ROW-Type Methods Applied to the Time Discretization of Device Equations

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1. Introduction. A correct simulation of the switching performance of semiconductor devices is becoming increasingly important in several fields of application. An important case is for example that of power devices, where large amounts of current are involved in driving reactive loads and the influence of parasitic effects should not be disregarded. A typical feature in the devices' switching behaviour is the coexistence of different time constants. In a power device this is true even when neglecting the surrounding circuit elements, because the sizes of the active zones may differ significantly from each other. Hence, when turning to the problem of numerically solving the system of PDE's describing the device's behavior, possibly coupled with those of the circuit elements, the choice of the solution method for the time dimension becomes very critical. The main purpose of this paper is describing the choice and successful application of a class of methods which have originally been devised for modeling, e.g., vehicle dynamics, circuits, or chemical reactions but, at least in the authors' knowledge, have not been used in the field of device analysis. They will be referred here as Rosenbrock-Wanner (ROW) type methods.

2. Theory. Formally, the PDE's describing the time-dependent semiconductor devices' behavior constitute a differential-algebraic system. Referring for instance to the well-known drift-diffusion model, the differential part is made of the two continuity equations for electrons and holes, while the algebraic part is Poisson's equation. After the spatial discretization has been performed and the boundary conditions have been imposed, the structure of the system turns out to be $\dot{\mathbf{y}} = \mathbf{f}(\mathbf{y}, \mathbf{z}), 0 = \mathbf{g}(\mathbf{y}, \mathbf{z})$. In our case, vector $\mathbf{y} = \mathbf{y}(t)$ is made of the values n_i, p_i, of the electron and hole concentrations at the nodes of the discretization grid, while vector $\mathbf{z} = \mathbf{z}(t)$ is made of the nodal values of the electric potential. Given consistent initial values $\mathbf{y}_0 = \mathbf{y}(t_0)$, $\mathbf{z}_0 = \mathbf{z}(t_0)$, the extension of the ROW method to the solution of the differential-algebraic system is achieved by embedding the algebraic part as $\varepsilon\dot{\mathbf{g}} = \mathbf{g}(\mathbf{y}, \mathbf{z})$ and then considering the limiting case $\varepsilon \rightarrow 0$. The details are given, e.g., in [1,2], along with the determination of the stability properties. Only the general form of the ROW iteration of order s is reported here, that is $\mathbf{y}(t_0 + \Delta t) = \mathbf{y}_0 + \sum_{i=1}^{s} c_i \mathbf{k}_i$, where c_i are fixed coefficients and $\mathbf{k}_i(\Delta t)$ are found by a modified, semi-implicit Runge-Kutta procedure. What must be stressed here is that this approach leads to a class of discretization methods which are essentially different from the standard ODE ones, and exhibit the rather promising feature of yielding a semi-implicit structure while keeping the stability properties of the implicit ones. Hence, it is worth investigating the performance of the extended ROW methods and carrying out some comparison with those used so far.

3. Implementation. The implementation of the ROW scheme has been carried out in the two-dimensional, drif-diffusion version of the in-house developed code `HFIELDS`. In the standard version, the time discretization in `HFIELDS` is achieved by means of the backward-Euler (BE) method. During the solution the code automatically selects the subintervals Δt of the prescribed time window(s) ΔT_i using a criterion based on the local truncation error. The application of the BE method at some t gives rise to a non-linear algebraic system, whose solution provides the unknown vectors $\mathbf{y}$, $\mathbf{z}$ at $t + \Delta t$. To avoid a new factorization of the system matrix at each Δt, the Jacobian matrix is kept unmodified for a number of consecutive Δt's and a suitable damping procedure is used in the RHS (because of the damping more than one evaluation of the RHS per Δt is needed in the average). The number of Newton iterations is further decreased by means of a projection scheme. Thanks to the above, the number of factorizations over the time windows is reduced in the average with respect to the number of solutions of the algebraic system, yielding a corresponding reduction in the overall computation time. Turning now to the ROW method, it will be shown below that its application brings a significant improvement in the solution speed with respect to the standard one, despite of the refinements which have been incorporated in the latter. The improvement is achieved by tackling directly the most expensive point of the procedure, i.e., the number of factorizations. In fact, the semi-implicitness of ROW makes one factorization per Δt sufficient. The ROW method used here is that of order 1, to be readily compared with the BE one since their precision is the same (i.e., order 1 in the time discretization). It is worth adding that both methods could be improved by introducing an iterative solver, especially in three-dimensional problems where the number of unknows is very large; on the other hand the number of time steps, hence the gain in the number of factorizations, would not be affected by this in either the BE or the order-1 ROW method.

4. Experiments and Results. The ROW method has been tested on the transient behaviour of a realistic power BJT [3]. A 1-μm, constant device width was assumed, and the emitter and collector voltages V_E and V_C were set at 0 and 1 V, respectively. The base voltage V_B, starting from a steady-state condition, was first switched from 0 to 1 V at $t = 0$ using a 1-psec linear ramp, was kept at 1 V for 5 μsec, then switched back to 0 V in 1 psec, and finally left there for 5 more μsec. The corresponding collector current I_C is shown in Fig. 1, where the continuous lines refer to BE and the dots to ROW. The negative value of I_C at very small t is due to the electrons injected into the collector to reduce the space charge at the base-collector junction. In a very short time I_C turns to positive values as the base-emitter junction enters the forward regime. Then I_C keeps

increasing until V_B is switched back to ground, which happens much before the steady-state condition is reached (this would take about 100 μsec). It is seen that I_C exhibits different time constants, related to the progressive increase of the carrier population in the base neutral region and in the junction regions. Different time constants can also be seen in the finer detail of the inset of Fig. 1. The positive peak at $t = 5$ μsec is due to the rebuilding of the space charge at the base-collector junction, though its amplitude is different than at $t = 0$ due to the larger capacitance. Finally, I_C decreases back to the reverse-bias value, again exhibiting different time constants. The final simulation time $t = 10$ μsec occurs much before reaching the steady-state condition.

As anticipated, the comparisons have been carried out using a ROW method of order 1, hence the total number of subintervals Δt was found to be about the same. Each half of the $I_C(t)$ curve of Fig. 1, made of one peak and a smoother portion, contributed about the same number of Δt, yielding 115 for the BE and 111 for the ROW method. However, while in the order-1 ROW method only one cycle factorization-RHS evaluation-solution is necessary at each Δt, hence the cycles amounted to 111 as well, the BE method required 201 solutions with factorization, 334 solutions with no factorization (hence a total of 535 solutions), and 700 RHS evaluations. This rather simple example shows that an appreciable gain is already achieved by the ROW method of order 1, whose implementation is by the way easier than that of BE. Further improvements are expected, on one side, using higher-order ROW methods and, on the other, in situations where the high-curvature portions of the $I(t)$ curves are much more numerous than in the example here. This case occurs, for instance, in oscillatory situations, typical of reactively-loaded power devices. To conclude, a time-discretization scheme has profitably been used in a new field of application, that of the transient simulation of semiconductor devices. As shown in the example presented here, its numerical accuracy compares quite well with that of the classical methods for ODE's, while its efficiency is superior. Moreover, the new method keeps the stability properties of the implicit ones, and its implementation is straightforward. It appears therefore a promising technique, worth further investigation in the device and the mixed-circuit/device simulations.

Acknowledgement: L. Colalongo profits by a fellowship provided by ST-Co.Ri.M.Me.

References

[1] J. R. Cash, *Semi-Implicit Runge-Kutta Procedures with Error Estimates for the Numerical Integration of Stiff Systems of ODE's*, J. of the ACM, Vol. 23, No. 3, July 1976, pp. 455-460.

[2] P. Rentrop, M. Roche, G. Steinebach, *The Application of Rosenbrock-Wanner Type Methods with Stepsize Control in Differential-Algebraic Equations*, Numerische Mathematik, Vol. 55, 1989, pp. 545-563.

[3] F. Gatti, A. Gnudi, G. Baccarani, G. Ferla, S. Aparo, *A New Methodology to Handle Mixed Circuit-Device Equation*, Proc. of the Fourth NUPAD Workshop, Seattle, May 1992, pp. 213–218.