

TCAD Sensitivity Analysis for Device Optimization

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Abstract—We explore the use of sensitivity analysis for technology computer-aided design (TCAD) optimization. By directly coupling device response to model parameters, our approach may be used to generate derivatives for gradient-based optimization. An example is presented for inverse modeling of a doping profile. We compare the number of simulations required, and accuracy, to a design of experiments (DOE) based optimization.

I. INTRODUCTION

To perform device optimization, a number of simulations are performed over a parameter space. When optimizing many parameters, a large number of simulations may be required to find the optimal parameter set. When derivatives with respect to the parameters are available, it is possible to reduce the number of simulations, since gradient methods offer better convergence in many circumstances [1].

TCAD sensitivity analysis couples the output response of devices with respect to fluctuations in the partial differential equations (PDE's) [2]. We extend this analysis by calculating the derivatives of the PDE's with respect to model parameters. Using the chain rule, we then compute the derivative of the output response of the device with respect to the parameters to optimize.

II. THEORY

We cast the problem of optimizing device parameters as a nonlinear least squares problem, using the objective function

$$S(\beta) = \frac{1}{2} \sum_{i=1}^M (f_i(\beta) - C_i)^2 = \frac{1}{2} r^T r \quad (1)$$

where we have M results to optimize, C_i is the i^{th} goal and $f_i(\beta)$ is the result using parameter set β .

The parameters are varied over their allowed range until $S(\beta)$ is minimized. Using the Gauss-Newton method [3], it is possible to find the parameter update using

$$\delta\beta = -\mathbf{H}^{-1} \mathbf{J}^T r \quad (2)$$

where

$$\mathbf{J}_{i,j} = \partial f_i(\beta) / \partial \beta_j \quad (3)$$

$$\mathbf{H} \approx \mathbf{J}^T \mathbf{J} \quad (4)$$

are referred to as the Jacobian and Hessian, respectively.¹

In device simulation, the simulation matrix, \mathbf{A} , is used to converge upon the dc solution. Each entry of this matrix is

$$\mathbf{A}_{i,j} = \partial g_i / \partial x_j \quad (5)$$

where g_i is a PDE being solved, and x_j is a solution variable.

If the simulation goal may be described in terms of x_k , we may find the sensitivity to perturbations in the PDE's [4]. This is by solving

$$\mathbf{A}^T y_k = e_k \quad (6)$$

¹While this method was chosen for its relative simplicity, more robust gradient-based optimization methods may be employed using the same Jacobian we describe here.

where e_k is a zero vector with a one in the row corresponding to x_k , and y_k is the vector relating a change in x_k to the residual in each PDE on the device.

The Jacobian entries are found from

$$\mathbf{J}_{k,j} = y_k^T \partial g / \partial \beta_j \quad (7)$$

where $\partial g / \partial \beta_j$ is a vector composed of the derivative of each PDE with respect to parameter β_j .

III. EXAMPLE

To demonstrate the approach, we optimize the doping profile for a 1 μm diode. Simulations are performed in DEVSIM using the drift-diffusion equations and the Shockley Read Hall (SRH) recombination model [5].

The donor doping profile for the diode is

$$N_D^+(x) = 0.5 \cdot 10^{N_0} \operatorname{erfc}[(x - x_0)/s_0] \quad (8)$$

and the acceptor doping profile is $N_A^- = 10^{15} \text{ cm}^{-3}$.

In this example, we optimize N_0 , s_0 , $x_0 \in \beta$. Using the values in Tbl. I, the bias is varied from 0 to 0.9 V. At each bias, a dc simulation is performed to calculate the current, $I(\beta)$. The sensitivity of $I(\beta)$ to fluctuations in the Poisson equation, y_k^φ , is solved using Eq. 6.

The derivative of the Poisson equation with respect to N_0 is then

$$\partial g^\varphi(x) / \partial N_0 = q \log(10) N_D^+(x) \quad (9)$$

where q is the electron charge. The derivatives with respect to s_0 and x_0 are calculated in a similar fashion. The derivatives of N_D^+ with respect to β are shown in Fig. 1.

The spatially dependent y_k^φ , and the derivatives of $I(\beta)$, are shown in Fig. 2 for a bias of 0.6 V. At each bias point, these derivatives are integrated over the device volume to calculate the parameter sensitivities shown in Fig. 3.

Using the parameters in Tbl. II as starting values, an optimization was performed with the goal being to match $I(\beta)$ simulated in Fig. 3. Since the residuals varied exponentially with bias, the current and its derivatives were scaled logarithmically so that

$$f_i(\beta) = \log(I_i(\beta)) \quad (10)$$

$$\partial f_i(\beta) / \partial \beta_j = 1/I_i(\beta) \cdot \partial I_i(\beta) / \partial \beta_j \quad (11)$$

Fig. 4 shows the convergence behavior using the constraints in Tbl. II. For this set of starting values, the optimization converged to an acceptable level within 15 simulations. In general, the convergence behavior depends on the starting values, and the constraints put on the simulation.

For comparison, a 15 run latin hypercube DOE was designed using the JMP statistical software [6] and the constraints in Tbl. II. A Gaussian process model, using the cubic correlation function, was fit to $S(\beta)$. It was minimized with a solution of $N_0 = 18.02$, $s_0 = 0.0195 \mu\text{m}$ and $x_0 = 0.207 \mu\text{m}$. In this case, $S(\beta) = 2.716 \cdot 10^{-3}$. In contrast, the same sum of squares was achieved within 7 runs using our approach.

IV. CONCLUSION

In this paper, we presented a method for simulating derivatives for use in optimization. Sensitivities to model parameters are found by coupling sensitivity analysis with analytic derivatives of the device PDE's.

The gradient information provided by our approach may be more accurate, and require fewer simulations, than finite difference approximations. Also, while our example was for doping profile parameters, we believe this approach is more generally applicable to other parameters in device PDE's. This is the subject of further investigation.

REFERENCES

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TABLE I
OPTIMIZATION PARAMETERS

Parameter	Value
N_0	18
s_0	$0.02 \mu m$
x_0	$0.2 \mu m$

TABLE II
STARTING PARAMETERS AND THEIR BOUND CONSTRAINTS

Parameter	Value	min.	max.
N_0	17	17	19
s_0	$0.01 \mu m$	0.01	0.05
x_0	$0.5 \mu m$	0.1	0.5

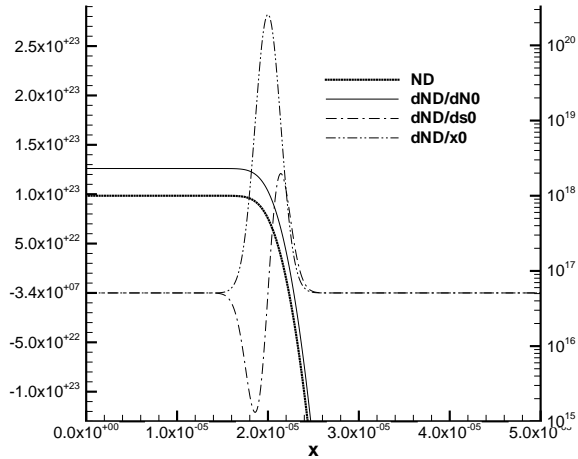


Fig. 1. The donor doping profile, $N_D^+(x)$, and $\partial N_D^+/N_0$ (log scale). Also, $\partial N_D^+/s_0$ and $\partial N_D^+/x_0$ (linear scale).

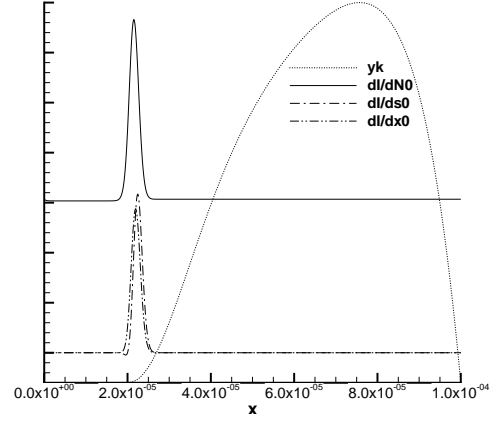


Fig. 2. Spatially dependent derivatives of $I(\beta)$ with respect to parameters. The dotted line is y_k^c . All lines shown in arbitrary units.

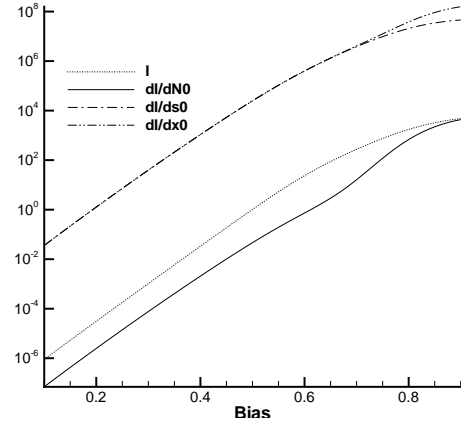


Fig. 3. $I(\beta)$, $\partial I(\beta)/\partial N_0$, $\partial I(\beta)/\partial s_0$ and $\partial I(\beta)/\partial x_0$ versus bias.

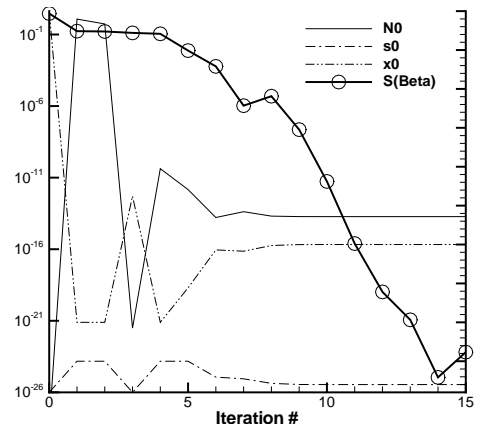


Fig. 4. Plot of $S(\beta)$ versus iteration number (log scale). The parameters are shown on a linear scale with arbitrary units.