Enabling Predictive Simulation through Embedded Sensitivity Analysis

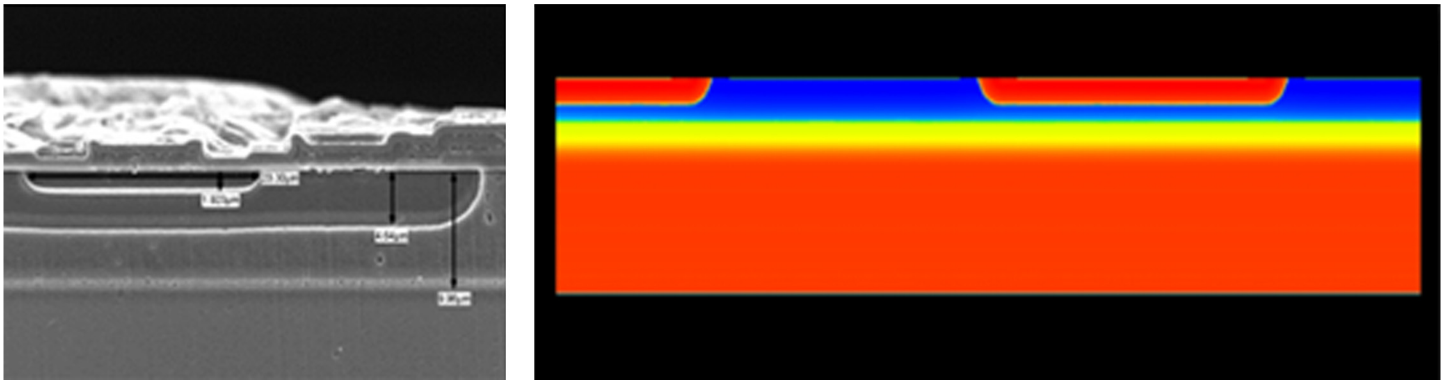

Figure 1: Left: Experimentally obtained micrograph of a stockpile bipolar junction transistor. Right: RAMSES/Charon simulation of the electric potential in the device.

Revolutionary approach uses automatic differentiation

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Computational simulation plays a critical role in the design, risk assessment, and qualification of complex engineering systems relevant to Sandia's mission. Examples include the design of re-entry vehicles and stable fusion reactors, the licensing of nuclear reactors and waste repositories, and the qualification of electronics in radiation environments. *Predictive* simulation entails significantly more analysis than high fidelity simulations, rather, it additionally requires verification of simulation code correctness, validation of the simulation's effectiveness at modeling the system, measuring the sensitivity of simulation results with respect to input data, and quantifying the effects of uncertainty in this data. Accordingly, simulation and analysis tools must provide these capabilities with reasonable execution times for predictive simulation to be feasible.

Computing derivatives, a staple of any freshman calculus course, provides the foundation for many analysis algorithms supporting predictive simulation. Derivatives, also called sensitivities, determine how a computation's results vary with it's inputs, and are useful in (1) estimating how errors and uncertainties in those inputs affect simulation outcomes, (2) highlighting which physics or subsystems are most important in a simulation, and (3) calibrating simulations against empirical data. Thus, estimating derivatives quickly and accurately is critical for predictive simulation. Traditional sensitivity approaches for complex large-scale production codes are based on running repeated simulations while varying inputs. While this approach is simple and convenient, it disregards much of the knowledge of the underlying system that could be leveraged for more efficient computations. Recently, Sandia has developed revolutionary technologies for "embedded" sensitivity analysis based on the ideas of automatic differentiation. Where simulations normally compute solution values, this technology re-uses the same simulation code-base but automatically produces sensitivities along with the solution. This new capability allows researchers to extract very accurate sensitivity information from simulation codes using less computing time than traditional approaches, but with minimal impact on the software development cycle. By leveraging this capability, Sandia researchers can develop and apply significantly more accurate and

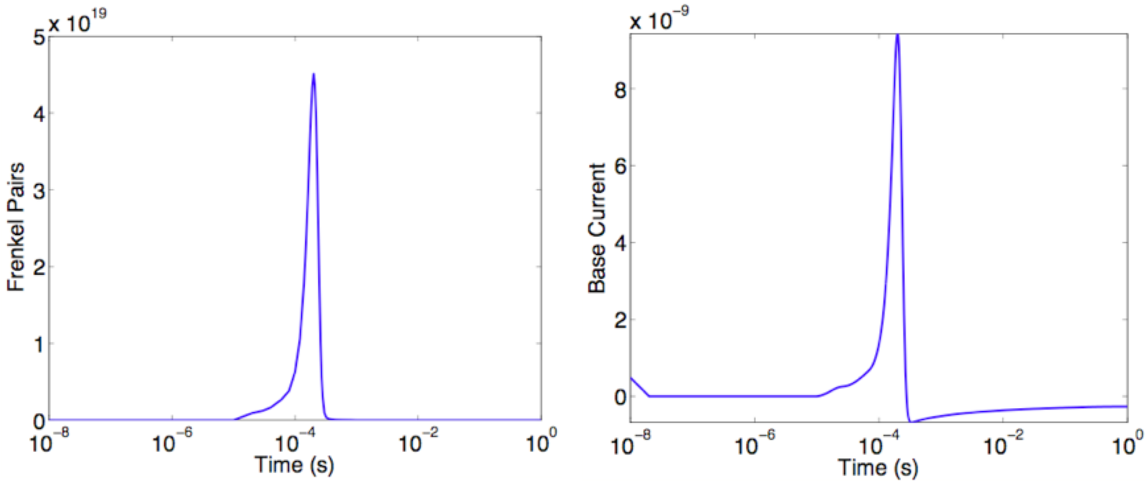

Figure 2: Left: Plot of the simulated radiation damage pulse, measured as the density of Frenkel pairs (defects in the device created by radiation) in the device from Figure 1, as a function of time.
Right: Resulting electric current flowing through the base contact of the device as computed by RAMSES/Charon.

efficient derivative-based analysis algorithms to even the most complex science and engineering problems.

This technology has recently been showcased in the simulation of radiation damage of an electrical circuit (Figure 1) as part of the Qualification Alternatives to the Sandia Pulse Reactor (QASPR) project. Figures 1 and 2 show a stockpile bipolar junction transistor along with computational simulation of the device under radiation provided by the RAMSES/Charon (RAMSES=Radiation, Analysis, Modeling, and Simulation for Electrical Systems) simulation code. Using the embedded sensitivity technology, coupled with a state-of-the-art transient sensitivity analysis tool currently under development, Sandia researchers were able to determine which of the 126 parameters in the radiation damage mechanism the operation of the device was most sensitive to (Figure 3). This improved understanding of the damage mechanisms, and indicated where further modeling efforts are required to increase simulation fidelity. Furthermore, this technique was demonstrated to be approximately *14 times faster* than traditional techniques, and significantly more accurate and robust as well.

This pivotal work is rapidly being incorporated into Sandia's next generation simulation software. It has impacted a variety of internal projects including security and strategic evaluations of the national natural gas network, rail gun design, circuit network design, and fundamental magnetohydrodynamics research. Externally, this work has fostered a strong collaboration in modeling advanced tactical lasers for the U.S. Air Force as well as potential impact to oil and gas exploration.

The automatic differentiation capabilities are available in the Sacado software package, part of Sandia's open-source Trilinos Software Framework, located at http://trilinos.sandia.gov/. The transient sensitivity analysis capability is provided by the Rythmos package, also part of Trilinos.

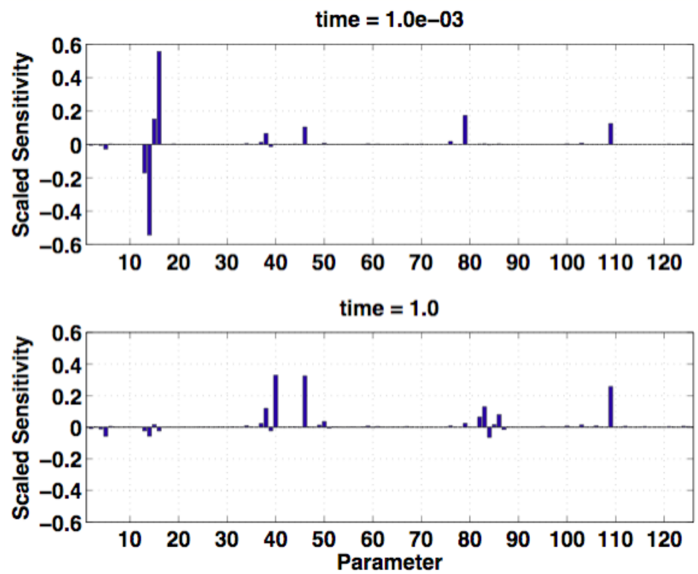

Figure 3: Plot of the scaled sensitivity of the base current from Figure 2 with respect to 126 parameters in the radiation damage mechanism, at early (top) and late (bottom) times after the radiation pulse. These results help focus future radiation damage mechanism research.

Sandia National Laboratories

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