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Solution of the nonlinear PDAEs by variational iteration method and its applications in nanoelectronics

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In this paper, the system of nonlinear partial differential-algebraic equations is solved by the well-known variational iteration method and the results with high accuracy are obtained by only one iteration. Furthermore, some nanoelectronics models are expressed by partial differential-algebraic equations and one of them is successfully solved by the proposed method. Although solving nonlinear PDAEs is difficult but it is shown that the variational iteration method using Taylor expansion is an efficient method to solve these nonlinear problems.

Key words: Nonlinear partial differential-algebraic equations, variational iteration method, nanoelectronics models.

INTRODUCTION

The mathematical model of dynamical systems often results from some network approach, which yields time-dependent systems of differential algebraic equations (DAEs). That is, we consider ideally joint lumped elements, without spatial coordinate, but with the topology information given by the incidences of these elements. In contrast, spatial physical effects are described by partial differential equations (PDEs) in space or time/space. Thus an enhanced model requires a coupling of DAEs and PDEs, which yields systems of so-called partial differential algebraic equations (PDAEs). Such systems of PDAEs arise in many technologies like mechanical engineering as coupled multibody systems with sole or flexible/plastic systems (Buttner and Simeon, 2003); in nanoelectronics and others (Ali et al., 2005; Bartel, 2004; Bodestedt and Tischendorf, 2007; Gunther and Feldmann, 1997).

Furthermore, the wording PDAE is also used for singular implicit PDEs, that is, where singular matrices arise in front of partial derivatives. In case of electronic circuits, a specific multivariate model yields an efficient representation of amplitude and/or frequency modulated signals including widely separated time scales. The

introduction of different time variables (for the occurring scales) transforms the circuit's DAE into a PDAE in the sense of a singular PDE.

In this paper, we present a different approach for solving PDAEs. The main aim of this paper is to use the variational iteration method (VIM), proposed by the Chinese mathematician (He, 1997) to find the solution of nonlinear PDAEs. The VIM and its modifications have successfully been applied to many situations (Ates and Yildirim, 2009; Ghorbani and Saberi-Nadjafi, 2009; Hosseini et al., 2010; Tatari and Dehghan, 2009). We have illustrated the efficiency and accuracy of this method by presenting some numerical examples and the last gives some applications of PDAEs.

VARIATIONAL ITERATION METHOD

The VIM, which is a modified general Lagrange's multiplier method, has been shown to solve effectively, easily and accurately a large class of nonlinear problems (Abbasbandy, 2007; Biazar and Eslami, 2010; He, 2008; Jafari et al., 2010; Mohyud-Din et al., 2009; Noor and Mohyud-Din, 2008; Soltanian et al., 2009). The main feature of the method is that the solution of a mathematical problem with linearization assumption is used as initial approximation or trial function. Then a

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more highly precise approximation at some special point can be obtained.

This approximation converges rapidly to an accurate solution. To illustrate the basic concepts of the VIM, we consider the following nonlinear differential equation:

$$Ly + Ny = g(x), \tag{1}$$

Where L is a linear operator, N is a nonlinear operator, and $g(x)$ is an inhomogeneous term. According to the VIM (He, 1999; He et al., 2010), we can construct a correction functional as follows:

$$y_{n+1}(x) = y_n(x) + \int_a^x \lambda [Ly_n(\tau) + Ny_n(\tau) - g(\tau)] d\tau, \quad n \geq 0, \tag{2}$$

Where λ is a general Lagrangian multiplier, which can be identified optimally via the variational theory, the subscript n denotes the n th-order approximation, y_n is considered as a restricted variation (He, 1999; He et al., 2010), that is $\delta y_n = 0$.

NUMERICAL EXAMPLE

In this section, to show the ability and efficiency of the proposed method an example is provided. In mentioned example, to perform the VIM, for natural number $\nu = 20$, every coefficient of function $g_k(x, t)$ is expressed by MTaylor series.

Consider the nonlinear PDAE system:

$$\begin{cases} u_t(x,t) - \frac{1}{t}u(x,t) + 2xtu(x,t) - t^2v_t(x,t) - 2\gamma(x,t) = g_1(x,t) \\ v_{xx}(x,t) + v_x(x,t) - 2tu(x,t) + u(x,t)e^{u(x,t)} - \gamma(x,t) = g_2(x,t) \\ v(x,t) + 2tu(x,t) + g_3(x,t) = 0 \end{cases} \tag{3}$$

With $u(x,0) = 1, u_t(x,0) = 0$.

Where $g_i(x, t), i = 1, 2, 3$ are computable to the exact solutions:

$$u(x,t) = \cos^2(x), \quad v(x,t) = \sin(x), \quad \gamma(x,t) = te^x. \tag{4}$$

To solve the PDAE, in the following we expand the coefficient of functions $g_i(x, t), i = 1, 2, 3$ at x, t by MTaylor expansion with $\nu = 20$.

To solve by means of He's variational iteration method, system (3) can be written as:

$$\begin{cases} v^{[n]}(x,t) = -2tu^{[n]}(x,t) - g_3(x,t), \\ y^{[n]}(x,t) = v_{xx}^{[n]}(x,t) + v_x^{[n]}(x,t) - 2tu^{[n]}(x,t) + u^{[n]}(x,t)e^{u^{[n]}(x,t)} - g_2(x,t), \\ u^{[n]}(x,t) = u^{[n]}(x,t) + \int_0^t \lambda(\tau) \left(u_{\tau\tau}^{[n]}(x,\tau) - \frac{1}{\tau}u_{\tau}^{[n]}(x,\tau) - 2xu_{\tau}^{[n]}(x,\tau) + \tau^2v_{\tau\tau}^{[n]}(x,\tau) - 2\tau\gamma^{[n]}(x,\tau) - \tilde{g}_1(x,\tau) \right) d\tau \end{cases}$$

Where $\tilde{u}^{[n]}(x, t)$ is considered as restricted variations, which mean $\delta \tilde{u}^{[n]}(x, t) = 0$. The Lagrange multiplier, therefore, can be identified as:

$$\lambda(\tau) = \frac{1}{2} \left(\tau - \frac{t^2}{\tau} \right)$$

and the following variational iteration formula is obtained:

$$\begin{cases} v^{[n]}(x,t) = -2tu^{[n]}(x,t) - g_3(x,t), \\ y^{[n]}(x,t) = v_{xx}^{[n]}(x,t) + v_x^{[n]}(x,t) - 2tu^{[n]}(x,t) + u^{[n]}(x,t)e^{u^{[n]}(x,t)} - g_2(x,t), \\ u^{[n]}(x,t) = u^{[n]}(x,t) + \int_0^t \frac{1}{2} \left(\tau - \frac{t^2}{\tau} \right) \left(u_{\tau\tau}^{[n]}(x,\tau) - \frac{1}{\tau}u_{\tau}^{[n]}(x,\tau) - 2xu_{\tau}^{[n]}(x,\tau) + \tau^2v_{\tau\tau}^{[n]}(x,\tau) - 2\tau\gamma^{[n]}(x,\tau) + \tilde{g}_1(x,\tau) \right) d\tau \end{cases}$$

Using initial solution $u^{[0]}(x, t) = 1$, we have:

$$\begin{cases} v^{[0]}(x,t) = tx - \frac{1}{6}t^3x^3 + \frac{1}{120}t^5x^5 - \frac{1}{5040}t^7x^7 + \frac{1}{362880}t^9x^9 + \dots \\ y^{[0]}(x,t) = t + tx + \frac{1}{2}t^2x^2 + \dots + \frac{1}{64023737280000}t^{18}x^{18} + \dots \\ u^{[0]}(x,t) = 1 - \frac{1}{2}t^4x^2 + \frac{1}{24}t^8x^4 - \frac{1}{720}t^{12}x^6 + \dots \end{cases} \tag{5}$$

Note that, the MTaylor series of the exact solutions (4) with order 20 are as:

$$\begin{cases} v(x,t) = tx - \frac{1}{6}t^3x^3 + \frac{1}{120}t^5x^5 - \frac{1}{5040}t^7x^7 + \frac{1}{362880}t^9x^9 + \frac{1}{39916800}t^{11}x^{11} + \dots \\ y(x,t) = t + tx + \frac{1}{2}t^2x^2 + \dots + \frac{1}{64023737280000}t^{18}x^{18} + \frac{1}{12164508832000}t^{19}x^{19} + \dots \\ u(x,t) = 1 - \frac{1}{2}t^4x^2 + \frac{1}{24}t^8x^4 - \frac{1}{720}t^{12}x^6 + \frac{1}{40320}t^{16}x^8 + \dots \end{cases} \tag{6}$$

It is easy to see that the obtained results in the first iteration (5) are same with the MTaylor expansion of the exact solutions (6) with $\nu = 20$, and this shows that a very suitable solution is obtained only with one iteration. Also it illustrates the high rate of convergence of the VIM

for this PDAE.

APPLICATIONS OF PDAEs

In this paper, we focus on PDAE models in nanoelectronics setting with PDE-enhancement of DAE models, rather than singular PDEs. Modified nodal analysis yields large systems of DAEs for ideal circuits (Gunther and Feldmann, 1997). We write such a system in the general form:

$$f: R^k \times R^k \times I \rightarrow R^k, f(Y, Y', t) = 0, t \in I := [0, T], \quad (7)$$

Where $Y: I \rightarrow R^k$ denotes unknown node voltages and branch currents. A consistent initial value $Y(0) = Y_0$ completes the usual electric network model. In addition, we formulate schematically a system of PDEs corresponding to a parasitic effect via an operator:

$$L: D \times I \times V \rightarrow R^m, L(x, t, v) = 0, x \in D \in R^d, t \in I, \quad (8)$$

With a solution $v: D \times I \rightarrow R^m$ in some function space V . Initial and/or boundary conditions have to be specified appropriately. Coupling the systems (7) and (8) using some variables/functions results in a PDAE. The coupling can be done via artificial variables, source terms, boundary conditions (BCs) or even more sophisticated constructions.

In the following classifications of some important PDAE models arising in ongoing research with in the field of nanoelectronics have been introduced.

After that an example of PDAE which mentioned in the above classifications has been solved to show the efficiency and accuracy of our proposed method.

Refined modeling

Usually semiconductors, transmission lines and other components with spatial distribution are given by sub circuits of lumped electric elements (companion models). To obtain a somewhat more precise model (also considering down-scaling phenomena), we replace one or several of these sub circuit descriptions by a PDE model for the corresponding electric effect in the network. These can be one or several semiconductor elements, which behave critical in an electronic network, and where it makes sense to simulate these elements more detailed. Another possibility is to replace a transmission line model based on DAEs by an according PDE. This is a natural way, which bypasses a huge number of more or less artificial parameters of the companion model.

This approach is called refined modeling. It has a special type of coupling. Boundary conditions for the

Ohmic contacts of the PDE model are the node potentials of the connect network nodes (Dirichlet condition). At the remaining boundaries in multiple dimensions, where there is no electric contract, one may have von-Neumann conditions with no flux or field conditions at insulated contacts. On the other hand, the output of the PDE model is an electric current, which is eventually a source term to the network's DAE. Abstractly, we obtain systems of the type

$$\begin{cases} AU_i + L_D U - h(U, t) = 0 & (PDE \text{ in } I \times D) \\ U|_{\Gamma_1} = g(Y) & (Dirichlet \ BC) \\ \frac{\partial}{\partial n} U|_{\Gamma_2} = h(Y) & (von-NeumannBC) \\ f(Y, Y', t) = \lambda(u) & (DAE \text{ in } I), \end{cases} \quad (9)$$

Where L_D represents a differential operator with respect to space. The involved PDE can be of mixed type (elliptic, hyperbolic and parabolic). Thereby, the coupling is performed via the input λ , and the boundary conditions g and h (where we have a decomposition of the boundary: $\partial D = \Gamma_1 \cup \Gamma_2$). Furthermore, analyzing complex systems (9) may yield simpler but still highly accurate companion models for the underlying component. In nanoelectronics, the PDAE systems, which have been considered in the literature or are part of ongoing research, can principally be categorized into the following cases:

1. Semiconductors: Here transistors are described by drift-diffusion or quantum mechanical equations coupled with the electric network. Existence and uniqueness results for no stationary and stationary drift-diffusion network systems are found in Ali et al., 2005; for an index analysis of the arising PDAE, we refer to Bodstedt and Tischendorf, 2007. Currently, efficient numerical codes are being developed.
2. Transmission line effects: Also down-scaling causes a decreasing distance of transmission lines and thus an undesired interaction arises. Telegrapher's equation describes the underlying physical effect. The coupling of PDEs and DAEs accords to the form (9). Now the involved PDE is exclusively of hyperbolic type, which implies a specific numerical treatment.
3. Electromagnetic fields: The DAEs (7) result from a network approach to avoid a simulation of the complete circuit using Maxwell's equations. However, if some crucial parts of the circuit demand a refined model, a separation from the network can be done. Thus we apply Maxwell's equations to represent the small part, whereas we use the network DAEs for the major part.

Multiphysical extension

This modeling is much more complex, since we do not

add a physical dimension to the electric network, but have a distributed additional effect:

1. Thermal aspects: The increase of the clock rate in chips causes a higher power loss in the electronic network. Thus we have to consider heat distribution and conduction between the circuit's elements. In contrast to the effects described above, the heat evolution runs in parallel to the time-dependence of voltages and currents. Thus a thermal network can be associated to the electric network. In the thermal part, specific 0D elements can be refined into elements with spatial distribution or elements can be located in macro structures. Combining the heat equation for the spatial elements with the network yields

$$\begin{cases} AU_t + L_D U - h(U, t) = s(x), & \text{PDE in } I \times D \\ U|_{\partial D} = g(x) & \text{(BC)} \\ f(Y, Y', t, \mu(u)) = 0 & \text{(DAE in } I), \end{cases} \quad (10)$$

In this case, the included PDE is of parabolic type (Fourier Law). The coupling is present in the source terms and boundary conditions s, μ, g : Here dissipated power is not only entering the boundary conditions, but is also a source term for the evolution equation; on the other hand, the temperature enters the electric network as parameter and thus causes a more general dependence. For further details, we refer to Bartel, 2004.

2. Electromagnetics: In principle, one can interpret an electromagnetic field influencing the complete circuit as a multiphysical case, too. Consequently, the contribution of the field to each component has to be modeled appropriately.

Example: Consider the nonlinear PDAE system in form (10):

$$\begin{cases} u_t(x, t) - u_{xx}(x, t) + v_x(x, t) + u^2(x, t) = g_1(x, t) \\ v_t(x, t) + u_x(x, t) = g_2(x, t) \\ y'(t) - 2v(x, t)z(t) = g_3(x, t) \\ z'(t) - 2te^{v(x, t)} = g_4(x, t) \\ z(t) - w(t) + v(x, t) = g_5(x, t) \end{cases} \quad (11)$$

With $u(0, t) = 1, v(0, t) = y(0) = z(0) = 0$.

Where $g_i(x, t), i = 1, 2, 3, 4, 5$ are computable to the exact solutions:

$$u(x, t) = e^{-tx^2}, v(x, t) = 1 - \cos(x), w(t) = t \sin(x), z(t) = \tan(x), w(t) = \frac{1}{Ht^2}. \quad (12)$$

To solve the PDAE (11), in the following we expand the coefficient of functions $g_i(x, t), i = 1, 2, 3, 4, 5$ at x, t by

MTaylor expansion with $\nu = 20$. To solve by means of He's variational iteration method, system (11) can be written as:

$$\begin{cases} v^{[n+1]}(x, t) = v^{[n]}(x, t) + \int_0^t \lambda_1(\tau) (v_\tau^{[n]}(x, \tau) + u_x^{[n]}(x, \tau) - \tilde{g}_2(x, \tau)) d\tau \\ u^{[n+1]}(x, t) = u^{[n]}(x, t) + \int_0^t \lambda_2(\tau) (u_x^{[n]}(x, \tau) - u_{xx}^{[n]}(x, \tau) + v_x^{[n]}(x, \tau) + (u^{[n]})^2(x, \tau) - \tilde{g}_1(x, \tau)) d\tau \\ w^{[n]}(t) = z^{[n]}(t) + v^{[n]}(x, t) - g_3(x, t) \\ z^{[n+1]}(t) = z^{[n]}(t) + \int_0^t \lambda_3(\tau) (z'(\tau) - 2e^{v(x, \tau)} - \tilde{g}_4(x, \tau)) d\tau \\ y^{[n+1]}(t) = y^{[n]}(t) + \int_0^t \lambda_4(\tau) (y'(\tau) - 2v^{[n]}(x, \tau)z^{[n]}(x, \tau) - \tilde{g}_5(x, \tau)) d\tau \end{cases}$$

By using the variational iteration method it is clear that $\lambda_1(\tau) = \lambda_2(\tau) = \lambda_3(\tau) = \lambda_4(\tau) = -1$. Finally by assuming $u^{[0]}(x, t) = 1, v^{[0]}(x, t) = y^{[0]}(t) = z^{[0]}(t) = 0$ the following results are obtained

$$\begin{cases} v^{[1]}(x, t) = -\frac{1}{2}t^2x^2 - \frac{1}{24}t^4x^4 + \frac{1}{720}t^6x^6 + \dots \\ u^{[1]}(x, t) = 1 - tx^2 + \frac{1}{2}t^2x^4 - \frac{1}{6}t^3x^6 + \dots + \frac{1}{720}t^6x^{12} + \dots \\ w^{[1]}(t) = 1 - t^2 + t^4 - \dots - t^{18} + \dots \\ z^{[1]}(t) = t + \frac{1}{3}t^3 + \frac{2}{15}t^5 + \dots + \frac{443861162}{18561569025}t^{19} + \dots \\ y^{[1]}(t) = t^2 - \frac{1}{6}t^4 + \frac{1}{120}t^6 - \dots + \frac{1}{3556874360}t^{18} + \dots \end{cases} \quad (13)$$

Note that, the MTaylor series of exact solution (12) with order 20 is as:

$$\begin{cases} v(x, t) = \frac{1}{2}t^2x^2 - \frac{1}{24}t^4x^4 + \frac{1}{720}t^6x^6 - \frac{1}{40320}t^8x^8 + \dots \\ u(x, t) = 1 - tx^2 + \frac{1}{2}t^2x^4 - \frac{1}{6}t^3x^6 + \dots + \frac{1}{720}t^6x^{12} - \frac{1}{5040}t^7x^{14} + \dots \\ w(t) = 1 - t^2 + t^4 - \dots - t^{18} + t^{20} - \dots \\ z(t) = t + \frac{1}{3}t^3 + \frac{2}{15}t^5 + \dots + \frac{443861162}{18561569025}t^{19} + \frac{1888846608}{19489600725}t^{21} + \dots \\ y(t) = t^2 - \frac{1}{6}t^4 + \frac{1}{120}t^6 - \dots + \frac{1}{3556874360}t^{18} - \frac{1}{812164508842000}t^{20} + \dots \end{cases} \quad (14)$$

The obtained results in the first iteration (13) are same with the MTaylor expansion of the exact solutions (14) with $\nu = 20$, and this shows that an high appropriate approximate solution can be obtained with only one iteration. Also it illustrates the high rate of convergence of the VIM for this PDAE.

CONCLUSION

In this paper, a new and effective approach has been proposed for solving nonlinear system of PDAEs. Appropriate solutions were obtained by only one iteration of the VIM. It was shown that some nanoelectronics models, which presented by PDAEs, can be easily solved by using VIM. Using the mentioned method for system of PDAEs with higher index could be a subject of further researches.

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