Statistical Enhancement of Terminal Current Estimation for Monte Carlo Device Simulation

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We present a new generalized Ramo-Shockley theorem (GRST) to evaluate contact currents, applicable to classical moment-based simulation techniques, as well as semiclassical Monte Carlo and quantum mechanical transport simulation, which remains valid for inhomogeneous media, explicitly accounts for generation/recombination processes, and clearly distinguishes between electron, hole, and displacement current contributions to contact current. We then show how this formalism may be applied to Monte Carlo simulation to obtain equations for minimum-variance estimators of steady-state contact current, making use of information gathered from all particles within the device. Finally, by means of an example, we demonstrate this technique's performance in acceleration of convergence time.

Keywords: Monte Carlo simulation, Terminal current calculation, Generalized Ramo-Shockley theorem

1 INTRODUCTION: THE RAMO-SHOCKLEY THEOREM

Through application of the method of Green functions in the quasi-electrostatic approximation, Shockley [1] and Ramo [2] introduced the original domain integration formula relating the currents induced on an arbitrary number of contacts to the motion of charges in multiple dimensions :

$$I^{(k)} = \sum_j q_j \mathbf{E}_j^{(k)} \cdot \mathbf{v}_j, \quad (1)$$

where the index k indicates the contact at which the current is to be evaluated, q_j and $\mathbf{v}_j$ represent particle charge and velocity, respectively, and the index j runs over all particles within the volume. The symbol $\mathbf{E}_j^{(k)}$ denotes the electric field at the position of particle j which would result if all charges were removed from the volume, and boundary conditions were imposed

such that all contacts are grounded with the exception of contact k , which is set to 1 Volt.

2 A GENERALIZED RAMO-SHOCKLEY THEOREM

One of the most fundamental properties of all types of transport are the continuity equations, which may be derived by taking moments of the appropriate transport equations. For classical and semi-classical systems, this is most often the Boltzmann Transport equation [3], and either the Wigner-Boltzmann equation [4] or the quantum Liouville equation [5] for quantum systems. The 0^{th} moments take on the following general form:

$$-\nabla \cdot \mathbf{j}_n = eG_n(\mathbf{r}) - e\dot{n}, \quad (2)$$

$$-\nabla \cdot \mathbf{j}_p = eG_p(\mathbf{r}) + e\dot{p}, \quad (3)$$

Furthermore, Maxwell's equations may be used to derive equally familiar identities for the displacement current $\mathbf{j}_d$ and total current $\mathbf{j}_t$:

$$-\nabla \cdot \mathbf{j}_d = \nabla \cdot (\mathbf{j}_n + \mathbf{j}_p) = -e(\dot{p} + \dot{n}) \quad (4)$$

$$-\nabla \cdot \mathbf{j}_t = 0, \quad (5)$$

where the variables n and p refer to the electron and hole free carrier densities, respectively. Let h_{kl} be a suitable set of test functions satisfying

$$h_{kl}|_{\Gamma_l} = 1, \quad h_{kl}|_{\Gamma_j} = 0, \quad j \neq l, \quad k = n, p, d, t, \quad (6)$$

where Γ denotes the boundary, consisting of both Neumann (Γ_N) and Dirichlet (Γ_D) parts, and $\Gamma_D = \cup_i \Gamma_i$. Upon multiplication of an equation of the form $-\nabla \cdot \mathbf{j}_k = R_k$ with a test function h_{kl} , integration by parts yields [6,7]:

$$(-\nabla \cdot \mathbf{j}_k, h_{kl}) = (R_k, h_{kl}), \quad (7)$$

$$-\int_{\Omega} h_{kl} \nabla \cdot \mathbf{j}_k dV = -\int_{\Gamma} h_{kl} \mathbf{j}_k d\mathbf{S} + \int_{\Omega} \nabla h_{kl} \cdot \mathbf{j}_k dV.$$

The definition of h_{kl} requires that the surface integral is equivalent to the contact current, because $h_{kl}|_{\Gamma_m} = \delta_{lm}$ and $(\mathbf{j}_k \cdot \hat{\mathbf{n}})|_{\Gamma_N} = 0$. Equations (2), (3), (4), (5), and (7), lead to the following formulas for the terminal currents at an arbitrary contact l :

$$I_{nl} = \int \nabla h_{nl}(\mathbf{r}) \cdot \mathbf{j}_n dV + e \int \dot{n} h_{nl}(\mathbf{r}) dV - e \int G_n(\mathbf{r}) h_{nl}(\mathbf{r}) dV, \quad (8)$$

$$I_{pl} = \int \nabla h_{pl}(\mathbf{r}) \cdot \mathbf{j}_p dV - e \int \dot{p} h_{pl}(\mathbf{r}) dV + e \int G_p(\mathbf{r}) h_{pl}(\mathbf{r}) dV, \quad (9)$$

$$I_{dl} = \int \nabla h_{dl}(\mathbf{r}) \cdot \mathbf{j}_d dV - \int h_{dl}(\mathbf{r}) \nabla \cdot (\mathbf{j}_n + \mathbf{j}_p) dV = \int \nabla h_{dl}(\mathbf{r}) \cdot \mathbf{j}_d dV + e \int (\dot{p} - \dot{n}) h_{dl}(\mathbf{r}) dV, \quad (10)$$

$$I_{tl} = \int \nabla h_{tl}(\mathbf{r}) \cdot (\mathbf{j}_n + \mathbf{j}_p + \mathbf{j}_d) dV. \quad (11)$$

This method is also applicable to terminal currents of quantities derived from higher-order moments of the carrier distribution functions, inhomogeneous media and high frequencies [8]. The steady-state form of these equations is obtained by setting all time derivatives equal to zero.

3 OPTIMIZED STEADY-STATE FORM OF THE GRST

Convergence time for steady-state particle-based simulation is limited by estimator variance. Minimizing the functional form of the steady-state terminal current estimator variances $\langle (\hat{I}_{kl} - \bar{I}_{kl})^2 \rangle$ with respect to the test functions h_{kb} under the assumption that fluctuations in particle trajectories about the spatially-dependent mean trajectory have only weak interparticle correlation, results in the following set of Euler-Lagrange equations:

$$\nabla \cdot \langle \delta \hat{\mathbf{j}}_k \otimes \delta \hat{\mathbf{j}}_k \rangle \cdot \nabla h_{kl}^{opt}(\mathbf{r}) = 0 \quad (12)$$

$$h_{kl}^{opt}|_{\Gamma_m} = \delta_{lm}, \quad h \in H^1, \quad k = n, p, t. \quad (13)$$

The quantity $\langle \delta \hat{\mathbf{j}} \otimes \delta \hat{\mathbf{j}} \rangle$ is the position-dependent current density variance tensor. In steady-state simulation, it has the following numerically convenient tensor and scalar approximations

$$\langle \hat{\mathbf{j}}_k \otimes \hat{\mathbf{j}}_k \rangle_{ii} \approx (\rho_k)^2 (v_{T,k,i}^2 - \bar{v}_{k,i}^2) \tau_{c,k} / (N_k t), \quad (14)$$

$$\| \langle \hat{\mathbf{j}}_k \otimes \hat{\mathbf{j}}_k \rangle \| \approx (\rho_k)^2 (v_{T,k}^2 - \bar{v}_k^2) \tau_{c,k} / (N_k t), \quad (15)$$

where the symbols ρ_k , $v_{T,k}$ and $\bar{v}_k$ are the charge density, thermal velocity and mean velocity, respectively, for particles of type k . N_k and $\tau_{c,k}$ are the grid-dependent mean type- k particle number and momentum relaxation time, and t is the simulation time. The corresponding terminal current estimators then become:

$$\hat{I}_{nl} = \int \nabla h_{nl}^{opt}(\mathbf{r}) \cdot \mathbf{j}_n dV - e \int G_n(\mathbf{r}) h_{nl}^{opt}(\mathbf{r}) dV, \quad (16)$$

$$\hat{I}_{pl} = \int \nabla h_{pl}^{opt}(\mathbf{r}) \cdot \mathbf{j}_p dV + e \int G_p(\mathbf{r}) h_{pl}^{opt}(\mathbf{r}) dV, \quad (17)$$

$$\hat{I}_{tl} = \int \nabla h_{tl}^{opt}(\mathbf{r}) \cdot (\mathbf{j}_n + \mathbf{j}_p) dV. \quad (18)$$

4 APPLICATION TO MOSFET SIMULATION

To extract current-voltage characteristics of an 0.5 μm n-Mosfet device, several simulations were performed with the Monte Carlo simulator Degas. Test functions for the terminal current estimators were computed

FIGURE 1 Simulated electron density and velocity profiles for a 0.5 micron MOSFET. $V_{gs} = 2$ V, $V_{ds} = 4.875$ V

FIGURE 2 Simulated and experimental $I_d - V_{ds}$ characteristics, along with convergence times for source, drain and substrate currents at $V_{ds} = 4.875$ V and $V_{gs} = 2$ V

from equations (12), (15) and (16), and used along with simulated carrier density and velocity profiles, such as shown in Fig. 1, to obtain the cumulatively time-averaged steady-state drain currents shown in Fig. 2. All simulations were run with 20000 electrons and 10000 holes. In comparison to the particle counting technique, convergence is reached with the optimized GRST method between 10 and 40 times faster for these examples.

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Biographies

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K. Gärtner was born in Zittau, Germany, on March 4, 1950. He studied theoretical physics in Dresden (Germany), and received a PhD in nuclear reactor physics. After working ten years in the field of neutron transport, he joined the Karl-Weierstraß-Institute for Mathematics in Berlin in 1982. Since this time, his main interest has been in numerical problems connected to PDE's and semiconductor device models. In 1992, he joined the Interdisciplinary Center for Supercomputing at the ETH, and since 1994 has been working with Prof. Fichtner at the ETH Integrated Systems Lab.

Nobuo Sasaki was born in Matsuyama, Japan, in 1949. He received the B.S. degree in Physics and Ph.D. degree in Electrical Engineering in 1971 and

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Wolfgang Fichtner received the Dipl. Ing. degree in physics and the Ph.D. degree in electrical engineering from the Technical University of Vienna, Austria, in 1974 and 1978, respectively. From 1975 to 1978, he was an Assistant Professor in the Department of Electrical Engineering, Technical University of Vienna. From 1979 through 1985, he worked at AT&T Bell Laboratories, Murray Hill, NJ. Since 1985 he is Professor and Head of the Integrated Systems Laboratory at the Swiss Federal Institute of Technology (ETH). In 1993, he founded ISE Integrated Systems Engineering AG, a company in the field of technology CAD. Wolfgang Fichtner is also a fellow of the IEEE and a member of the Swiss National Academy of Engineering.