Efficient Shooting Method Based on Leading Dynamics Determination by QR Decomposition

Federico Bizzarri[1], Angelo Brambilla[1], Giambattista Gruosso[1], and Giancarlo Storti Gajani[1]

Politecnico di Milano, DEI, p.za Leonardo da Vinci, 32, 26013 Milano, Italy
bizzarri,brambill,gruosso,storti@elet.polimi.it

Abstract In this paper an improved version of the conventional shooting method based on the Newton iterative algorithm is presented. One of the main drawbacks of the shooting method is due to the determination of the fundamental matrix by means of a product of partial matrices that limits its application to medium size circuits. Fundamental matrix free approaches have been presented in literature, they are based on the use of the GMRES method that lowers the computational effort from that of matrix by matrix product to that of matrix by vector product. In this paper a different approach is presented that exploits the properties of the QR decomposition to determine the leading dynamics of the circuit, i.e. the working modes represented by the eigenvectors of the circuit fundamental matrix associated to the Floquet exponents with the smaller negative real part. This can drastically reduce the number of matrix by vector products as in the GMRES method, but still makes available the main and most useful portion of the fundamental matrix, which is a key element, for example, in the determination of the stability of circuits working in a steady state condition.

1 Introduction

The shooting method, in contrast to harmonic balance, is well suited to compute the steady state behaviour of strong non-linear circuits and its importance has been recently strengthened to the reliable extension of this approach to mixed-signal problems [2]. Its "engine" is based on a time domain analysis that solves the DAE modeling the circuit with a variable time step integration method [1, 5]. Time domain analyses computes the residue, i.e. the difference among state variable values at the beginning and at the end of the integration time interval, and the sensitivity matrix, also known as the fundamental matrix **M**, that relates variations of state variables at the end of the integration period to those at the beginning. One of the main drawbacks of the shooting method is that its application is limited to medium size circuits. This is due to the fact that **M** is derived as a product of partial matrices each computed at each integration time step of the time domain analysis. If we assume that the circuit is characterised by N state variables and that the integration is performed on S time points, the effort to compute **M**, which in general is full, is proportional to $S \times N^3$ [7]. The introduction of the "matrix free" shooting methods based on GMRES sensibly reduces the computational effort [6]. The GMRES method builds the Krylov base $\mathscr{B} = \left[\mathbf{Mp}, \mathbf{M}^2\mathbf{p}, \ldots, \mathbf{M}^n\mathbf{p}\right]$ where $\mathbf{M} \in \mathbb{R}^{N\times N}$ and $\mathbf{p} \in \mathbb{R}^N$ is a "tentative" vector. If $\mathscr{B}$ spans the solution of the steady state problem with respect to a given error threshold, the solution is found in n matrix by vector products with a total cost $S \times n \times N^2$. The gain is thus proportional to a factor $(N-n)$. Consider now

$$\begin{cases} \dfrac{d\mathbf{x}}{dt} + G(\mathbf{x},t) = 0 \\ \mathbf{x}(t+T) - \mathbf{x}(t) = 0 \end{cases} \tag{1}$$

where $G(\mathbf{x},t) : \mathbb{R}^{N+1} \to \mathbb{R}^N$, models the vector field, $\mathbf{x} \in \mathbb{R}^N$ is the solution, $t \in \mathbb{R}^+$ represents time and $T \in \mathbb{R}^+$ is the working period. Assume to solve Eq. (1) in the time domain with the simple Implicit Euler integration method and consider one integration time step of length $h \in \mathbb{R}^+$, from t_n to $t_{n+1} = t_n + h$, we have

$$\mathbf{x}(t_{n+1}) - \mathbf{x}(t_n) + hG(\mathbf{x}(t_{n+1}), t_{n+1}) = 0.$$

By deriving this equation with respect to the $\mathbf{x}(t_0)$ initial condition we obtain

$$\frac{d\mathbf{x}(t_{n+1})}{d\mathbf{x}(t_0)} - \frac{d\mathbf{x}(t_n)}{d\mathbf{x}(t_0)} + h\frac{G(\mathbf{x}(t_{n+1}), t_{n+1})}{d\mathbf{x}(t_{n+1})}\frac{d\mathbf{x}(t_{n+1})}{d\mathbf{x}(t_0)} = 0$$

from which the sensitivity of $\mathbf{x}(t_{n+1})$ with respect to $\mathbf{x}(t_0)$ can be immediately computed as

$$\frac{d\mathbf{x}_{n+1}}{d\mathbf{x}_0} = \overbrace{\left(\mathbb{1}_N + h\frac{dG(\mathbf{x}_{n+1}, t_{n+1})}{d\mathbf{x}_{n+1}}\right)^{-1}}^{\mathbf{M}_{n+1}} \frac{d\mathbf{x}_n}{d\mathbf{x}_0} \tag{2}$$

where $\mathbb{1}_N$ is the order N identity matrix and subscript $_n$ refers to time instant t_n. To compute product **Mp**, either the $\mathbf{M}_n$ matrices with $n = [1, \ldots, S]$ in Eq. (2) or the $\mathbf{x}_n$ solution vectors must be stored and this can be problematic when dealing with large circuits. The implementation chosen in our simulator PAN [2] follows the second solution to minimise memory usage. Therefore, to compute **Mp**, $G(x_{n+1}, t_{n+1})$ is reevaluated at each time point, the $\mathbf{M}_{n+1}$ matrix is recomputed (at the cost of one LU factorisation) and the

[2] Our simulator PAN is available at the URL: http://brambilla.ws.dei.polimi.it.

$$\mathbf{M}_{n+1}\prod_{k=1}^{n}\mathbf{M}_k\mathbf{p} \tag{3}$$

left matrix by vector product is performed.

2 The proposed approach

According to Floquet theory, matrix $\mathbf{M}$ can be decomposed as

$$\mathbf{M}=\sum_{k=1}^{\mathrm{N}} e^{\lambda_k T}\mathbf{v}_k\mathbf{u}_k^{\mathrm{T}} \tag{4}$$

where λ_k are the Floquet exponents of $\mathbf{M}$ and $\mathbf{u}_k$, $\mathbf{v}_k$ are the corresponding right and left eigenvectors [3]. The boundary value problem defined in Eq. (1) can be solved with the Newton iterative method

$$\mathbf{x}_0^{p+1}=\mathbf{x}_0^p-\left(\sum_{k=1}^{\mathrm{N}} e^{\lambda_k T}\mathbf{v}_k\mathbf{u}_k^{\mathrm{T}}-\mathbb{1}_{\mathrm{N}}\right)^{-1}\left(\mathbf{x}_{\mathrm{S}}^p-\mathbf{x}_0^p\right)$$

where p is the iteration index and $\mathbf{x}_0^p$ is an approximation of the initial condition. If we sort in decreasing order the Floquet exponents and set to 0 those having a real part considerably less than $\Re(\lambda_1)$ we have

$$\widetilde{\mathbf{x}_0}^{p+1}=\mathbf{x}_0^p-\left(\widetilde{\mathbf{M}}-\mathbb{1}_{\mathrm{N}}\right)^{-1}\left(\mathbf{x}_{\mathrm{S}}^p-\mathbf{x}_0^p\right)$$

where $\widetilde{\mathbf{M}}=\sum_{k=1}^{\mathrm{N-L}} e^{\lambda_k T}\mathbf{v}_k\mathbf{u}_k^{\mathrm{T}}\in\mathbb{R}^{\mathrm{N}\times\mathrm{N}}$ is a rank L matrix that represents the *leading dynamics* of the system modeled by Eq. (1) and $\widetilde{\mathbf{x}}_0^{p+1}$ is the approximated new tentative solution computed by the Newton method.

Apparently, the "truncated" matrix $\widetilde{\mathbf{M}}$ can be derived only after having performed the complete matrix product (3). On the other hand the leading dynamics of the circuit can be computed by exploiting properties of the QR decomposition as shown in the sequel. Consider the product shown in Eq. (3) performed using only the first $\mathrm{S}_1<\mathrm{S}$ time samples. Consider the $\mathbf{Q}_{1,S1}\mathbf{R}_{1,S1}=\mathbf{M}_{1,S1}\mathbf{P}_{1,S1}$ QR decomposition where $\mathbf{R}_{1,S1}\in\mathbb{R}^{\mathrm{N}\times\mathrm{N}}$ is upper triangular and $\mathbf{P}_{1,S1}$ is a permutation matrix sorting the diagonal of $\mathbf{R}_{1,S1}$ in decreasing order. We set to 0 the $r_{i,j}$ entries of $\mathbf{R}$ such that $r_{i,i}<\alpha|r_{1,1}|$. It can be shown that $|r_{i,i}|>|r_{i,j}|$ with $j>i$ so that $\mathrm{N}-\mathrm{L}$ last columns of $\mathbf{Q}_{1,S1}$ can be *dropped* in the subsequent left matrix product performed to compute the fundamental matrix. A QR decomposition can be performed after a predefined number of integration time steps. The structure of $\mathbf{R}$ can be thus checked to see if other columns of the related $\mathbf{Q}$ matrix can be dropped. At the end of this process, i.e. at the end of the integration process along the T working period, we have performed no more than $\mathrm{S}\times(\mathrm{N}-\mathrm{M})\times\mathrm{N}^2$ matrix by vector products (as with GMRES), with the advantage of having computed a version of $\widetilde{\mathbf{M}}$ representing the leading dynamics of the system, i.e. that has the same $(\mathrm{N}-\mathrm{L})$ eigenvalues and eigenvectors of the $\mathbf{M}$ fundamental matrix and, finally, with the advantage of avoiding the storage of partial matrices or solutions.

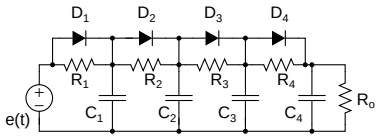

Figure 1. The schematic of the fourth order nonlinear ladder circuit. $\mathtt{C_x}=1\,\mu\mathrm{F}$, $\mathtt{R_x}=1\,\mathrm{k}\Omega$, $\mathtt{e(t)}=10\sin(200\pi t)$.

3 Simple simulation example

The schematic of a simple example circuit is shown in Fig. 1. It is a nonlinear ladder circuit with 4 state variables. The working period of the circuit is $T=10\,\mathrm{ms}$. After $T/4$, a QR decomposition of $\mathbf{M}_{1,\mathrm{S1}}$ gives

$$\mathbf{R}_{1,\mathrm{S1}}=\begin{bmatrix}-0.1 & 0 & -0.1 & -0.1\\ 0 & 9.7\times10^{-4} & -7.0\times10^{-4} & 9.2\times10^{-4}\\ 0 & 0 & -2.0\times10^{-6} & 8.6\times10^{-7}\\ 0 & 0 & 0 & 1.8\times10^{-9}\end{bmatrix}$$

Setting $\alpha=10^{-3}$, the last two rows of $\mathbf{R}_{1,\mathrm{S1}}$ can be set to 0, i.e. the leading dynamics is adequately spanned by the first two columns of $\mathbf{Q}_{1,\mathrm{S1}}$. The maximum relative error in computing the Floquet multipliers of $\mathbf{M}$ is less than 6×10^{-4} showing the effectiveness of the proposed method. This approach has been applied also to the oscillator described in [4] characterized by about 500 state variables. With the proposed approach, choosing $\alpha=10^{-7}$, the leading dynamics is spanned by only 41 columns of $\mathbf{Q}$ just after $T/10$.

References

1. Brambilla A., Gruosso G., and Storti Gajani G. Fssa: Fast steady-state algorithm for the analysis of mixed analog/digital circuits. *IEEE Trans. on CAD*, 29(4):528–537, Apr 2010.
2. F. Bizzarri, A. Brambilla, and G.S. Gajani. Phase noise simulation in analog mixed signal circuits: An application to pulse energy oscillators. *Circuits and Systems II: Express Briefs, IEEE Transactions on*, 58(3):154 –158, March 2011.
3. Miklós Farkas. *Periodic motions*. Springer-Verlag New York, Inc., New York, NY, USA, 1994.
4. S. Gagliolo, G. Pruzzo, and D. D. Caviglia. Phase noise performances of a cross-coupled cmos vco with resistor tail biasing. In *SBCCI05, 18th Annual Symposium on Integrated Circuits and System Design. Florianopolis, Brazil.*, pages 149–153, NEW YORK, NY, September 4-7 2005. ACM Press.
5. K. Kundert. *The Designer's Guide To Spice And Spectre*. Kluwer Academic Publishers, New York, NY, USA, 1995.
6. Y. Saad and H. Schultz. Gmres: A generalized minimal residual algorithm for solving non symmetric linear systems. *SIAM Journal on Scientific and Statistical Computing*, 7:pp. 856–869, July 1986.
7. J. Stoer. *Einfuhrung in die Numerische Mathematik*. Springer Verlag, Berlin - Heidelberg - New York, 1972.