping is being developed, which can handle complete circuit blocks across the levels from circuit performance through the underlying fabrication processes. Models to represent etching, deposition, oxidation, diffusion and stress analysis from process steps that are necessary in the creation of electrical devices are also being developed. The focus is however not on developing yet another point tool, but on creating a computational prototyping environment that can accommodate new and existing physical models and numerical methods, as well as eliminate the interface barriers in communication and abstraction between different levels of tools. The software maintainability and configurability are derived from object-oriented (OO) design, and large computational requirements are tackled by intelligent abstraction and parallel programming. This next-generation TCAD environment is designed to strongly link to and interact with the manufacturing process and therein provide system designers with practical methods to prototype, examine and conceptualize the underlying physical properties of new technology. Better trade-off decisions in a timely manner are projected with the fast moving semiconductor technology base.

2. Overview:

To achieve the goals of 1-2-3D computational prototyping of fabrication processes, many design aspects of the TCAD tool and framework need to be carefully considered:

1. **Flexible definition of physical models**. Impurity profiles are still the predominant design factors for advanced IC technology [1]. Interaction among dopants, defects and material interface is still under intensive investigation and new models are necessary to capture the essential physical effects. A new code ALAMODE (A LAyered MOdel Development Environment) using object-oriented design with models defined through the dial-an-operator method is developed under this project. A posteri error estimation capability is also provided

for each operator in support of adaptive gridding.

2. **Accurate and robust boundary movement**. Conventional boundary movement algorithms such as the string method and the cell method suffer from unreliable heuristics for developing, mass conservation, and curvature-dependent rate calculation. The level-set method [2] which solves the Hamilton-Jacobi equation on a static non-interface-conformal volume grid is robust and accurate for complex geometry movement, with a reasonably small penalty on computational efficiency. The level-set method is added to Stanford Profile Emulator for Etching and Deposition in IC Engineering (SPEEDIE) in this project, which conforms to the SUPREM OO7 open framework.

3. **Numerical techniques for oxidation**. The success of Si VLSI technology has deep roots in the good quality of silicon dioxide for insulation and masking. Oxidation is a very critical process step, but has been modeled in a quite ideal manner without consideration of large deformation and visco-elastic-thermal constitutive models. In addition to oxide shape, in-situ and residual stress analysis for oxidation has become increasingly important for advanced transistor and isolation structures. A self-consistent treatment for stress-dependent oxidant diffusion, visco-elastic models and surface reaction/ segregation kinetics has been developed in this project with the level-set method to remove the interface conformity constraint. The finite deformation approximation is used to allow more robust and efficient time stepping schemes

4. **Numerical stability for diffusive-reactive systems**. The maximum principle (or more generally the ordering principle) for the diffusive-reactive system of equation needs to be satisfied for numerical stability in transient prediction and asynchronous parallelization [3]. For 1D and 2D cases, element technology for the maximum principle can be easily established. However, for 3D cases the constraints on element quality become much more stringent. A rigorous analysis on the element technology that satisfies the maximum principle is investigated in this project.

5. **Common representation and functionality for geometry and gridding**. The TCAD tools for various process steps need to communicate to one another through a unified geometry/gridding representation and they also share numerous geometry/gridding requirements. A 1-2-3D geometry/ field server prototype that conforms with the minimal SWR (semiconductor wafer representation) specification [4] has been developed in this project to demonstrate feasibility and to support technological examples used in the tools mentioned above. Functionalities including conformal gridding, consistent field management, boundary movement and smoothing, and solution adaptivity are provided to physical tools such as ALAMODE. A 3D conformal gridding tool from Stanford, CAMINO based on quad/oct-tree is implemented and demonstrated for complex structures.

6. **Rapid geometrical prototyping**. Full 3D process simulation of a large chip area may still be too expensive even for a very powerful HPC stations. Rapid prototyping based on geometrical manipulation of 1D and 2D simulated and measured profiles, mask information and designer's intuition is still very useful. This heterogeneous approach reduces overall complexity and provides fully compatible geometry for further processing and analysis. A virtual integrated process (VIP) framework is developed in this project and can exchange geometry information with the minimal SWR server.

3. ALAMODE --- dial-an-operator for coupled diffusive-reactive systems of equation:

To accurately simulate modern semiconductor process steps, TCAD tools must include a variety of physical models and numerical methods. Increasingly complex physical formulations are required to account for effects that were not important in previous generations of technology. As a specific example, the impurity diffusion mechanisms owing to point defects and damage kinetics are not well understood, and thus flexibility in definition of models is highly desirable. An object-oriented approach has been applied to implementing a 1-2-3D finite-element dial-an-operator PDE solver, which is named as ALAMODE (A LAyered MOdel Development Environment). The object-oriented design provides for specification of PDE-based models via a dial-an-operator approach. As shown in the information model (Figure 2), a model can be composed by building systems of equations from a library of operators and functions. This information model along with the operator and function libraries implemented in ALAMODE has been sufficient for representation of virtually all equation-based thermal

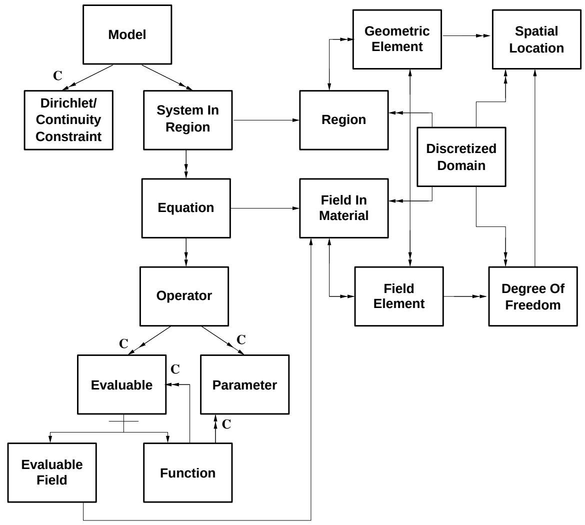

Figure 2: Detailed information model used in the design and implementation of ALAMODE (A LAyered MOdel Development Environment) for support of dial-an-operator TCAD tool development.

diffusion models considered by current research.

The front-end to ALAMODE is an extended TCL (tool control language) interpretor which provides both the model description layer (complete with access to the numerical discretization) as well as a rich set of simulation control including access to robust ODE integration algorithms as well as to geometry and field manipulation primitives. Although the TCL interface is low level compared to abstractions available in more traditional simulation tools, the generality provides much wider applicability. Because TCL is a full-featured scripting language, user-defined procedures can be written to provide a more user-friendly interface for those who do not need to access the low-level layers.

As an example, we solve a system of five reactive-diffusive equations for phosphorus diffusion [5]. This five-species model contains the diffusion, recombination and kinetic reaction of phosphorous, interstitial, vacancy, pairs of phosphorous-interstitial and phosphorous-vacancy. The profiles developed during a 10 minute, 900˚C anneal are shown below. Multi-species reactive-diffusive systems, similar to the one shown, are becoming increasingly important to model low temperature and rapid thermal annealing as well as implant damage enhanced diffusion. The physical model can be completely described in a simple TCL script. The results are shown in Figure 3 and have been compared favorably with the 1D PEPPER diffusion simulation tool [5]. Other examples include boron segregation (benchmarked with SUPREM IV), 1D and 2D SUPREM mesh and 3D CAMINO mesh [6], and diffusion in poly-silicon by considering the average grain boundary growth/ recombination. Another example of ALAMODE is demonstrated for boron diffusion [7]. The new boron model includes reactions of point defects and defect-dopant pairs, considering their charge states, and the dopant inactivation by the introduction of a boron clustering reaction. The six transport equations and complex constitutive models for diffusive and reactive terms have been completely described in the TCL extension language without any modification and compilation of the source code. Rate of convergence and level of accuracy are comparable to the original implementation for the specific model.

In the dial-an-operator regime, since the stiffness of the coupled system of equations is determined by the user, numerical stability of the simulation demands more robust time stepping and nonlinear iterative schemes. Although it is unlikely to have a universal solution for all types of PDEs, the reactive-diffusive systems can be reasonably treated with the second order TR-BDF2 time discretization [6] using an estimate of the local truncation error (LTE) to control the size of the timesteps. This discretization has been very successful in integrating moderately stiff diffusion models, but it had not been applied to highly stiff fully kinetic models. The control of temporal error via the LTE estimates is usually sufficient “load control” to guarantee convergence of the Newton solve. When applied to fully kinetic models, however, the traditional LTE estimators are also sufficiently conservative to avoid overshoot in the TR substep which

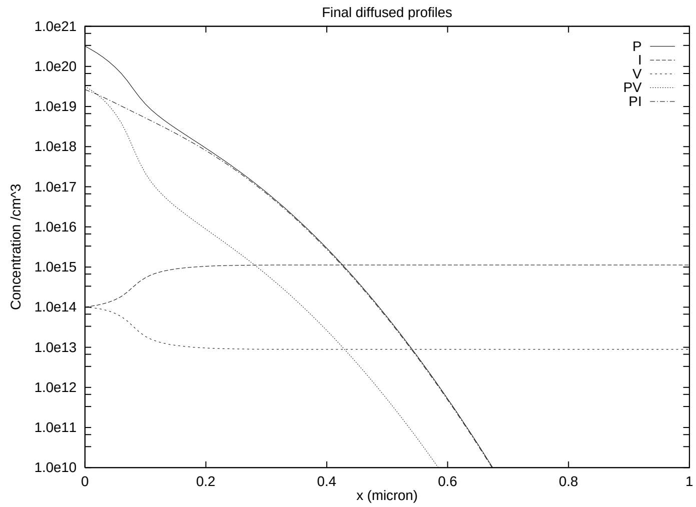

Figure 3: ALAMODE simulation results (log concentration vs. distance) for phosphorous diffusion using a five-species model [5].

would drive concentrations negative, but additional heuristics needed to be developed to avoid difficulties in the BDF2 substep. When the models are modified to conform to these heuristics, TR-BDF2 provides a very robust temporal discretization for solving fully kinetic systems.

A hierarchy of spatial error estimators, including implicit/explicit and inter-/intra-element methods, are formulated and partially connected to ALAMODE. Error fields for explicit inter-/intra-element contributions are verified for the diffusion equation. Time domain error estimation for general trapezoidal schemes including local and global discretization errors has also been formulated. The local truncation error is based on the divided difference approximation and the global error is calculated using the mass and Jacobian matrices in the nonlinear iteration. The formulation is tested against the standard van der Pol equation for nonlinear systems. The conventional constant-step backward Euler method, although stable and convergent, is not only less efficient owing to unnecessary fine steps in slow transient regions, but also heavily polluted by global errors and hence very inaccurate after a fast transient region. Along with the error estimator implementation, access to strong forms of operators are built, which will later be extended to Galerkin-Least-Square (GLS) implementation.

The semi-discrete finite element discretization for a reactive diffusion equation may encounter numerical problems, where concentration becomes negative, if the amplification matrix, even though positive-definite, contains negative elements operating on very large concentration gradients. Negative concentrations are not only unphysical, but may also cause numerical problems in reaction and recombination terms. To guarantee that concentration remains positive for all time steps, the spatial flux discretization has to satisfy the maximum principle. We have analytically derived the criteria for the maximum principle in the diffusion equation in 1D, 2D and 3D. In 1-D, mass lumping is most effective with arbitrary spatial discretization. However, in 2D and 3D, mass lumping is not sufficient without constraints on geometrical elements. For various element types including triangles, quads, bricks, prisms and tetrahedra, a formal analysis is performed to give geometrical constraints for satisfying the maximum principle.

It is established that the waveform relaxation technique is stable and efficient for large sets of ordinary differential equation (ODE) systems as in circuit simulation. Parallelization based on waveform relaxation is attractive since the calculation on subsystems can be asynchronous. Application of waveform relaxation for partial differential equations (PDE) with subsystems partitioned by domain decomposition with controllable overlap regions is very promising for parallelization of the reactive-diffusive systems, since stability and rate of convergence are directly related to the maximum principle (the ordering principle if the reactive term is strong). This will be continuously investigated in the follow-on ParaSCOPE project.

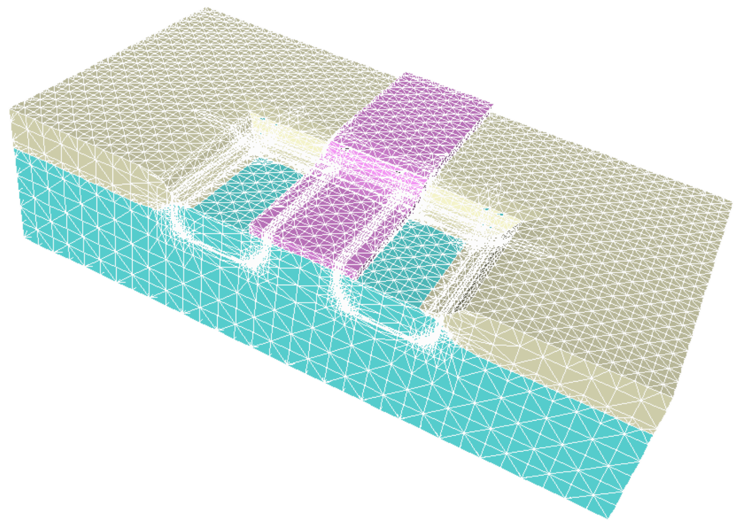

Figure 4: Grid for a MOSFET based on CAMINO and ALAMODE solutions for 3D dopant diffusion of source and drain regions.

4. Minimal set of Semiconductor Wafer Representation (SWR) with supporting geometry/grid capabilities:

From the late 1980s, an intensive effort has been conducted on TCAD tool communication. Two major directions have been considered. First, the TCAD tools will communicate based on standard file format. Two file formats have been standardized: SUPREM structure file and that in support of VISTA [8]. This approach, also easily implemented in each tool by an I/O wrapper, does not provide any functionality or guarantee consistency. The second approach is the Semiconductor Wafer Representation (SWR), which specifies not only access methods for wafer information, but also provides functionalities such as gridding, boundary movement, Boolean operations, etc. SWR is deeply specified for the methods in each class (geometry, field, attribute, etc.) and literally requires a new implementation for both clients and server. Ever since the first procedure interface documented in late 1992, there is no practical implementation until now.

For the next decade, it is still expected that many algorithmic improvements on numerical methods and computational geometry for 3D problems will be proposed. An open environment for plug-in new gridding algorithms is necessary for server longevity. Under the SprintCAD project, we have taken a hybrid direction to take advantage of the previous two approaches. A minimalistic SWR is defined with sufficient access and functionality, but only the global access method is specified (similar to Berkeley SPARSE package), not the class. It is much easier for existing gridders and tools to write socket procedural interfaces to conform to the minimal SWR 0.3 specification, while there are still a rich set of functionalities, including conformal gridding, boundary movement and smoothing, adaptation to an error field and consistent field storage. Coarse-grain parallelization of the SWR is under continuous study in a follow-on project, including the joint effort with Bell Labs using the PROPHET tool discussed below.

A first prototype of geometry/field server in 2D conformed to minimal SWR specification is the FOREST tool developed by our group. Later on the level-set boundary movement for geometry, CAMINO (quad/oct tree) and EUCLID (unstructured triangles and tetrahedra) have been developed according to minimal SWR. Examples for gridded device structure are shown in Figure 4. Simulation tools such as ALAMODE and SPEEDIE have been connected to the gridders according to the minimal SWR specification and an inter-operable suite of TCAD tools has been shown in the SUPREM OO7 framework, consistent with our vision in Figure 1.

Test cases of 3D multi-region MOS structures gridded by CAMINO have been validated with the Fermi diffusion model implemented in ALAMODE. The Oct-tree based tetrahedral mesh contains anisotropic refinement capabilities and can take general boundary-representation geometry. The generalized oct-tree mesh generation algorithm enables mesh refinement and de-refinement in different directions at various regions. A

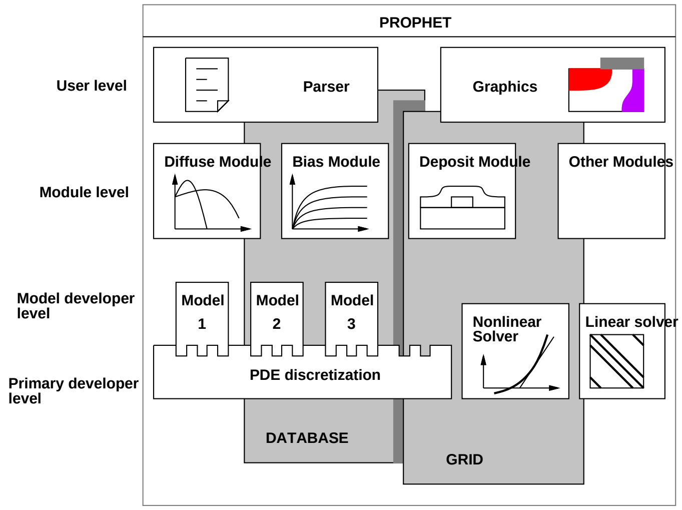

Figure 5: A block structure of PROPHET.

vector level control function is computed and indicates the directions for which the refinement will be performed. In a contour based refinement scheme, the level control function indicates the directions as the gradient, while in an error estimator based scheme, it indicates the direction where the error will be maximally reduced. Every octant can be refined in either one, two or three dimensions. After the tree is generated, detailed tetrahedralization algorithms are implemented to match the complex geometry and ensure mesh conformity. Then after each simulation step, the vector level control function is re-calculated according to the new gradient or error, and the mesh is adapted to reflect the changing areas of simulation significance. With the tree structure, interpolation error is also greatly reduced since the meshes before and after the adaptation share many common nodes. Grid quality required by the maximum principle is also derived.

5. PROPHET -- A program and high-level development platform for PDE system solver targeted specifically for IC device and process simulation:

PROPHET was originally developed in Bell Labs (formerly with AT&T and now as part of Lucent Technologies) as an IC process simulation program with user-expandable set of diffusive-reactive PDEs. Figure 5 shows a block diagram of the PROPHET simulator. In addition to the usual user level and developer level perspectives on the simulator, there is also a model developer perspective, which simplifies the addition of new models both by scripting and by a simple interface for new routines. Underlying and communicating with all levels are the database and grid structures. It has several unique features:

1. The simulator has already seen extensive use in simulating Bell Labs' state-of-the-art CMOS technology, and to develop what is now the standard model of transient dopant diffusion (TED) in silicon.

2. The spatial discretization of the simulation domain can be carried on in either 1-2-3 dimensions and both finite element and finite difference methods are available.

3. The control flow for solving PDEs in the system can be altered at the user discretion at the input level. The control flow includes grouping of equations for Newton iteration and the solving sequence of equations in Gummel sequential loop.

4. Easy ability to switch in sparse linear solvers from various sources. Both direct and iterative solvers are routinely applied to problems assembled by PROPHET.

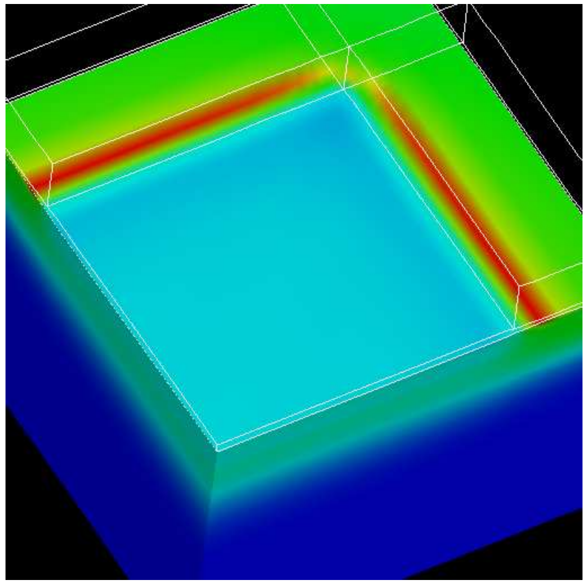

Figure 6: An example of TED simulation with PROPHET.

Figure 6 shows an example of TED simulation with PROPHET. A cross section of a waffle-gate MOS shows dopant pileup effects due to TED at the gate edges, but not at its corners. This leads to different threshold voltage in waffle-gate devices compared to stripe-gate devices [9].

In collaboration with Stanford University in the ParaSCOPE project (Parallel Shared Computational Prototyping Environment), supported by DARPA, the Bell Labs group is helping to further develop PROPHET in directions that support: shared tool infrastructure (the server-based architecture of OO7), incorporation of capabilities for parallelization and the overall creation of a developer's platform to test new physical models. One such example in the domain of device analysis is the hydrodynamic (HD) model for high energy (i.e. hot) carrier transport in semiconductor devices which became popular a decade ago. More generally, the demand for having a more flexible device simulator that can accommodate new PDEs is becoming apparent. For example, in optoelectronic device simulation, Helmholtz equation, which is in the domain of eigenvalue problems, and photon rate equation are required to be solved in addition to the electrical semiconductor equations. Even in the mainstream silicon technology base, for accurate simulation of deep sub-micron silicon MOSFETs with gate oxide thickness below 10 nm, the quantum mechanical correction to the carrier confinement and transport in the channel region can no longer be ignored. The rigid structure of traditional device simulators such as PISCES is not adequate for this purpose. Not only much more man power has to be spent in adding new models/equations in the original code, the effort is also very much error-prone.

There is a parallelism between PROPHET and ALAMODE discussed in Section 3. Both are targeted to explore the use of pre-fabricated building blocks to define a new system of equations, and both were developed with IC process simulation as their primary application. The difference lies on the code structure -- ALAMODE used object-oriented programming style while PROPHET was written largely in C. (PROPHET also targets the task of adding new physical modules through a simple interface which requires no knowledge of the simulator's data structures.) With the migration of embracing the device simulation into the same code structure as for process simulation, PROPHET is gradually transformed to be a platform and simulation tool for IC technology modeling, including the device simulation capabilities. The efforts under the umbrella of ParaSCOPE show great promise in providing a means for quick prototyping of electric behavior based on the structural information.

Since the launching of ParaSCOPE in 1996, under the joint effort of Stanford, Bell Labs, and a complementary (DARPA-funded) project with UT Austin, device simulation capabilities for steady state analysis using the drift-diffusion transport model has been realized in PROPHET. During the process of implementation, much has been learned about the data and code structure of PROPHET. The database in PROPHET has also been overhauled to better serve the dual purpose of process and device simulation. The overall changes and architectural structure of PROPHET can be briefly summarized as follows. PROPHET is a simulation tool for both users and model/system developers. At the user level, the usage is exactly the same as conventional TCAD tools from both universities and software vendors. Users specify the structure, processing/bias condition, analysis mode (dc and transient) together with the meshing, required equations and their solution method (Gummel or Newton), all within the capabilities of "hard-wired" equation set in the code. However, PROPHET is also designed for developers at both model and system levels. The task of developers is to add something (either models or equations, or both) new and un-available to the users in the code before analyzing the individual structures.

This development task is carried out largely at the scripting (i.e., input file) level. The basic building blocks (or agents) in PROPHET for describing PDEs are so-called terms, which are actually terms in the mathematical form of the equation. Thus term covers both the operator (such as the divergence) and the operand. PROPHET has a large collection of terms commonly encountered in IC process simulation. If a new equation (PDE) can be described using the terms already available in the data base, the user/developer doesn't need to touch the source code. Everything, including the new system specification and actual structure analysis, is done at the user-input file (or script) level. If, however, the new term(s) are required in describing a PDE to be included in the simulation system, it is the developer's responsibility to write dedicated C routine (i.e. function) for each new term, and modify a few files to reflect the addition of new terms to the database. The effort in code-writing is minimal, involving only the description of terms using fundamental variables (i.e. solutions to be solved) and a few derivatives. All other detail operations such as the spatial and time discretization are hidden from the developers.

This level of abstraction of simulation tools is much like the popular commercial math packages such as Mathematica and Matlab. However, PROPHET can solve realistic engineering problems, in a discrete space, with virtually arbitrary structure, while pure math packages can only deal with continuum, well described (meaning using analytic formulas) system of PDEs. The current effort of the PROPHET project (i.e. ParaSCOPE) is focused on enhancement of device simulation capabilities, including adding new terms required by the device simulation and expanding the existing infrastructure as necessary when the equation type is expanded from diffusive-reactive to include strongly diffusive-advective and eigenvalue problems.

There are a broad range of further enhancements that are being considered for PROPHET and in support of creating a model developer's platform for research. Some of these involve basic underlining infrastructure such as adaptive meshing and error control, efficient and robust numerical algorithm while others move more specifically into application and model developer issues such as calibration and materials characterization. Within both the scope and spirit of the ParaSCOPE project (as well as the companion 21st Century Computation Prototyping of Semiconductor Devices project, also supported by DARPA), the use of internet for both information dissemination and collaborative development are being strongly encouraged. Hence, for further detailed information about both the PROPHET and ALAMODE projects, the interested reader is referred to the web site (http://www-tcad.stanford.edu/tcad/programs.html).

6. Conclusion:

The SPRINTCAD project has made several paradigm-shifting breakthroughs in both numerical algorithms and software implementation. A prototype of TCAD framework, which is flexible in physical model definition, interoperable for tool communication, and capable in 1-2-3D geometrical functionalities, has been implemented and successfully transferred and used in the national labs, industrial companies and universities for practical VLSI fabrication technology modeling. Initial efforts on parallelization have shown great promise for the follow-on ParaSCOPE project, which will further exploit common protocols and functionalities in coarse-grain parallel computing for semiconductor process and device simulation tools.

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