A-Stability of Multirate Integration Methods, with Application to Parallel Semiconductor Device Simulation*

M. Reichelt† F. Odeh‡ J. White§

Abstract

In this paper we present a few theoretical and experiment results on applying multirate integration algorithms to solving the differential-algebraic equations generated by spatial discretization of the semiconductor device equations.

1 Introduction

Spatial discretization of the time-dependent partial differential equations used to model semiconductor devices generates large sparsely-coupled systems of index one semi-explicit differential-algebraic equations (DAE's)[1]. The solution to these systems can be computed using the waveform relaxation (WR) method, a technique which is a generalization of algebraic relaxation schemes to differential equations[2]. As the WR algorithm decomposes systems of differential equations into subsystems which can be solved independently, the algorithm has easily exploited parallelism[3]. When using WR on a parallel computer, it is likely that the different subsystems will be assigned to different processors. In that case, communication can be avoided, and overall computational efficiency improved, if each of the separated subsystems can be solved with independently determined timesteps.

Using different timesteps for different subsystems implies that a *multirate integration* method has been used to solve the system. In this paper, we present a few theoretical and experimental results about using multirate integration to solve semiconductor equations. We start in the next section with background material on semiconductor equations, WR, and multirate integration. In section 3, we give a multirate WR convergence theorem, and then use it to prove a multirate A-stability result in Section 4. In Section 5, we give some experimental results on using multirate WR to simulate MOS semiconductor devices, and in Section 6 we give conclusions and acknowledgements.

2 Background Material

The drift-diffusion model for transport in a semiconductor is a coupled system consisting of the Poisson equation and electron and hole current-continuity equations,

$$\nabla^2 u + c_1 (p - n + D) = 0 \quad (1)$$

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†Research Laboratory of Electronics, Mass. Inst. Tech.

‡I.B.M. T. J. Watson Research Center

§Research Laboratory of Electronics, Mass. Inst. Tech.

$$(2)\qquad \nabla^2 n - \nabla n \nabla u - n\nabla^2 u = c_2 \frac{\partial n}{\partial t}$$

$$(3)\qquad \nabla^2 p + \nabla p \nabla u + p\nabla^2 u = c_3 \frac{\partial p}{\partial t}$$

where u is the normalized electrostatic potential, n and p are electron and hole concentrations, D is a background doping concentration, and c_1, c_2, and c_3 are physical constants [4].

A common approach to spatially discretizing (1), (2), and (3) is to use a finite-difference formula to discretize the Poisson equation, and an exponentially-fit, finite-difference formula to discretize the continuity equations [5]. At each node of an m-node uniform mesh,

$$(4)\qquad \sum_j [u_i - u_j] - w^2 c_1 (p_i - n_i + D_i))$$

$$(5)\qquad \sum_j [n_i B(u_i - u_j) - n_j B(u_j - u_i)] = \frac{c_2}{w^2}\frac{dn}{dt}$$

$$(6)\qquad \sum_j [p_i B(u_j - u_i) - p_j B(u_i - u_j)] = \frac{c_3}{w^2}\frac{dp}{dt}$$

where w is the spatial discretization step; now $u, n, p \in \Re^m$ are vectors of normalized node potential, electron concentration, and hole concentration; and the sums in the three equations are over either two, four or six neighboring nodes for one, two or three dimensional analysis respectively. The Bernoulli function, $B(x) = x/(e^x - 1)$, is used to exponentially fit the potential variation to electron and hole concentration variations, and effectively upwinds the current-continuity equations.

To analyze multirate stability, we will consider linearizations of the spatially discretized drift-diffusion model of the form

$$(7)\qquad \boldsymbol{D}\dot{x}(t) = \boldsymbol{A}x(t) \quad x(0) = x_0$$

where $t \in [0, \infty)$, $x(t) \in \Re^N$, $\boldsymbol{D}, \boldsymbol{A} \in \Re^{N\times N}$, and $\boldsymbol{D}$ is a diagonal matrix whose diagonal entries are either one or zero, where the zeros correspond to the algebraic equations associated with the discretized Poisson equation.

If $\boldsymbol{A}$ is partitioned (possibly after reordering equations) as in

$$(8)\qquad \boldsymbol{A} = \begin{bmatrix} \boldsymbol{A}_{1,1} & \boldsymbol{A}_{1,2} & \dots & \boldsymbol{A}_{1,M} \\ \cdot & \cdot & \cdot & \cdot \\ \cdot & \cdot & \cdot & \cdot \\ \cdot & \cdot & \cdot & \cdot \\ \boldsymbol{A}_{M,1} & \boldsymbol{A}_{M,2} & \dots & \boldsymbol{A}_{M,M} \end{bmatrix}$$

where $\boldsymbol{A}_{ij} \in \Re^{N_i \times N_j}$ and $\sum_{i=1}^{M} N_i = N$, then the above partitioning is said to be *stable* if $\boldsymbol{D}_{ii}\dot{x}_i(t) = \boldsymbol{A}_{ii}x_i(t)$ is a stable DAE. The characterization of the partitioned matrix given below is a slight generalization of block diagonal dominance [6].

DEFINITION 2.1. *The partitioned matrix $\boldsymbol{A}$ is said to satisfy the dominance condition with respect to a given norm if the positive matrix $\boldsymbol{P} \in \Re^{M\times M}$, whose diagonal elements are zero and whose off-diagonal elements are given by*

$$(9)\qquad \boldsymbol{P}_{ij} = \|\boldsymbol{A}_{ii}^{-1}\| \|\boldsymbol{A}_{ij}\|,$$

has a spectral radius less than one.

When Gauss-Jacobi Waveform Relaxation[2] (WR) is applied to solve (7) given a partitioning of A, the iteration update equation for x^{k+1} given x^k is

$$D_{ii}\dot{x}_i^{k+1}(t) = A_{ii}x_i^{k+1}(t) + \sum_{j\neq i} A_{ij}x_j^k(t). \tag{10}$$

where the superscript k is the WR iteration index, $i \in \{1, ..., M\}$ is the partition index, $x_i^k(t), x_i^{k+1}(t) \in \Re^{M_i}$, and $x_i^{k+1}(0) = x_{i_0}$. If the partitioned A satisfies the dominance condition, then results from [7] can be used to easily prove the following theorem.

THEOREM 2.1. *If the matrix A in (7) is stably partitioned, and the partitioning satisfies the dominance condition in definition (2.1), then given any two arbitrary waveforms x^k and y^k on $[0, \infty)$ which match the initial conditions of (7), the x^{k+1} and y^{k+1} waveforms computed from (10) satisfy*

$$\|x^{k+1} - y^{k+1}\| \leq \gamma \|x^k - y^k\| \tag{11}$$

where $\gamma < 1$ is independent of x^k and y^k.

Approximately solving (10) with a fixed-timestep backward-difference formula results in a discretized WR iteration update equation,

$$\sum_{l=0}^{p} \alpha_l D_{ii} x_i^{k+1}[m-l] = h_i \left[A_{ii}x_i^{k+1}[m] + \sum_{j\neq i} A_{ij} I_{mh_i}\left(\{x_j^k\}\right)\right] \tag{12}$$

where p is the order of the integration method, the α_l's are the integration method coefficients, h_i is the timestep used to compute x_i, $x_i^{k+1}[m]$ is the discrete approximation to $x_i^{k+1}(mh_i)$, and $I_t(\{x_j^k\})$ is some interpolation operator which maps $t \in \Re^+$ and sequence $\{x_j^k\}$ on $\Re^{N_j}$ to a vector in $\Re^{N_j}$.

If the iteration in (12) converges, the resulting sequence, $\{x\}$, will satisfy

$$\sum_{l=0}^{p} \alpha_l D_{ii} x_i[m-l] = h_i \left[A_{ii}x_i[m] + \sum_{j\neq i} A_{ij} I_{mh_i}(\{x_j\})\right] \tag{13}$$

for $i \in \{1, ..., M\}$, and this discrete system is said to be a multirate integration method for solving (7) [8].

There are no general multirate A-stability results which hold given any partitioning of a stable system, and counter-examples exist even for the backward-Euler algorithm [9]. Instead, we will consider results that depend on the properties of the partitioned matrix.

DEFINITION 2.2. *A multirate method of the form of (13) is A-stable for a given partitioned $A \in \Re^{N\times N}$ if for any set of positive timesteps $\{h_1, ..., h_M\}$ and any initial conditions*

$$\lim_{m\to\infty} x_i[m] = 0 \tag{14}$$

for all $i \in \{1, ..., M\}$.

Though multirate integration methods don't necessarily inherit the stability properties of the integration methods used in solving the subsystems, the A-stability of the subsystem integration methods is essential for multirate A-stability.

DEFINITION 2.3. *A multirate method of the form of (13) is partition-by-partition A-stable for a given partitioned $A \in \Re^{n\times n}$ if the solution to*

$$\sum_{l=0}^{p} \alpha_l D_{ii} x_i[m-l] = h_i A_{ii} x_i[m] \tag{15}$$

is such that for all $i \in \{1, ..., M\}$, $\lim_{m\to\infty} x_i[m] = 0$ *for any initial condition and any positive* h_i.

The following lemma and theorem are used in subsequent sections.

LEMMA 2.1. *If the* α*'s in (12) correspond to the first or second order backward-difference formulas, then*

$$\min_{|z|=1} Re\left(\sum_{l=0}^{p} \alpha_l z^l\right) \geq 0 \tag{16}$$

where z *is a complex scalar and* $Re(\cdot)$ *denotes the real part.*

THEOREM 2.2. *A multirate integration method of the form of (13) is multirate A-stable for any stable and stably partitioned system of the form of (7) if the multirate method is partition-by-partition A-stable, and if the iterations defined by (10) and (12) converge to the exact solution of (7) and (13) respectively, uniformly on* $[0, \infty)$ *and* $\{0, 1, ..., \infty\}$ *respectively.*

The proofs of Lemma (2.1) and Theorem (2.2) are quite straightforward, and can be found in [10]. Note that the proof of Theorem (2.2) involves interchanging limits, hence uniformity of convergence on the infinite interval is required.

3 A Multirate WR Convergence Theorem

Most results about multirate A-stability approach the problem directly, and either require some form of timestep synchronization, or apply only to first-order integration methods [8, 11]. Theorem (2.2) connects multirate A-stability to multirate WR convergence, and as we will show in the next section, this connection can be exploited to prove multirate A-stability for unsynchronized second-order schemes. First, however, it is necessary to verify multirate WR convergence, and that is the subject of this section.

To prove the convergence theorem, we will use the following specialized norm.

DEFINITION 3.1. *Given an infinite sequence* $\{x\}$ *on* $\Re^N$, *the quantity*

$$|||\{x\}|||_h \equiv ||x[0]||_2 + \sqrt{\frac{1}{h}\sum_{m=1}^{\infty} \langle (x[m] - x[m-1]), (x[m] - x[m-1]) \rangle} \tag{17}$$

is a norm for any positive h. *In addition, if*

$$|||\{x\}|||_1 < \infty, \tag{18}$$

we say that $\{x\}$ *has bounded variation.*

The theorem below is a minor generalization of a result in [10].

THEOREM 3.1. *If the partitioned matrix* $\boldsymbol{A} \in \Re^{N\times N}$ *in (12) is stably and normally partitioned, and if the multirate method in (12) uses linear interpolation and a first or second-order backward-difference integration formula, then for any two sets of sequences with bounded variation,* $\{x_i^k\}$, $\{y_i^k\}$, $i \in \{1, ..., M\}$, *such that* $x^k[0] = y^k[0] = x_0$,

$$|||\{x_i^{k+1} - y_i^{k+1}\}|||_{h_i} \leq \sum_{j\neq i} ||\boldsymbol{A}_{ii}^{-1}|| ||\boldsymbol{A}_{ij}|| |||\{x_j^k - y_j^k\}|||_{h_j}, \tag{19}$$

where x_i^{k+1} *and* y_i^{k+1} *are given by (12).*

Proof. Given $\{x^k\}$ and $\{y^k\}$, the difference between $\{x^{k+1}\}$ and $\{y^{k+1}\}$ can be derived from (12) and is

$$\sum_{l=0}^{p} \alpha_l \boldsymbol{D}_{ii}\delta_i^{k+1}[m-l] = h_i\left[\boldsymbol{A}_{ii}\delta_i^{k+1}[m] + \sum_{j\neq i} \boldsymbol{A}_{ij} I_{mh_i}\left(\{\delta_j^k\}\right)\right] \tag{20}$$

where $\delta_i^k[m] \equiv x_i^k[m] - y_i^k[m]$.

Subtracting (20) at $m-1$ from (20) at m yields

$$(21)\quad \sum_{l=0}^{p} \alpha_l D_{ii}(\delta_i^{k+1}[m-l] - \delta_i^{k+1}[m-l-1]) = \\ h_i A_{ii}(\delta_i^{k+1}[m] - \delta_i^{k+1}[m-1]) + h_i \sum_{j\neq i} A_{ij}\left(I_{mh_i}\left(\{\delta_j^k\}\right) - I_{(m-1)h_i}\left(\{\delta_j^k\}\right)\right)$$

Applying the z-transform to (21) and reorganizing,

$$(22)\quad \mathcal{Z}(\delta_i^{k+1}[m] - \delta_i^{k+1}[m-1]) = \\ \left(\left[\sum_{l=0}^{p} \alpha_l z^{-l}\right] D_{ii} - h_i A_{ii}\right)^{-1} h_i \sum_{j\neq i} A_{ij} \mathcal{Z}\left(I_{mh_i}\left(\{\delta_j^k\}\right) - I_{(m-1)h_i}\left(\{\delta_j^k\}\right)\right).$$

Taking the l_2 norm of both sides and applying the Cauchy-Schwarz inequality leads to

$$(23)\quad \|\mathcal{Z}(\delta_i^{k+1}[m] - \delta_i^{k+1}[m-1])\|_2 \leq \\ M_i \sum_{j\neq i} \|A_{ij}\|_2 \left\|\mathcal{Z}\left(I_{mh_i}\left(\{\delta_j^k\}\right) - I_{(m-1)h_i}\left(\{\delta_j^k\}\right)\right)\right\|_2.$$

where

$$(24)\quad M_i = h_i \left\|\left(\left[\sum_{l=0}^{p} \alpha_l z^{-l}\right] D_{ii} - h_i A_{ii}\right)^{-1}\right\|_2$$

From Parseval's relation and Definition (3.1),

$$(25)\quad \|\mathcal{Z}(\delta_i^{k+1}[m] - \delta_i^{k+1}[m-1])\|_2 = \sqrt{h_i}|||\{\delta_i^{k+1}\}|||_{h_i},$$

as $\delta_i^k[0] = 0$ for all i and k.

Combining (24) and (25),

$$(26)\quad |||\{\delta_i^{k+1}\}|||_{h_i} \leq M_i \sum_{j\neq i} \|A_{ij}\|_2 \; |||\{I_{mh_i}\left(\{\delta_j^k\}\right)\}|||_{h_i} \leq M_i \sum_{j\neq i} \|A_{ij}\|_2 \; |||\{\delta_j^k\}|||_{h_j},$$

where the term $\{I_{mh_i}\left(\{\delta_j^k\}\right)\}$ is used informally to denote the sequence whose m^{th} element is given by $I_{mh_i}\left(\{\delta_j^k\}\right)$, and the rightmost inequality follows from the lemma in the appendix of [10].

To bound M_i, we note that as A_{ii} is normal and D_{ii} is a diagonal matrix of either ones or zeros,

$$(27)\quad \left\|\left(\left[\sum_{l=0}^{p} \alpha_l z^{-l}\right] D_{ii} - h_i A_{ii}\right)^{-1}\right\|_2 \leq \max_{|z|=1} \rho\left(\left(\left[\sum_{l=0}^{p} \alpha_l z^{-l}\right] D_{ii} - h_i A_{ii}\right)^{-1}\right).$$

where $\rho(\cdot)$ denotes the spectral radius of the argument. From Lemma (2.1) and the stability of A_{ii},

$$(28)\quad \max_{|z|=1} \rho\left(\left(\left[\sum_{l=0}^{p} \alpha_l z^{-l}\right] D_{ii} - h_i A_{ii}\right)^{-1}\right) \leq \rho\left((h_i A_{ii})^{-1}\right) = \frac{1}{h_i}\|A_{ii}^{-1}\|_2,$$

The bound on M then implies

$$|||\{\delta_i^{k+1}\}|||_{h_i} \le \sum_{j\neq i} \|A_{ii}^{-1}\| \|A_{ij}\|_2 \ |||\{\delta_j^k\}|||_{h_j} \tag{29}$$

proving the theorem. □

COROLLARY 3.1. *If A in (12) is stably and normally partitioned so that the partitioned A has the dominance property with respect to the l_2 norm, and if the multirate method in (12) uses linear interpolation and a first or second-order backward-difference integration formula, then the multirate WR algorithm converges uniformly on the infinite interval.*

Corollary (3.1) follows directly from Theorem (3.1) and Definition (2.1).

4 Near-zero Current

When analyzing semiconductor devices which operate using small currents, (1), (2) and (3) can be solved efficiently by iterating between a modified Poisson equation and the current-continuity equations [5]. The modification of the Poisson equation involves a change of variables motivated by exact analysis of the zero current case, and this change of variables yields a nonlinear Poisson equation, but leaves the current-continuity equations unmodified [12]. Note also that in the case where the currents are very close to zero, the potential derived by solving the nonlinear Poisson equation can be used as a given in the current-continuity equation. With this as motivation, in this section, we consider using a multirate method to solve (5) given u.

To begin, note the following about equation (5).

LEMMA 4.1. *For any given u, (5) represents a linear ODE of the form*

$$\dot{n}(t) = A(u)n(t) \tag{30}$$

where a partitioning of $A(u)$ into scalar equations is both a stable partitioning, and satisfies the dominance condition (Definition (2.1)).

Proof. Since the Bernoulli function $B(x) > 0$ for all x, $A(u)_{ii} < 0$ for all i, and therefore a scalar partitioning of $A(u)$ is a stable partitioning. The transpose of $A(u)$ is irreducibly diagonally dominant [6], and therefore a scalar partitioning of $A(u)$ has the dominance property.

THEOREM 4.1. *When applied to solving (5) partitioned into scalar equations, a multirate integration method which uses linear interpolation and a first or second order backward-difference integration formula is multirate A-stable.*

Proof. From Lemma (4.1), partitioning of (5) into scalar equations is a stable partitioning, and first and second-order backward difference methods are partition-by-partition A-stable. Also from Lemma (4.1), the scalar partitioning of (5) satisfies the dominance property, and therefore Theorem (2.1) and Corollary (3.1) imply that both the continuous and discretized WR algorithms converge uniformly on the infinite interval. All the conditions of Theorem (2.2) are therefore satisfied, thus guaranteeing multirate A-stability. □

5 Experimental Results

In this section we compare the computational efficiency of using a WR-based multirate algorithm to a more standard direct method of solving the two-dimensional semiconductor device equations given in (4),(5) and (6). The WR-based algorithm is a block red/black Gauss-Seidel waveform-relaxation Newton scheme using vertical line blocks, where the equations governing nodes in the same block are solved simultaneously using the first and second-order backward-difference formulas, an iterative timestep refinement strategy, Newton's method and sparse Gaussian elimination [13, 14, 15]. For the direct method, the first and second-order backward-difference formulas, Newton's method and sparse Gaussian elimination were applied to the entire problem. The program was written in C, and all experiments were run on an IBM RS/6000 model 540 workstation.

The three MOS devices of Figure 1 were used to construct six simulation examples, each device being subjected to either a drain voltage ramp with the gate held high (the **D** examples), or a gate voltage ramp with the drain held high (the **G** examples). Each device was spatially discretized on an irregular tensor-product mesh, i.e. the mesh lines were placed closer together at points where u, n and p were expected to exhibit rapid spatial variation. Dirichlet boundary conditions were imposed by a gate contact and by ohmic contacts at the drain, the source, and along the bottom of the substrate. Neumann reflecting boundary conditions were imposed along the left and right edges of the meshes. For all examples, the source and substrate contacts were fixed at 0 V. The drain-driven **kD** test setup is illustrated in Figure 2.

device	description	mesh
kar	abrupt junction	19×31
ldd	lightly-doped drain	15×20
soi	silicon-on-insulator	18×24

FIG. 1. *Description of MOS devices.*

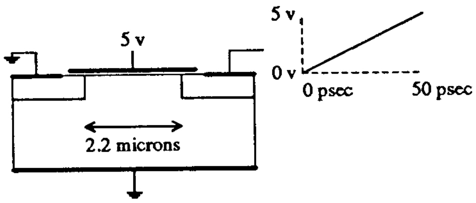

FIG. 2. *Illustration of the drain-driven* **kD** *example.*

example	direct	WRN/r	(iters)
kD	697.08	501.66	(315)
kG	2622.29	563.75	(215)
lD	147.47	296.48	(353)
lG	439.22	253.19	(268)
sD	208.77	96.68	(235)
sG	130.75	95.61	(161)

FIG. 3. *CPU times for direct and the multirate WRN method, simulating a drain ramp and a gate ramp applied to the three devices.*

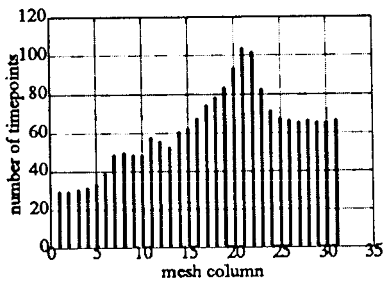

FIG. 4. *Number of timepoints per vertical mesh line, showing the multirate behavior in the* **kD** *example.*

The table of Figure 3 shows the CPU times required by direct solution and the multirate WRN algorithm with timestep refinement. The results show that in most cases, WRN with timestep refinement is competitive with direct methods, and as noted in [3], waveform relaxation methods are more easily parallelized.

Figure 4 shows that the blocks consisting of different vertical mesh lines required different numbers of timesteps, because more timepoints were needed to resolve the widening of the drain depletion region than are needed to resolve the source end of the device. This indicates that in practice some multirate behavior exists within a device that can be exploited by a multirate integration method.

6 Conclusions and Acknowledgements

In this paper we demonstrated that the multirate WRN algorithm may be a practical technique for parallel semiconductor device simulation, and that WR is also a useful analytic tool for analyzing the stability properties of multirate integration methods. The authors apologize for several somewhat cryptic sections, but space was limited. Finally, the authors wish to thank A. Elfadel for a valuable discussion on Lemma 1, and S. Skelboe for several valuable discussions.

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