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Mathematical Modelling and Simulation of Electrical Circuits and Semiconductor Devices

Proceedings of a Conference held at the Mathematisches Forschungsinstitut, Oberwolfach, July 5-11, 1992

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Preface

Progress in today's high-technology industries is strongly associated with the development of new mathematical tools. A typical illustration of this partnership is the mathematical modelling and numerical simulation of electric circuits and semiconductor devices.

At the second Oberwolfach conference devoted to this important and timely field, 35 scientists from around the world, mainly applied mathematicians and electrical engineers from industry and universities, presented their new results.

The contributions to this conference are presented in this proceedings. They cover electric circuit simulation, device simulation and process simulation, including discussions on experiences with standard software packages and improvements of such packages.

In electric circuit simulation three different types of problems can be distinguished depending on the size of a circuit: small circuits with less than 20 basic elements and an oscillating behaviour; middle-sized circuits up to 500 elements; very large circuits. Today the simulation of middle-sized circuits is well understood. Current focal points for oscillating circuits include new discretization schemes, limit cycle computation and the transient phase. Parallel methods and multirate strategies are suggested and tested for the very large circuits.

In the semiconductor area special lectures were given on new modelling approaches, numerical techniques and existence and uniqueness results. Among these, for example, mention is made of mixed finite element methods, an extension of the Baliga-Patankar technique for a three dimensional simulation, and the connection between semiconductor equations and the Boltzmann equations.

The editors are grateful to Georg Denk and Peter Rentrop for their effective and efficient help in organizing the conference.

The editors

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Circuit Simulation

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A new efficient numerical integration scheme for highly oscillatory electric circuits

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Abstract. This paper presents a new numerical integration scheme for second order ordinary differential equations which can integrate highly oscillating electric circuits with high efficiency. This is shown by numerical results. The discretization scheme is based on the principle of coherence proposed by Hersch which will be described shortly. The analysis reveals important properties of the new method such as consistency. Some problems (e. g. cancellation) make an efficient implementation difficult, solutions are given.

AMS Subject Classification: 65L05, 65L06.

Key words: ordinary differential equations, oscillatory solutions, multistep method, consistency, convergence, circuit simulation.

1. Introduction

Circuit simulation is a standard task for the computer aided design of electronic circuits. However, there are two types of circuits which need special proceeding: These are very large circuits (e. g. memory chips) and highly oscillating circuits (e. g. quartz oscillators). The first type can be handled by the exploitation of latency [7, 8]. Oscillating circuits require a quite different approach, see e. g. [16]. In the paper presented here, a new discretization scheme will be described that is able to use some information about the ordinary differential equation (ODE) to compute highly oscillatory solutions with high efficiency.

Most integration schemes solve the general initial value problem

$$y'(x) = f(x, y(x)), \quad y(x_0) = y_0 \text{ with } y : \mathbf{R} \to \mathbf{R}^n.$$

As no special information about the ODE is given, they require a large amount of computing time for the integration of highly oscillatory ODEs: Every oscillation of y has to be followed which leads to very small integration steps and subsequently to rounding errors. This is the motivation for special integration schemes for special ODEs.

An ODE describing oscillatory behavior with possible damping can be written as

$$y''(x) + a\,y'(x) + b\,y(x) = f(x, y(x)), \quad y(x_0) = y_0,\ y'(x_0) = y_0', \tag{1}$$

with $a,\ b \in \mathbb{R}$, $y : \mathbb{R} \to \mathbb{R}^n$. As this equation does not reflect the standard form $y'(x) = f(x, y(x))$ for an ODE, standard techniques for the construction of a numerical integration scheme cannot be used. A transformation of (1) into standard notation would yield to a loss of the special information about the ODE which is given by the parameters a and b.

One approach for this special ODE was used by Deuflhard [6] for the construction of an extrapolation scheme. His work is based on the *principle of coherence* [11, 12]. This principle will also be used in this paper for the construction of a multistep formula for (1) and will be described in the next section.

If the parameter a in (1) equals 0, the ODE is called *special second order ODE.* For this kind of ODE many approaches can be found in literature. One of the first investigators were Stiefel and Bettis [20] who modified the polynomial ansatz of Cowell's method in order to take oscillatory solutions into account. Here, some part of the polynomial basis is replaced by trigonometric functions. A generalization of this approach has been used by Skelboe [19] for the simulation of mildly nonlinear electric circuits. As the ODEs describing the circuit are given in standard notation $z'(x) = g(x, z(x))$, the additional information about the frequency has to be passed to the algorithm in an appropriate manner.

Another approach for the numerical computation of special second order ODEs is the adaptation of parameters of the discretization scheme. This has be done for the construction of multistep schemes [1, 3, 18] as well as for Runge-Kutta-Nyström type methods [14, 15].

2. The principle of coherence

The principle of coherence was formulated by Hersch [12] as "Successive approximations should not contradict each other". This yields some conditions on the coefficients of a numerical method which have to be fulfilled. The main idea will become clear by the following example: Consider the ODE $z''(x) + \lambda z(x) = 0$, $\lambda > 0$. A standard approach for this ODE is the difference equation

$$z(x-h) - A(h)z(x) + z(x+h) = 0. \tag{2}$$

Here, $A(h)$ is the coefficient of the method and it depends on the step size h. If the step size is multiplied with 2, the difference equation is

$$z(x-2h) - A(2h)z(x) + z(x+2h) = 0.$$

A formula for the step size $2h$ can be constructed also by a linear combination of three equations of type (2), centered at $x-h$, x, and $x+h$, resp. This leads to the expression

$$z(x-2h) - (A(h)^2 - 2)z(x) + z(x+2h) = 0. \tag{3}$$

Comparing (3) with (2) gives the coherence condition $A(2h) = A(h)^2 - 2$ which has to be satisfied for a coherent discretization scheme. This condition holds for $A(h) = 2\cos(\kappa h)$ with $\kappa \in \mathbb{R}$. For $h \to 0$ this leads to $\kappa = \sqrt{\lambda}$, as the difference equation should reflect the differential equation. The coherent approximation of $z''(x) + \lambda z(x) = 0$ is

$$z(x-h) - 2\cos(\sqrt{\lambda}h)z(x) + z(x+h) = 0$$

instead of the classical approach yielding

$$z(x-h) - (2 - \lambda h^2)z(x) + z(x+h) = 0.$$

The mathematical approach for the construction of coherent discretization schemes is the transformation of the homogeneous part of the ODE (in the example $z''(x)+\lambda z(x)$) into a difference equation. The solution of the latter one fulfills the ODE, too. The principle of coherence can be used for the construction of a number of integration schemes depending on the kind of the homogeneous part to be considered. In Table 1, some of the basic discretization formulas for equidistant step sizes are given. The well-known Adams-Bashforth/Moulton schemes can be found as well as the Cowell/Störmer methods, they belong to the homogeneous parts $y'(x)$, and $y''(x)$, resp.

homogeneous part	discretization scheme
$y'(x)$	$y(x+h) = y(x)$
$y'(x) + b\,y(x)$	$y(x+h) = \exp(-b\,h)y(x)$
$y''(x)$	$y(x+h) = 2y(x) - y(x-h)$
$y''(x) + b^2 y(x)$	$y(x+h) = 2\cos(b\,h)y(x) - y(x-h)$
$y^{(4)}(x)$	$y(x+2h) = 4y(x+h) - 6y(x) + 4y(x-h) - y(x-2h)$
$y^{(4)} - b^4 y(x)$	$y(x+2h) = (2\cosh(b\,h) + 2\cos(b\,h))y(x+h)$ $- (2 + 4\cosh(b\,h)\cos(b\,h))y(x)$ $+ (2\cosh(b\,h) + 2\cos(b\,h))y(x-h) - y(x-2h)$

Table 1: Coherent discretization schemes due to Hersch [11].

The construction of the coherent discretization scheme for the ODE (1) is complicated by the dependency on the values of a and b. As the transformation of the homogeneous part of the ODE into a difference equation is done via the calculus of distribution and the distribution depends on the fundamental solutions $g_1(x)$ and $g_2(x)$ of the homogeneous ODE, there exist five different cases. These cases are given in Table 2. The most important case is $b \neq 0$, $b > a^2/4$ giving oscillatory solutions and will be considered in the following. For this case, the coherent discretization scheme is

$$y(x+h) = 2\,\exp(-\alpha\, h)\,\cos(\beta\, h) y(x) - \exp(-2\,\alpha\, h) y(x-h).$$

Please note that there is no evaluation of $y'(x)$ necessary despite the term $ay'(x)$ in (1). A derivation of this formula for the non-equidistant case can be found in [4, 5].

		$g_1(x)$	$g_2(x)$
$b=0$	$a=0$	1	x
$b=0$	$a\neq 0$	1	$\exp(a\,h)$
$b\neq 0$	$b>a^2/4$	$\exp(\frac{a}{2}\,x)\cos(\sqrt{b-a^2/4}\,x)$	$\exp(\frac{a}{2}\,x)\sin(\sqrt{b-a^2/4}\,x)$
$b\neq 0$	$b=a^2/4$	$\exp(\frac{a}{2}\,x)$	$x\,\exp(\frac{a}{2}\,x)$
$b\neq 0$	$b<a^2/4$	$\exp(\frac{a}{2}\,x)\cosh(\sqrt{a^2/4-b}\,x)$	$\exp(\frac{a}{2}\,x)\sinh(\sqrt{a^2/4-b}\,x)$

Table 2: Fundamental solutions for the homogeneous part of (1).

Up to now, the inhomogeneous part $f(x, y(x))$ of (1) has not taken into account. With an approach similar to classical multistep methods as the Cowell/Störmer family, the following ansatz is used for a discretization scheme with $k+1$ function evaluations:

$$\sum_{i=k-2}^{k} \alpha_i y(x_{n+i}) = h^2 \sum_{i=0}^{k} \beta_i f(x_{n+i-s}, y(x_{n+i-s})). \tag{4}$$

α_i, $i = k-2, k-1, k$, denotes the coefficients derived from the transformation of the homogeneous part, β_i, $i = 0, \ldots, k$, describes the unknown coefficients for the right-hand side. For an explicit method the parameter s equals 1; an implicit scheme is characterized by $s = 0$. The unknowns β_i in this ansatz are computed in such a way that the formula (4) is exact for $f(x, y(x)) \in\ < x^0, x^1, \ldots, x^k >$. Due to the non-standard form of (1), the coherent discretization scheme is more complicated than standard methods. This is especially true for the important case of non-equidistant step sizes.

3. Consistency of the new method

For the theoretical analysis of the coherent discretization scheme, standard theorems for numerical analysis found in textbook (see e. g. [21]) can not be used without modification. This is due to the form of the ODE (1) which is solved by the method. The analysis becomes even more complicated as the coefficients α_i, β_i of the method depend on the step size h even in the case of equidistant step sizes. This is in contrast to classical multistep methods.

To make notation simple, the following definitions are introduced: A multistep method which solves the general second order ODE $z(x)'' = g(x, z(x), z'(x))$ can be written as

$$\sum_{i=0}^{k} a_i z(x_{n+i}) = h \sum_{i=0}^{k} b_i z'(x_{n+i-s}) + h^2 \sum_{i=0}^{k} c_i g(x_{n+i-s}, z(x_{n+i-s}), z'(x_{n+i-s}))$$

with $a_i = a_i(h)$, $b_i = b_i(h)$, $c_i = c_i(h)$, and $x_{n+i} = x_n + ih$ for the equidistant case. This defines the operator

$$\mathcal{L}[z, x_{n+k}, h] := \sum_{i=0}^{k} a_i z(x_{n+i}) - h \sum_{i=0}^{k} b_i z'(x_{n+i-s}) - h^2 \sum_{i=0}^{k} c_i g(x_{n+i-s}, z(x_{n+i-s}), z'(x_{n+i-s})),$$

and the *characteristic polynomials*

$$\rho(x; h) := \sum_{i=0}^{k} a_i(h) x^{i+s}, \quad \sigma(x; h) := \sum_{i=0}^{k} b_i(h) x^i, \quad \tau(x; h) := \sum_{i=0}^{k} c_i(h) x^i.$$

The consistency of a method with coefficients depending on the step size h even in the equidistant case was computed by Lyche [17] for the special ODE $y^{(r)}(x) = g(x, y(x))$. This fits into the notation used above if $r = 2$ and $b_i = 0$ for $i = 0, \ldots k$. Following Lyche, $a_i(h)$ and $c_i(h)$ are expanded in Taylor's series around h yielding

$$a_i(h) = \sum_{j=0}^{q} a_{i,j} h^j + \mathcal{O}(h^{q+1}), \qquad c_i(h) = \sum_{j=0}^{q} c_{i,j} h^j + \mathcal{O}(h^{q+1}).$$

Expanding $z(x_{n+i})$ in Taylor's series around x_n, we find after some rearranging

$$\mathcal{L}[z, x_{n+k}, h] = \sum_{i=0}^{q} \left(\sum_{j=0}^{i} C_{j,i-j} z^{(j)}(x_n) \right) h^i + \mathcal{O}(h^{q+1})$$

with

$$\begin{aligned}
C_{j,i} &= \frac{1}{j!} \left(0^j a_{0,i} + 1^j a_{1,i} + \ldots + k^j a_{k,i} \right) \quad \text{for } j = 0, 1, \\
C_{2,i} &= \frac{1}{2!} \left(a_{1,i} + 2^2 a_{2,i} + \ldots + k^2 a_{k,i} \right) \\
&\quad - \left(c_{0,i} + c_{1,i} + \ldots + c_{k,i} \right), \\
C_{j,i} &= \frac{1}{j!} \left(0^j a_{0,i} + 1^j a_{1,i} + \ldots + k^j a_{k,i} \right) \\
&\quad - \frac{1}{(j-2)!} \left(0^{j-2} c_{0,i} + 1^{j-2} c_{1,i} + \ldots + k^{j-2} c_{k,i} \right) \\
&\qquad \text{for } j = 3, 4, \ldots
\end{aligned}$$

This leads to (see [17])

Definition 1: *The operator $\mathcal{L}[z, x_{n+k}, h]$ of a multistep method solving $z''(x) = g(x, z(x))$ is said to be of* order of consistency p, *if $C_{j,i} = 0$ for $0 \leq i + j \leq p + 1$ and $C_{j,i} \neq 0$ for some i, $j \geq 0$ such that $i + j = p + 2$.*

The main difference to the classical definition of order of consistency is the appearance of more terms $z^{(j)}(x_n)$ for one h-order. This makes the analysis complicated as well as tedious. The following theorem makes the computation of p simpler, especially if programs for computer algebra are used:

Theorem 2: *The operator $\mathcal{L}[z, x_{n+k}, h]$ of a multistep method solving $z''(x) = g(x, z(x))$ is said to be of order of consistency p if*

$$C_j(h) = C_{j,p+2-j} h^{p+2-j} + \mathcal{O}(h^{p+3-j})$$

holds for $j = 0, \ldots, p + 1$. $C_j(h)$ is defined as

$$\begin{aligned}
C_j(h) &= \frac{1}{j!}\left(0^j a_0(h) + 1^j a_1(h) + \ldots + k^j a_k(h)\right) \quad \mathit{for} j = 0, 1, \\
C_2(h) &= \frac{1}{2!}\left(a_1(h) + 2^2 a_2(h) + \ldots + k^2 a_k(h)\right) \\
&\quad - \left(c_0(h) + c_1(h) + \ldots + c_k(h)\right), \\
C_j(h) &= \frac{1}{j!}\left(0^j a_0(h) + 1^j a_1(h) + \ldots + k^j a_k(h)\right) \\
&\quad - \frac{1}{(j-2)!}\left(0^{j-2} c_0(h) + 1^{j-2} c_1(h) + \ldots + k^{j-2} c_k(h)\right) \\
&\qquad \mathit{for}\ j = 3, 4, \ldots
\end{aligned}$$

Proof: The coefficients $C_j(h)$ are expanded in Taylor's series by expanding the coefficients $a_i(h)$ and $c_i(h)$ in Taylor's series around h. This leads to

$$C_j = C_{j,0} + hC_{j,1} + h^2 C_{j,2} + \ldots + h^{p+2-j} C_{j,p+2-j} + \mathcal{O}(h^{p+3-j}).$$

For a method of order p, Definition 1 yields

$$C_{j,n} = 0 \quad \text{für } 0 \leq n \leq p + 1 - j,$$

which reduces the Taylor's series of $C_j(h)$ to

$$C_j = h^{p+2-j} C_{j,p+2-j} + \mathcal{O}(h^{p+3-j}).$$

□

With the help of the characteristic polynomials, the computation of the order of consistency can be simplified even more:

Theorem 3: *The operator $\mathcal{L}[z, x_{n+k}, h]$ of a multistep method solving $z''(x) = g(x, z(x))$ is said to be of order of consistency p if*

$$\rho(e^h; h) - h^2 \cdot \tau(e^h; h) = \tilde{C}_{p+2} h^{p+2} + \mathcal{O}(h^{p+3}), \quad \tilde{C}_{p+2} \neq 0.$$

C_{p+2} is defined as

$$\tilde{C}_{p+2} = \sum_{j=0}^{p+2} C_{j,p+2-j}.$$

Proof: Consider the special case $z(x) = e^x$. For a discretization scheme of order p, the following expression holds:

$$\mathcal{L}[e^x, x_{n+k}, h] = h^{p+2} \sum_{j=0}^{p+2} C_{j,p+2-j} e^{x_n} + \mathcal{O}(h^{p+3}).$$

On the other hand,

$$\mathcal{L}[e^x, x_{n+k}, h] = e^{x_n} \left(\rho(e^h, h) - h^2 \cdot \tau(e^h, h) \right).$$

The Taylor's series of $\rho(e^h, h) - h^2 \cdot \tau(e^h, h)$ yields after some calculation

$$\rho(e^h, h) - h^2 \cdot \tau(e^h, h) = \sum_{i=0}^{q} \left(\sum_{j=0}^{i} C_{j,i-j} \right) h^i + \mathcal{O}(h^{q+1}).$$

If the integration scheme is of order p, then — according to Definition 1 —

$$C_{j,i-j} = 0 \quad \text{for } 0 \leq i \leq p+1.$$

This cancels the terms $h^0, \ldots, h^{p+1}$ and

$$\rho(e^h, h) - h^2 \cdot \tau(e^h, h) = \sum_{i=p+2}^{q} \left(\sum_{j=0}^{i} C_{j,i-j} \right) h^i + \mathcal{O}(h^{q+1})$$

is the final expression. This finishes the proof. □

To compute the order of consistency of the discretization scheme presented here, Theorem 3 has to be generalized to take the term $ay'(x)$ in (1) into account. Before this can be done, the ODE (1) has to be transformed into standard notation which reads as $z''(x) = g(x, z(x), z'(x))$. This requires the definitions

$$a_i(h) := \alpha_i(h) - \beta_i(h) h^2 b, \; b_i(h) := \beta_i(h) a h, \; c_i(h) := \beta_i(h).$$

Theorem 4: *The operator $\mathcal{L}[z, x_{n+k}, h]$ of a multistep method solving*

$$z''(x) = g(x, z(x), z'(x))$$

is said to be of order of consistency p if

$$\rho(e^h; h) - h \cdot \sigma(e^h; h) - h^2 \cdot \tau(e^h; h) = \tilde{C}_{p+2} h^{p+2} + \mathcal{O}(h^{p+3}), \quad \tilde{C}_{p+2} \neq 0.$$