Numer. Math. (1998) 79: 203–212

Numerische
Mathematik

Electronic Edition

Simulating digital circuits numerically – a charge-oriented ROW approach

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Received January 22, 1996 / Revised version received January 28, 1997

Summary. A ROW type approach is considered for integral form DAEs arising in charge-oriented nodal analysis of digital networks. These network equations define very special index-2 systems that can be solved by Rosenbrock-Wanner (ROW) methods suitable for semi-explicit index-1 systems without order reduction. To obtain charge conservation, the charge variables are projected on the linear charge constraint. In contrast to the semi-explicit index-1 case, all order conditions for the algebraic variables up to order p have to be fulfilled for a method of order p. CHORAL, an embedded charge-oriented method of order (2)3, is introduced and compared with DASSL and RODAS for two industrial applications, the NAND gate and the two-bit adding unit.

Mathematics Subject Classification (1991): 65L05

1. Introduction

TCAD based electric circuit simulation tools commonly use a charge oriented approach to describe especially intrinsic charge flow effects in MOS transistors physically correct [2, 4]. Considering the important class of circuits without flux storing elements, this ansatz yields stiff differential-algebraic equations of integral form

$$(1)\quad \mathcal{F}(x,\dot{q}) = A\cdot\dot{q}(x) - f(x) = 0 \quad \text{on} \quad t\in[0,T], \qquad x(0)=x_0$$

as network equations[1]. The system (1) can be described as follows: The vector $x \in \mathbb{R}^n$ of unknowns consists of all node potentials at current defining elements. The m terminal charges $q_i(x)$, $m \approx 3n$, given as functions of node potentials, are assembled at each node by the incidence matrix $A \in \{-1, 0, 1\}^{n \times m}$. In general, A has *not* full row rank. The total time derivative $\dot{q}_i(x) = \mathrm{d}q_i(x)/\mathrm{dt}$ describes the charge flow caused by the i-th terminal charge $q_i(x)$. At each node j, the current $[A \cdot \dot{q}(x)]_j$ due to the charge flow is related to the sum of all other static currents $f_j(x)$ by Kirchhoff's current law. Note that circuits with time dependent input signals yield autonomous network equations of type (1) as usual by introducing t as an additional unknown.

Charge-oriented network equations are commonly solved by the direct BDF ansatz [1,2,9] in industrial network simulation packages. This approach has the drawback that the step size control is based on charges, but the user is only interested in the nodal voltages. The accuracy in the nodal voltages is only checked in the Newton-Raphson iteration, or error estimates in x have to be computed from estimates in q. In this paper, we introduce Rosenbrock methods that directly offer an error control and step size prediction based on nodal voltages. We restrict ourselves to the important class of digital circuits, which are generally described by network equations of the following special type:

(2a) The Jacobian $Aq'(x)$ is smooth and has constant image along the solution. In general, the rank s of A is larger than the rank r of $Aq'(x)$.

(2b) The matrix pencil $\{Aq'(x), f'(x)\}$ is regular and has index 1 of nilpotency along the solution.

(2c) The initial values are consistent, i. e.

$$f(x(0)) \in \mathrm{Im}\,(Aq'(x(0))), \qquad y(0) = q(x(0)),$$

Though the first assumption may not be fulfilled along the whole solution, it holds piecewise within every operation region of the transistor. The second property can be achieved for digital circuits by appropriate modeling and regularization techniques.

In the following section, we show that these network equations define very special index-2 systems that can be solved by Rosenbrock methods for semi-explicit index-1 systems without order reduction. We introduce CHORAL, an embedded ROW method of order (2)3,which uses a projection of the differential variables. Finally, this method is compared with DASSL

[1] Here, and in the following, $\dot{}$ denotes the total time derivative and $'$ the partial derivative with respect to x: $A\dot{q}(x) = Aq'(x)\dot{x}$

and RODAS for two industrial applications: NAND gate and two-bit adding unit.

2. Charge-oriented network equations for digital circuits

Using the integral form structure in (1), it is natural to introduce charges, technically demanded in semiconductor physics, as additional state variables. Now (1) is enlarged into the differential-algebraic system

$$A \cdot \dot{y} = f(x) \tag{3a}$$

$$0 = y - q(x) \tag{3b}$$

of linear-implicit form. This system is equivalent to an index-2 system with the very special property that all index-2 variables are constant: Decomposing the matrix A as

$$A = S \begin{pmatrix} I_s & 0 \\ 0 & 0 \end{pmatrix} T$$

with the identity I_s and nonsingular constant matrices $S \in \mathbb{R}^{n\times n}$ and $T \in \mathbb{R}^{m\times m}$, the assumption (2a) yields that $s-r$ of the first s components of $S^{-1}Aq(x)$ are constant along the solution. Without loss of generality, we can assume that the components $s-r+1$ up to s of $S^{-1}Aq(x)$ are constant. Hence system (3) can be transformed into the semi-explicit system

$$\dot{\widetilde{y}}_1 = \widetilde{f}_1(x), \qquad 0 = \widetilde{y}_1 - \widetilde{q}_1(x) \tag{4a}$$

$$\dot{\widetilde{y}}_2 = \widetilde{f}_2(x), \qquad 0 = \widetilde{y}_2 - \widetilde{q}_2(x) = \widetilde{y}_2 - const \tag{4b}$$

$$0 = \widetilde{f}_3(x), \qquad 0 = \widetilde{y}_3 - \widetilde{q}_3(x) \tag{4c}$$

via constant regular matrix transformations, where the components of $(\widetilde{q}_1(x), \widetilde{q}_2(x), \widetilde{q}_3(x))^{\mathrm{t}} = Tq(x)$, $(\widetilde{y}_1(x), \widetilde{y}_2(x), \widetilde{y}_3(x))^{\mathrm{t}} = Ty(x)$ and $(\widetilde{f}_1(x), \widetilde{f}_2(x), \widetilde{f}_3(x))^{\mathrm{t}} = S^{-1}f(x)$ have dimensions r, $s-r$ and $n-s$. The differential index of system (3) depends on the dimension of $\widetilde{y}_2$:

- In classical capacitance-oriented MOS modeling, $s = r$ holds, and dim $\widetilde{y}_2 = 0$. System (4) is thus an index-1 Hessenberg system, since the matrix $(\widetilde{q'}_1(x), \widetilde{f'}_3(x))^{\mathrm{t}}$ is regular by condition (2b).
- If charge-oriented MOS models are used, generally $s > r$ holds [4], and dim $\widetilde{y}_2 > 0$: the algebraic equation $0 = \widetilde{y}_2 - const$ occurs, which does not depend on the algebraic variables $\widetilde{y}_3$ and x. The index is 2, since the matrix $(\widetilde{q'}_1(x), \widetilde{f'}_2(x), \widetilde{f'}_3(x))^{\mathrm{t}}$ is regular by condition (2b).

Hence digital MOS circuits yield charge-oriented network equations (3) that are equivalent to the index-2 system (4) via constant regular matrix transformations. Rosenbrock methods are invariant with respect to such

transformations. Since $\widetilde{y}_2 = const$ holds, these components are integrated exactly by a ROW method, and the numerical solution is thus identical to that when the same Rosenbrock method is applied to

$$\dot{\widetilde{y}}_1 = \widetilde{f}_1(x), \qquad 0 = \widetilde{y}_1 - \widetilde{q}_1(x) \tag{5a}$$

$$0 = \widetilde{f}_2(x), \qquad 0 = \widetilde{y}_2 - const \tag{5b}$$

$$0 = \widetilde{f}_3(x), \qquad 0 = \widetilde{y}_3 - \widetilde{q}_3(x). \tag{5c}$$

This is a semi-explicit index-1 problem. Rosenbrock methods for semi-explicit index-1 problems can also be applied to the special type (3) of charge-oriented network equations of index 2 — no order reduction takes place.

3. ROW approach for charge-oriented network equations

A ROW method with stage number s applied to the linear-implicit system (3) reads [8, 10]

$$x_1 = x_0 + b^{\mathrm{t}} k, \tag{6a}$$

$$y_1 = y_0 + b^{\mathrm{t}} l, \tag{6b}$$

with weights $b := (b_1, \ldots, b_s)^{\mathrm{t}}$ and increments $k := (k_1, \ldots, k_s)^{\mathrm{t}}$, $l := (l_1, \ldots, l_s)^{\mathrm{t}}$ defined by

$$\begin{pmatrix} A & -\gamma h f'(x_0) \\ -\gamma I & \gamma q'(x_0) \end{pmatrix} \cdot \begin{pmatrix} l_i \\ k_i \end{pmatrix} = \tag{6c}$$

$$\begin{pmatrix} hf(\sum_{j=1}^{i-1} \alpha_{ij} k_j) + hf'(x_0) \sum_{j=1}^{i-1} \gamma_{ij} k_j \\ y_0 - q(\sum_{j=1}^{i-1} \alpha_{ij} k_j) + \sum_{j=1}^{i-1} (\alpha_{ij} + \gamma_{ij}) l_j - q'(x_0) \sum_{j=1}^{i-1} \gamma_{ij} k_j \end{pmatrix}$$

where $\alpha_{ij} = 0$ for $i \geq j$, $\gamma_{ij} = 0$ for $i > j$ and $\gamma_{ii} = \gamma \neq 0$, $i, j = 1, \ldots, s$. x_1 and y_1 are the approximations to the solution at time h with $x(0) = x_0$, $y(0) = y_0$. The increments are uniquely defined by the linear system (6c): the matrix

$$\begin{pmatrix} 0 & Aq'(x_0) - \gamma h f'(x_0) \\ -\gamma I & \gamma q'(x_0) \end{pmatrix}$$

obtained after one block Gaussian elimination step is nonsingular for sufficient small step sizes h, since the matrix pencil $\{Aq'(x), f'(x)\}$ is regular due to condition (2b). The linear structure of the charge constraint (3b) allows for k_i to be computed independently from $l_1, \ldots, l_{i-1}$. To fulfill charge conservation during integration, the differential variables y are projected at each grid point in the integration interval $[0, T]$ on the charge constraint:

$$y_m := q(x_m), \qquad m = 1, 2, \ldots, T/h \tag{6d}$$

Convergence and order conditions. As shown in Sect. 2, classical convergence theory for semi-explicit index-1 problems can be applied to the ROW method (6a,6c,6d) for the index-2 system (3). Owing to the projection (6d), the local error $q(x_1) - q(x(h))$ must be $\mathcal{O}(h^{p+1})$ to obtain convergence order p. For arbitrary charge functions, this conditions leads to the requirement $x_1 - x(h) = \mathcal{O}(h^{p+1})$. Since the special structure of the Hessenberg index-1 system (5) cannot be exploited, we have the following theorem:

Theorem 1. *To obtain order p for the network equations (3), the coefficients of the Rosenbrock method (6a,6c,6d) have to fulfill all order conditions for the algebraic variables up to order p in general index-1 Hessenberg systems.*

Proof. To prove this theorem, it is sufficient to show that despite the special structure of (5), all order conditions for the general index-1 Hessenberg system have to be fulfilled for a ROW method of order p.

We consider system (5) as a special case of an index-1 Hessenberg system

$$\begin{aligned} \dot{z} &= f(x) \\ 0 &= g(x,z) = Bz + \bar{g}(x) \end{aligned}$$

with $f_z \equiv 0$ and $B \in \{0,1\}^{2n-r \times r}$. Using the notation of Roche [11], the elementary differentials for the following trees are vanishing:

$$\begin{aligned} &[v_1,\ldots,v_m,u_1,\ldots,u_n]_z \qquad \text{for } m \geq 1,\ n \geq 0 \qquad (f_z \equiv 0)\,, \\ &[v_1,\ldots,v_m,u_1,\ldots,u_n]_x \quad \text{for } m \geq 1,\ m+n \geq 2 \quad (g_z \equiv B)\,, \end{aligned}$$

with $v_1,\ldots,v_m$ denoting trees in DAT_z, and $u_1,\ldots,u_n$ in DAT_x. The equivalence $\Phi_i([v]_x) = \Phi_i(v)$, however, yields

$$\begin{aligned} \Phi_i([v_1,\ldots,v_m,u_1,\ldots,u_n]_z) &= \Phi_i([[v_1]_x,\ldots,[v_m]_x,u_1,\ldots,u_n]_z)\,, \\ \Phi_i([v_1,\ldots,v_m,u_1,\ldots,u_n]_x) &= \Phi_i([[v_1]_x,\ldots,[v_m]_x,u_1,\ldots,u_n]_x)\,. \end{aligned}$$

Since the number of meagre nodes is equal in both cases, the order conditions coincide for the corresponding trees. But the order conditions for the trees of type $[[v_1]_x,\ldots,[v_m]_x,u_1,\ldots,u_n]_z$ and $[[v_1]_x,\ldots,[v_m]_x,u_1,\ldots,u_n]_x$, resp., cannot be dropped in the special case (5). Hence all order conditions for an index-1 Hessenberg are necessary.

The order conditions for index-1 Hessenberg systems can be found, e. g., in [10]. For $p = 1, 2, 3$ and 4 one, three, eight and 24 order conditions are required to get a local error of $\mathcal{O}(h^{p+1})$ for the algebraic variables.

Implementation of CHORAL. One notes that the coefficient sets of RODAS [6, 12], the state-of-the-art Rosenbrock method for linear-implicit index-1 problems, are constructed according to the demands made in theorem 1. Hence they yield embedded ROW methods of order (3)4 to solve charge-oriented network equations of type (3). On account of the low smoothness

properties of transistor models, as well as of the low accuracy demands required by the user, an embedded method of order (2)3 seems to be more suitable.

The corresponding scheme, CHORAL, has four stages and only three function evaluations. To avoid a constant term in the error estimate due to inconsistent initial values, both methods are chosen as stiffly accurate [6]. The implementation of CHORAL is tailored to the time-dependent network equations

$$A\dot{q}(x,t) - f(x,t) = 0 \tag{7}$$

of the special type $q(x,t) = \bar{q}(x, s_1(t))$ and $f(x,t) = \bar{f}(x, s_1(t)) + s_2(t)$, which arise in charge-oriented nodal analysis of digital circuits without inductive behavior. $s_1(t)$ denotes the time-dependent input voltages, whereas $s_2(t)$ describes the time-dependent current sources. Only linear systems of dimension n have to be solved:

$$x_1 = x_0 + \sum_{i=1}^{s} d_i \kappa_i,$$

with the increments κ_i given by the linear system

$$\left(A\frac{\partial q}{\partial x} - h\gamma \frac{\partial f}{\partial x} \right) \Bigg|_{x_0,t_0} \kappa_i = A\left(q(x_0,t_0) - q(a_i, t_0 + h\alpha_i)\right) +$$
$$h\sum_{j=1}^{i} \beta_{ij} f(a_j, t_0 + h\alpha_j) + h\sum_{j=1}^{i-1} \beta_{ij} \frac{\partial f}{\partial x}(x_0,t_0)\kappa_j +$$
$$h^2 \tau_i \frac{\partial f}{\partial t}(x_0,t_0) - h\gamma_i A \frac{\partial q}{\partial t}(x_0,t_0).$$

Here we have used with $\mathcal{G} = (\gamma_{ij})_{i,j=1}^{s}$, $\mathcal{A} = (\alpha_{ij})_{i,j=1}^{s}$, $\mathcal{B} = \mathcal{A} + \mathcal{G}$ and $\mathcal{S} = (\sigma_{ij})_{i,j=1}^{s} := \mathcal{A}\mathcal{G}^{-1}$ the transformed increments $\kappa = \mathcal{G}k$ and the abbreviations

$$\alpha_i = \sum_{j=1}^{i-1} \alpha_{ij}, \quad \gamma_i = \sum_{j=1}^{i} \gamma_{ij}, \quad \tau_i = \sum_{j=1}^{i} \beta_{ij}\gamma_j$$

$$\text{and } a_i = x_0 + \sum_{j=1}^{i} \sigma_{ij}\kappa_j \,.$$

The corresponding coefficient set of CHORAL is given in Table 1. Since the usual error estimate (see, e. g., [10]) for stiffly-accurate embedded ROW methods is used, a reliable error control and step size selection are offered that are based on node potentials. No heuristic techniques are necessary to recompute errors from charges into node potentials.

Table 1. Coefficients for CHORAL

$\gamma = 0.5728160624821349$	$\beta_{21} = -2.0302139317498051$
$d_1 = \widehat{d}_1 = \sigma_{21} = \sigma_{31} = \sigma_{41} = 1/\gamma$	$\beta_{31} = 0.2707896390839690$
$d_2 = \widehat{d}_2 = \sigma_{32} = \sigma_{42} = 0.0$	$\beta_{32} = 0.1563942984338961$
$d_3 = \widehat{d}_3 = \sigma_{43} = 1.0$	$\beta_{41} = 2/3$
$d_4 = 1.0$	$\beta_{42} = 0.08757666432971973$
$\alpha_2 = 1.0$	$\beta_{43} = -0.3270593934785213$
$\alpha_3 = 1.0$	$\gamma_1 = \gamma$
$\alpha_4 = 1.0$	$\gamma_2 = -2.457397870$
$\tau_1 = 0.3281182414375370$	$\gamma_3 = 0$
$\tau_2 = -2.57057612180719$	$\gamma_4 = 0$
$\tau_3 = -0.229210360916031$	
$\tau_4 = 1/6$	

The method is compatible with circuit simulation packages such as TITAN [2]: model evaluation, direct sparse matrix solvers and multi rate techniques already implemented in the numerical integration kernel can be used efficiently. This is confirmed by the numerical results in the next section.

4. Technical application: NAND gate and two-bit adding unit

The NAND gate is a logical subcircuit that connects two input signals by the *n*ot *and*-operation. It is part of the two-bit adding unit, a digital circuit which adds two two-digit binary numbers and one carry-in bit. The result is a three-digit binary number. This device is the basis for more complex adder units in CPUs. Its implementation in MOS-technique consists of three NOR gates, one NAND gate, one ORANI gate and five ANDOI gates. See [3] for a detailed description of the models[2].

Using charge-oriented nodal analysis, the two-bit adding unit is described by 175 node potentials as unknowns, and the NAND gate by 14. Neglecting artificial load capacitances, the index of system (1) is one for both problems.

CHORAL is compared with DASSL [1], representing the standard integration software in circuit simulation packages, and different coefficient sets implemented in RODAS [6]. The first set RODAS1 is given in [6], RODAS2 is a modification with stronger damping behavior. The third set RODASP was constructed by Steinebach [12] to get order four also for linear parabolic

[2] The model for the two-bit adding unit is available as FORTRAN77 subroutines at the CWI test set for IVP solvers [7] via WWW at the page http://www.cwi.nl/cwi/projects/IVPtestset.shtml. The NAND gate model is available by the author via e-mail

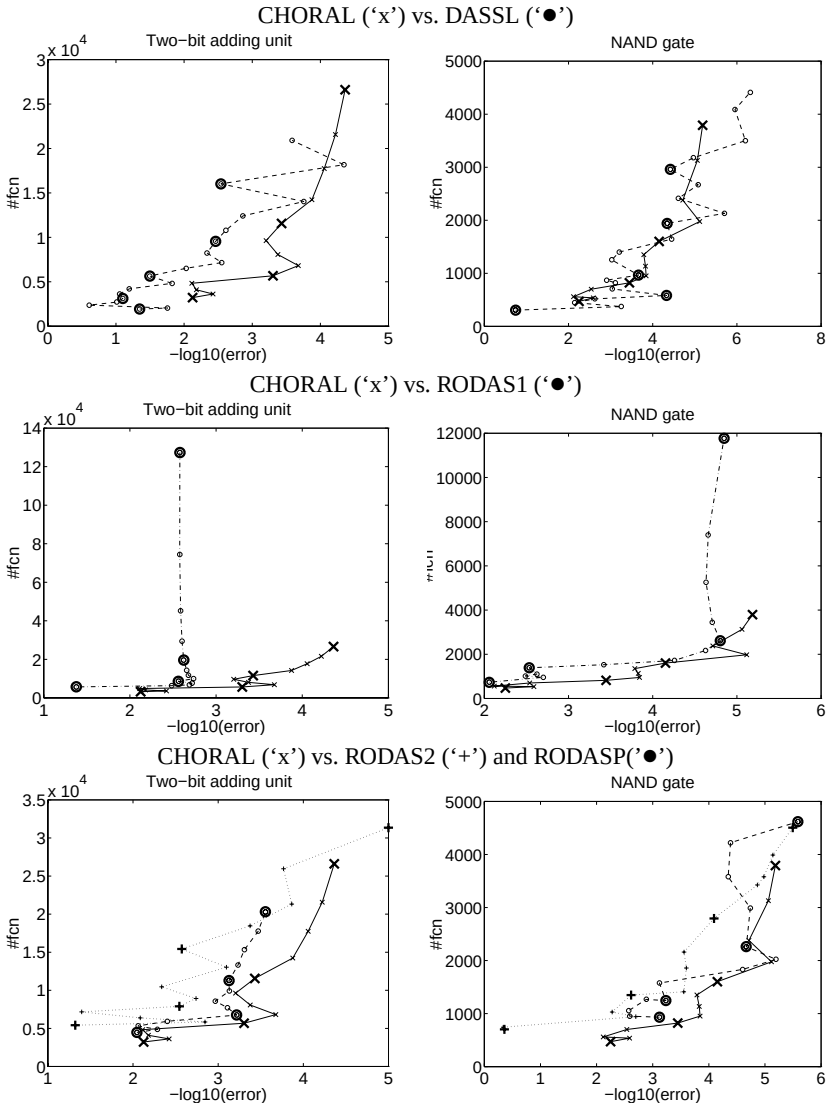

Fig. 1. Work-precision diagram for two-bit adding unit (left) and NAND-gate (right). We used: $rtol = 10^{-1+m/4}$ with $m = 0, 1, \ldots, 12$ for CHORAL and RODAS, and $m = 0, 1, \ldots, 20$ for DASSL. The highly accurate reference solutions are obtained by RADAU5 [6] with $rtol = atol = 10^{-12}$

systems, avoiding order reduction phenomena for method of lines applications. All coefficient sets represent an A-stable stiffly accurate embedded ROW method of order 4(3) with six stages that fulfill the demands of Theorem 1. Hence they can be applied on systems of type (1), if the assumptions made in (2) hold.

In Fig. 1 we present the work-precision diagram (cf. [6], for example), relating the achieved accuracy (Euclidian norm of relative errors in all components) to the number `fcn` of function evaluations for the two-bit adding unit (left) and the NAND gate (right)[3]. This number is a reasonable measure for the computation costs, since the costs for model evaluation generally exceed the costs for the linear algebra part in common circuit simulation tools [2].

All methods except RODAS1 show a robust behavior for both problems, with CHORAL being the most efficient method for non stringent accuracy demands required in network analysis. RODAS1, however, seems to react very sensitive to the model discontinuities for higher tolerances. These are mainly caused by changing operation regions of the transistors during integration; the used transistor model due to Shichman and Hodges [5] is not smoothly fitted at the boundaries of different operation regions. Consequently, each transistor introduces several discontinuity points caused by its modeling. Due to our experience, it does not make sense to detect and localize these points in order to restart the integration, i. e. to apply the so-called switching point technique from optimal control [13].

Acknowledgements. The author thanks P. Rentrop for his encouragement and support, as well as U. Feldmann and E. Hairer for helpful discussions.

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