An efficient physics-based CAD approach to evaluate the sensitivity of GaAs devices with respect to process parameters

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Abstract
The paper presents an efficient technique for evaluating the DC sensitivity of GaAs monopolar or bipolar devices through a two-carrier drift-diffusion model. The sensitivity analysis is based on the Brannin’s method for the sensitivity analysis of electrical networks. Numerical results are presented concerning two topics: the behaviour of the distributed sensitivity within MESFET devices and the sensitivity-based statistical MESFET analysis with respect to random variations of the technological parameters, which is the basis of yield-driven device optimization.

Introduction
Physics-based design and yield optimization of GaAs microwave devices have been the object of great interest during the last few years [1]. Such topics rely on efficient physics-based simulation techniques aimed at evaluating the sensitivity $S^2_{\gamma} = \partial \gamma / \partial \sigma$ of the device electrical performance $\gamma$ with respect to a small-amplitude variation of the physical and/or technological parameter $\sigma$. In fact, yield estimate and optimization require the physics-based models to efficiently provide not only the expected values for the electrical device performances, but also the self- and joint probability distributions of the deviations between actual and expected values. On the other hand, an efficient use of physics-based numerical models for the device optimization with respect to technological parameters calls for an estimate of the gradient of the electrical device performances with respect to the latter, thus enabling the use of gradient-based optimization approaches.

The computational burden of physics-based models suggests that evaluating $S^2_{\gamma}$ by numerical differentiation is inaccurate and time consuming. Similarly, estimating the statistical distribution of the electrical performances resulting from randomly distributed input data by means of repeated analyses is unfeasible. Nevertheless, in the case of small physical parameter changes, the statistical characterization of the electrical parameters could be approximated through the first-order expression: $\Delta \gamma = S^2_{\gamma} \Delta \sigma$, where $\Delta \sigma$ is a random variable describing the spread of technological parameter $\sigma$ with respect to its expected value, $\Delta \gamma$ is the resulting random deviation of $\gamma$ (see [2] for a discussion).

An efficient technique for evaluating the sensitivity of monopolar devices has been proposed by Ghione and Filicori [3]; the approach is based on a Green’s function formulation of the sensitivity, whereby this parameter is evaluated as the volume integral of a distributed local sensitivity $s^2_{\gamma}(\tau)$, which in turn is expressed in terms of a perturbation source $f(\tau)$ and of a Green’s function $G(\tau)$. The Green’s function is then efficiently evaluated through the help of the adjoint approach [3]. The approach described in this paper is a generalization of the adjoint technique based on Brannin’s method for the sensitivity and noise analysis of electrical networks [4], originally developed by some of the present authors in [5] with application to the multidimensional noise modelling of semiconductor devices. In what follows, stress will be laid on the formulation of the problem and on the applications of the sensitivity approximation to the statistical analysis of microwave solid-state devices. Examples of technological optimization of a microwave FETs will be presented elsewhere.

Formulation and computational approach
This section is devoted to a formal treatment of the sensitivity analysis within a discretized bipolar drift-diffusion model. Only the sensitivity of the DC parameters will be discussed here; for the AC sensitivities see [3].

Let us suppose that the drift-diffusion model, together with its boundary conditions, has been suitably discretized [6]; thus, the electron and hole concentrations $n$ and $p$ and the potential distribution $\psi$ become arrays of nodal values. Let us formally denote the drift-diffusion set of equations and the boundary conditions as:

$$\begin{align*}
F(\psi, n, p, \dot{n}, \dot{p}; \sigma) &= 0, \\
\chi(\psi, n, p; s, \sigma) &= 0,
\end{align*}
$$

where $F$ is a nonlinear system of dimension $3 \times N$, $N$ being the number of discretization nodes. The set of discretized boundary conditions (of dimension $3 \times M$, where $M$ is the number of device terminals) is denoted through the system $\chi = 0$; $\dot{\alpha} = \partial \alpha / \partial t$ ($\alpha = n, p$) and $s(t)$ is a set of external electrical sources applied at the device terminals. Finally, both the device equations and the boundary conditions depend on a suitable parameter set $\sigma$, including physical and technological parameters.
such as the mobility models, the doping level at each discretization nodes, the device geometrical dimensions and so forth. Both the discretized equations and boundary condition systems are ordered so as to be written as $\mathbf{F} = \{F^{(\psi)}, F^{(n)}, F^{(p)}\}$ and $\mathbf{X} = \{\chi^{(\psi)}, \chi^{(n)}, \chi^{(p)}\}$, where $F^{(\psi)}$ is the discretized Poisson equation, $F^{(n)}$ the discretized electron continuity equation, $F^{(p)}$ the discretized hole continuity equation, and $\chi^{(\psi)}, \chi^{(n)}$ and $\chi^{(p)}$ are the related boundary conditions.

Let the electrical source term be a DC bias $s_0$. If the parameter set $\sigma$ undergoes a small time-independent variation $\Delta \sigma$ with respect to its nominal value $\sigma_0$, the resulting discretized potential and carrier concentration distributions can be written as:

$$\alpha = \alpha_0 + \Delta \alpha \quad \alpha = \psi, n, p$$

where $\alpha_0$ is the DC response with nominal parameters and $\Delta \alpha$ is the DC perturbation due to the parameter variation, which can be analyzed in the linear approximation. As discussed in [3], $\Delta \sigma$ is proportional to $\Delta \alpha$. The linear system defining these unknowns can be obtained by a Taylor expansion of (1), yielding:

$$\begin{bmatrix} F^{(\psi)}_\alpha & F^{(n)}_\alpha & F^{(p)}_\alpha \\ F^{(\psi)}_n & F^{(n)}_n & F^{(p)}_n \\ F^{(\psi)}_p & F^{(n)}_p & F^{(p)}_p \end{bmatrix} \begin{bmatrix} \Delta \psi \\ \Delta n \\ \Delta p \end{bmatrix} = - \begin{bmatrix} F^{(\psi)}_\alpha \\ F^{(n)}_\alpha \\ F^{(p)}_\alpha \end{bmatrix} \Delta \sigma,$$

$$\begin{bmatrix} \chi^{(\psi)}_\alpha & \chi^{(n)}_\alpha & \chi^{(p)}_\alpha \\ \chi^{(\psi)}_n & \chi^{(n)}_n & \chi^{(p)}_n \\ \chi^{(\psi)}_p & \chi^{(n)}_p & \chi^{(p)}_p \end{bmatrix} \begin{bmatrix} \Delta \psi \\ \Delta n \\ \Delta p \end{bmatrix} = - \begin{bmatrix} \chi^{(\psi)}_\alpha \\ \chi^{(n)}_\alpha \\ \chi^{(p)}_\alpha \end{bmatrix} \Delta \sigma$$

(2)

where $F^{(\beta)}_\alpha$ is the partial derivative of $F^{(\beta)}(\beta = \psi, n, p)$ with respect to $\alpha$ evaluated at the DC operating point $(\psi_0, n_0, p_0, 0; \sigma_0)$, and $\chi^{(\beta)}_\alpha$ has a similar meaning.

According to Eq. (2), the DC parametric variation of the model variables is the linear response to source terms linearly dependent on the parameter variation. For equation $\beta (\beta = \psi, n, p)$, such a source term is denoted as:

$$f^{(\beta)} = \sum_{k=1}^{N_p} f^{(k)}_\beta \Delta \sigma_k$$

where $N_p$ is the number of parameters considered and $f^{(k)}_\beta$ is an array of nodal values deriving from discretization. The lumped procedure associated to a finite-box discretization scheme suggests to use $f^{(k)}_\beta \approx f^{(k)}_\beta(\xi_k) \Omega_k$, where $f^{(k)}_\beta(\xi_k)$ is a space-dependent function and $\Omega_k$ is the control volume associated to node $i$. According to the kind of parameter variation considered, the source term can appear as a charge variation in Poisson equation (i.e. $f^{(\psi)} \neq 0$, $f^{(n)} = f^{(p)} = 0$), or as a scalar current term impressed in the right-hand side of the electron or hole continuity equations. The former case arises for doping variations, while the latter occurs e.g. for mobility variations.

Let us suppose that $f^{(\beta)} (\beta = \psi, n, p)$ is a discretized $\delta$ function, i.e. $f^{(\beta)} = 1$ on node $i$ and $f^{(\beta)} = 0$ elsewhere. From (2), we can therefore express the response to $f = (f^{(\psi)}, f^{(n)}, f^{(p)})$ in such case as:

$$\Delta \psi_j = \sum_{\beta=\psi, n, p} G^{(\beta)}_{\psi, j}$$

$$\Delta n_j = \sum_{\beta=\psi, n, p} G^{(\beta)}_{n, j}$$

$$\Delta p_j = \sum_{\beta=\psi, n, p} G^{(\beta)}_{p, j}$$

where $j$ denotes the observation node of coordinate $\tau_j$ and $G^{(\beta)}_{a, j}$ is the response in the variable $a$ (potential, electron or hole concentration) caused by a DC unit source impressed in equation $\beta$; this is, by definition, the discretized Green's function relating a source term in equation $\beta$ to the observed variable $a$. The Green's function corresponding to a source term in the continuity equation yields, for open-circuit boundary conditions on the induced perturbation solution, the so-called scalar impedance field (see [3] and references therein).

The expression of the device DC sensitivities, i.e. the solution of (2) as superposition integrals, is now straightforward. Let us suppose that the discretized Green's functions $G^{(\beta)}_{a, j}$ are available; then, since the problem is linear, the small-change DC sensitivity of any set of external electrical variables can be expressed, with no lack of generality, through the help of the small-signal parameters of the device evaluated in DC and of a linearly independent set of sensitivities. For example, let us consider the set of potentials at the device terminals, $e_i, i = 1, \ldots, M$ and their open-circuit variations. Let us suppose that $N_p$ parameters $\sigma_1, \ldots, \sigma_{N_p}$ are varied; the induced DC variation in the open-circuit potentials will then be:

$$\Delta e_i = \sum_{k=1}^{N_p} \sum_{j=1}^{M} \left( \sum_{\beta=\psi, n, p} G^{(\beta)}_{\psi, j} f_k^{(\beta)}(\tau_j) \Omega_j \right) \Delta \sigma_k$$

$$= \sum_{k=1}^{N_p} \left( \sum_{j=1}^{M} s^{e_i}_{\sigma_k}(\tau_j) \Omega_j \right) \Delta \sigma_k = \sum_{k=1}^{N_p} S^{e_i}_{\sigma_k} \Delta \sigma_k$$

where $s^{e_i}_{\sigma_k}$ is the sensitivity of $e_i$ with respect to $\sigma_k$, expressed as the volume integral of a distributed DC sensitivity $s^{e_i}_{\sigma_k}$. The distributed sensitivity is an interesting result of the Green's function formulation, since it enables to gain a deeper insight on the regions of the device that are more critical with respect to the variation of a given technological parameter. Moreover, if random parameter variations occurring in the device volume are considered, the statistical properties of the induced variations can only be obtained through a distributed formulation.
Figure 1: Distributed sensitivity of uniformly doped epitaxial MESFET: variation of the short-circuit DC drain current due to a 10% variation of the local doping. The device terminals are located at a 0.3 \( \mu \)m depth.

Figure 2: Green's function relative to a DC short-circuit drain current variation for an epitaxial MESFET caused by a point charge injection in the device volume. The device terminals are located at a 0.3 \( \mu \)m depth.

A direct solution of the linear system \( (2) \) requires \( N \) back solves, but the numerical approach described in [5] enables to obtain the relevant information with \( M \) back solves only, where \( M \) is the number of open-circuited device terminals, thereby yielding the same numerical advantage of the adjoint approach. The main advantage of this numerical technique with respect to the latter is its direct applicability to any model derived by the discretization of a system of partial differential equations (see [5] and references therein).

The numerical approach to the sensitivity evaluation was implemented within the BOSS bipolar drift diffusion GaAs finite-boxes device simulator developed at Politecnico di Torino. The simulator includes also the DC and frequency-domain small-signal and physics-based noise analysis. Typical computation times for a 1500 node simulation are 30 s for the DC solution on a HP 735/125 workstation; the computation of the DC sensitivities requires about 5 s, thus introducing a negligible overhead.

Results and discussion

As a first example, we consider a simple, epitaxial MESFET with gate length \( L_g = 0.5 \) \( \mu \)m, gate width \( W = 100 \) \( \mu \)m, active layer thickness \( a = 0.2 \) \( \mu \)m. The epi-layer doping is uniform and equal to \( N_D = 10^{17} \) cm\(^{-3}\) while the S.I. buffer layer has been simulated for a thickness of 0.1 \( \mu \)m and modelled as an ideal, undoped material. For the operating point \( V_{DS} = 3 \) V, \( V_{GS} = 0 \) V we computed the DC sensitivity of the short-circuit current with respect to distributed doping variations \( \Delta N_D(x) \) occurring in each of the discretization nodes. Fig.1 shows the small-change variation of the drain current in short-circuit conditions (i.e. keeping \( V_{DS} \) constant) due to a 10% variation of the doping with respect to the nominal value; this means that a smaller absolute variation has been considered for the buffer layer, where the doping is already low. The small-change current variation is proportional to the distributed sensitivity, and turns out to be maximum in correspondence of the velocity-saturated region of the MESFET. On the other hand, the sensitivity is low below the device contacts, where the device behaviour is mainly ohmic. The shape of the sensitivity profile is a direct consequence of the Green's function expressing the open-circuit potential variation induced by the injection of a nodal charge. A related quantity, the short-circuit DC current variation induced by the injection of a nodal charge, is presented in Fig. 2, which clearly shows that a charge variation has a larger effect when it takes place near the end of the channel. As expected in DC conditions, the corresponding short-circuit gate current small-change variations are negligible.

The statistical analysis of the electrical device performances with respect to small random variations of the technological parameters can be formulated in a straightforward manner on the basis of the sensitivity analysis. For the sake of simplicity, we consider statistical variations of the saturation DC current and of the threshold voltage \( V_T \) due to a statistical spread in the energy of a single-implant profile. Other cases can be treated analogously.

For a single-implant MESFET, the drain current formally depends on the applied bias and on the projected range and straggle of the doping implant, which in turn depend on the implant energy. According to its definition, \( I_{DSS} \) is the drain current evaluated for \( V_{GS} = 0 \) V and \( V_{DS} \) fixed to a constant value; one easily derives, from a first-order approximation, that the \( I_{DSS} \) variation \( \delta I_{DSS} = I_{DSS} - < I_{DSS} > \) is a random variable having the same statistical distribution as \( \delta E \), and whose variance is given by:

\[
<\delta I_{DSS}^2> = \left( \frac{\partial I_D}{\partial R_p} \frac{\partial R_p}{\partial E} + \frac{\partial I_D}{\partial E} \right)^2 <\delta E^2>,
\]

where \( <z> \) is the mean value of \( z \), \( E = <E> + \delta E \) is the implant energy and all the derivatives are evaluated at the mean value. In the same way, the MESFET
threshold voltage $V_T$, defined as that $V_{GS}$ value (for $V_{DS}$ held constant) such that $I_D$ is equal to a suitably small value $I_0$, undergoes a statistical variation with variance:

$$\langle \delta V_T^2 \rangle = \frac{1}{G_m^2} \left( \left( \frac{\partial I_D}{\partial V_{GS}} \right)^2 + \left( \frac{\partial I_D}{\partial V_{DS}} \right)^2 \right) \langle \delta V_{GS}^2 \rangle,$$

where $G_m = \frac{\partial I_D}{\partial V_{GS}}$ denotes the device DC transconductance.

As an example of application, we consider an implant process wherein the implant energy exhibits a random variation with respect to the nominal value. We assume a Gaussian distribution with an average energy of 90 keV and a standard deviation of 10 keV. The energy dependence of the implant parameters follows the model described in [7]. For a MESFET device having gate length $L_g = 0.5 \mu m$, gate width $W = 100 \mu m$ and an implanted dose $D = 2 \times 10^{12} \text{ cm}^{-2}$, we then evaluate the resulting statistical distribution of the saturation current and of the threshold voltage, defined with reference to a current equal to 0.1 mA. The statistical distribution of the saturation current and threshold voltage can be evaluated in closed form from the distribution of $\delta E$. The results are reported in Fig. 3, where the continuous curves have been normalized so that their area is the same as for the corresponding histogram. As a reference solution, the statistical distribution was estimated through direct Montecarlo analysis carried out on the physical model. In the first case, the estimated standard deviation is found to be 1.15 mA (with the sensitivity approach) and 1.19 mA (with the Montecarlo analysis); in the second case, one has 0.32 V and 0.325 V, respectively. It is clear that, if the statistical spread of the input parameter is not too high, the sensitivity analysis provides results in excellent agreement with the much more time consuming direct Montecarlo analysis.

Conclusion

An efficient sensitivity analysis technique is presented. Within the framework of a two-carrier drift-diffusion physical model, the method enables to evaluate the small-change sensitivity of the DC electrical device performances with respect to variations of technological or physical parameters. The results thereby obtained can be exploited in the parametric optimization of devices and in the statistical analysis with respect to random parameter variations, which is the basis for yield estimate and optimization. Further work will concern the implementation of the small-change sensitivity of AC parameters, whose theory is discussed in [3], and the extension to non-stationary transport models.

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References