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Jacobian Calculation Using the Multidimensional Fast Fourier Transform in the Harmonic Balance Analysis of Nonlinear Circuits

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Abstract **— A technique is developed whereby the gradient of frequency-domain simulation variables may be analytically determined using time-domain derivative information and the multidimensional fast Fourier transform. It is shown that this technique can be efficiently implemented when a circuit is driven by any number of incommensurate input frequencies. A harmonic balance simulator is constructed which uses this technique to determine the entries of the Jacobian matrix which are needed in a quasi-Newton iteration scheme. A significant reduction of simulation time is observed when compared with a harmonic balance simulator that uses matrix-multiplication-based transforms.**

I. INTRODUCTION

In the harmonic balance method of nonlinear analog circuit simulation, the linear subcircuit is analyzed in the frequency domain and the nonlinear subcircuit in the time domain. For simulations with multifrequency excitation, the time-domain and frequency-domain analyses have been interfaced using either the almost periodic discrete Fourier transform (APDFT) method [1], [2] or the multidimensional fast Fourier transform (NFFT) method [3]. The advantage of the APDFT is that computer implementation is relatively simple for an arbitrary number of incommensurate input frequencies. On the other hand the NFFT algorithm is computationally more efficient and exhibits superior numerical stability. An alternative method to that used by Rizzoli *et al.* [3] is presented here in which the Jacobian is calculated using the NFFT. This method has the advantage that frequency-domain derivatives may be computed for every frequency contained in the transform. It can also be used in conjunction with the block Newton iteration scheme [4].

II. HARMONIC BALANCE

Harmonic balance analysis proceeds by first selecting a set of frequency-domain analysis variables at every edge/node which is common to both the linear and nonlinear portions of the circuit. The frequency-domain independent variable is $\boldsymbol{X}$, and for impedance (admittance) type elements $\boldsymbol{X}$ is a set of current (voltage) phasors, while the dependent variable, $\boldsymbol{Y}$, is a set of voltage (current) phasors. Lowercase variables will be used to indicate time-domain quantities.

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The independent and dependent variables at a single node or edge will be denoted by the subscript n. Absence of this subscript will indicate the collection of *all* independent or dependent variables in the simulation. For example, $\boldsymbol{X}_n$ represents the frequency-domain independent variable containing all analysis frequencies at the nth node/edge, and $\boldsymbol{y}$ is the collection of the time-domain dependent variables at *every* node/edge and sample time.

The objective of the harmonic balance procedure is to "balance" the response of the nonlinear elements ($\boldsymbol{Y}$) to that of the linear elements ($\tilde{\boldsymbol{Y}}$). Defining the forward and inverse transform operators as $\mathcal{F}$ and $\mathcal{F}^{-1}$ respectively, the "balance point" is determined iteratively as follows. During each iteration and at each analysis node/edge an updated estimate of $\boldsymbol{X}_n$ is inverse Fourier transformed into the time domain,

$$\boldsymbol{x}_n = \mathcal{F}^{-1}(\boldsymbol{X}_n) \tag{1}$$

and applied as input to the constitutive relations of a nonlinear element. This yields the time-domain response ($\boldsymbol{y}_n$) for the present iterate of the dependent variable:

$$\boldsymbol{y}_n = \boldsymbol{h}(\boldsymbol{x}_n). \tag{2}$$

This is then Fourier transformed to the frequency domain,

$$\boldsymbol{Y}_n = \mathcal{F}(\boldsymbol{y}_n) \tag{3}$$

and compared with the response of the linear circuit to generate the error function E, $E = \|\boldsymbol{E}\|$ where $\boldsymbol{E} = [E_{k,n}] = [Y_{k,n} - \tilde{Y}_{k,n}]$; the subscript k denotes the frequencies and n the edges/nodes of elements $E_{k,n}$ of the matrix $\boldsymbol{E}$.

The error function is minimized by iteratively selecting better estimates for all independent variables. Generally, methods using first derivative information, known as quasi-Newton methods, are preferred. For each iteration the updated version of all independent variables is calculated using

$$^{\iota+1}\boldsymbol{X} = {}^{\iota}\boldsymbol{X} - ({}^{\iota}\boldsymbol{J}^{-1})({}^{\iota}\boldsymbol{E}) \tag{4}$$

where the leading superscript is the iteration index and ${}^{\iota}\boldsymbol{J} = {}^{\iota}(\partial \boldsymbol{E}/\partial \boldsymbol{X})$ is the Jacobian matrix or an approximation to the Jacobian matrix.

III. NFFT

The harmonic balance algorithm can be generalized to signals having N incommensurate input frequencies by using a multidimensional Fourier transform. The operations in (1) and (3) then become

$$x_{\boldsymbol{m},n} = \frac{1}{|\boldsymbol{M}|} \sum_{k_1=0}^{M_1-1} \sum_{k_2=0}^{M_2-1} \cdots \sum_{k_N=0}^{M_N-1} X_{k,n} \cdot \exp \frac{2\pi}{j} \left(\frac{k_1}{M_1} m_1 + \frac{k_2}{M_2} m_2 + \cdots + \frac{k_N}{M_N} m_N \right) \tag{5}$$

and

$$Y_{\boldsymbol{k},n} = \sum_{m_1=0}^{M_1-1} \sum_{m_2=0}^{M_2-1} \cdots \sum_{m_N=0}^{M_N-1} y_{\boldsymbol{m},n} \cdot \exp 2j\pi \left(\frac{m_1}{M_1} k_1 + \frac{m_2}{M_2} k_2 + \cdots + \frac{m_N}{M_N} k_N \right) \tag{6}$$

where $|\boldsymbol{M}| = \Pi^N |M_i|$ and the subscripts $\boldsymbol{k}$ and $\boldsymbol{m}$ are multi-indices which represent $[k_1 k_2 \cdots k_N]$ and $[m_1 m_2 \cdots m_N]$ respec-

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tively. The operations in (5) and (6) are most efficiently implemented using an NFFT. In this algorithm, the complex frequency-domain coefficients, $X_{k,n}$ and $Y_{k,n}$, may be thought of as belonging to an N-dimensional frequency space (elements of an N-dimensional matrix). Each dimension in this space corresponds to a particular input frequency. The frequency-domain coefficient indexed by $\boldsymbol{k}$ corresponds to the amplitude of a phasor having frequency $\omega_{\boldsymbol{k}} = \omega_1 k_1 + \cdots + \omega_N k_N$. The phase factors $2\pi m_l k_l / M_l$ come from the product $\omega_{k_l}\tau_{m_l}$, where $\omega_{k_l} = \omega_l k_l$ and the discrete evaluation times are $\tau_{m_l} = 2\pi m_l/\omega_l$. To satisfy the Nyquist sampling criterion we let the k_lth index reference frequencies up to the $(M_l/2-1)$th harmonic of ω_l (coefficients for negative, Nyquist, and dc frequencies account for the other $M_l/2+1$ terms). Similarly the time-domain coefficients $x_{\boldsymbol{m}}$ and $y_{\boldsymbol{m}}$ can be viewed as elements of a multidimensional sample matrix and the phase associated with harmonics of the ω_lth input frequency varying as we traverse the matrix along the lth dimension (i.e., as the index m_l increases the phase associated with the ω_lth frequency advances).

We thus have a multidimensional time space and the signals $\boldsymbol{y}_n$ and $\boldsymbol{x}_n$ cannot be related to any real physical signal. The time-domain constitutive relationships of nonlinear elements are constrained to be algebraic, i.e., have no memory, due to the absence of an identifiable sequence of time samples. This is not a restriction, as Newton-based harmonic balance simulators generally require that constitutive relations be algebraic. Nonlinear inductors, capacitors, and other elements having constitutive relations involving derivatives with respect to time are handled through multiplication by an appropriate power of $j\omega$ in the frequency domain.

In the remainder of this paper we shall consider the data to be arranged in matrices. An example of the notation which will be used is

$$\frac{\partial \boldsymbol{y}_n}{\partial x_{\boldsymbol{m},n}} = \left[\frac{\partial y_p}{\partial x}\right]_n.$$

The left side of the equation states that we are taking the partial derivative of the matrix of the time-domain dependent variable ($\boldsymbol{y}$) at all sample instants with respect to the dependent variable at one particular sample instant ($x_{\boldsymbol{m}}$). Here boldface type and the absence of a subscript indicate a vector or matrix quantity with the index varying throughout the range of the (suppressed) subscript. Lightface type and the presence of a subscript indicate that we are selecting one particular scalar value. When differentiation is performed, the node index n indicates that we are performing this operation at one particular node/edge of the dependent variable and one particular node/edge of the independent variable. The node/edge in each case may be different but we will use the same n in each case to avoid additional complexity. On the right side of the previous equation, the square brackets indicate a matrix, each element of which is indicated by the enclosed quantity. In this example, matrix elements are indexed by the subscript $\boldsymbol{p}$ and derivatives are taken with respect to the independent variable at a single sample instant. When subscripts are present inside the brackets they are free to vary over their range; absence of a subscript indicates a single fixed element. Note that the subscript convention for variables outside brackets is the opposite to that used for matrix elements.

IV. Jacobian Calculation

The harmonic balance procedure requires determination of the frequency-domain derivatives $\partial \boldsymbol{Y}/\partial \boldsymbol{X}$. These can be calculated from the time-domain derivatives

$$\boldsymbol{g}_n = [g_{\boldsymbol{pm}}]_n = \left[\frac{\partial y_p}{\partial x_{\boldsymbol{m}}}\right]_n = \left[\frac{\partial h(x_p)}{\partial x_{\boldsymbol{m}}}\right]_n \tag{7}$$

which are available from the nonlinear device time-domain constitutive relations. We may express (7) as

$$\boldsymbol{g}_n = \left[\delta_{\boldsymbol{pm}} g_{\boldsymbol{pm}}\right]_n \tag{8}$$

where $\delta_{\boldsymbol{pm}}$ is the Kronecker delta. A consequence of algebraic time-domain constitutive relationships is that an element $g_{\boldsymbol{pm}} = 0$ if $\boldsymbol{p} \neq \boldsymbol{m}$. Here we develop a procedure for calculating the frequency-domain derivatives from the time-domain derivatives when an NFFT is used to accomplish transformation. Difficulties arise because of the multidimensional nature of the data and the fact that the transform is accomplished by a linear operator rather than through multiplication by a matrix.

From (6) we see that each frequency-domain coefficient $Y_{k,n}$ is a function of all time-domain samples, the $y_{\boldsymbol{m},n}$'s. Similarly, from (5), we see that each time-domain sample $x_{\boldsymbol{m},n}$ is a function of all frequency domain coefficients, the $X_{\boldsymbol{k},n}$'s. This indicates that the transform should operate on the coefficients as if they were a vector rather than an N-dimensional matrix (as implied by the multiple indices). Thus the collection of all frequency-domain or time-domain coefficients will be treated here as a vector. This will be indicated by a hat ($\hat{\ }$) above the frequency- or time-domain coefficient. For example, $\hat{\boldsymbol{x}}_n$ represents a vector containing all the instantaneous coefficients, $x_{\boldsymbol{m},n}$, and is obtained by concatenating the rows of $\boldsymbol{x}_n$. We will assume that the rightmost index in $\boldsymbol{k}$ and $\boldsymbol{m}$ changes most rapidly, that each index is more significant than the index to its right, and that the lth index counts modulo M_l. The exact order used to concatenate the N-dimensional matrix into the vector is immaterial as long as a convention is set and followed consistently.

With the data represented in a column vector, the forward and inverse transforms (5) and (6) can be symbolically accomplished by matrix multiplication. The transform matrix ($\hat{\Gamma}$) and the inverse transform matrix ($\hat{\Gamma}^{-1}$) will always be two-dimensional matrices regardless of the number N. Thus

$$\hat{\boldsymbol{Y}}_n = \hat{\mathscr{F}}(\boldsymbol{y}_n) = \hat{\Gamma}\hat{\boldsymbol{y}}_n \tag{9}$$

and

$$\hat{\boldsymbol{x}}_n = \hat{\mathscr{F}}^{-1}(\boldsymbol{X}_n) = \hat{\Gamma}^{-1}\hat{\boldsymbol{X}}_n \tag{10}$$

where $\hat{\mathscr{F}}$ indicates Fourier transformation followed by concatenation. The transform and inverse transform matrices are

$$\hat{\Gamma} = [\gamma_{\boldsymbol{mk}}] \tag{11}$$

$$\hat{\Gamma}^{-1} = [\gamma_{\boldsymbol{km}}^{-1}] \tag{12}$$

and the terms $\gamma_{\boldsymbol{mk}}$ and $\gamma_{\boldsymbol{km}}^{-1}$ can be found directly by inspection of (5) and (6):

$$\gamma_{\boldsymbol{mk}} = \exp\frac{2\pi}{j}\left[m_1\frac{k_1}{M_1} + \cdots + m_N\frac{k_N}{M_N}\right]$$

$$\gamma_{\boldsymbol{km}}^{-1} = \frac{1}{|\boldsymbol{M}|}\exp 2\pi j\left[k_1\frac{m_1}{M_1} + \cdots + k_N\frac{m_N}{M_N}\right].$$

Using the chain rule

$$\frac{\partial \hat{\boldsymbol{Y}}_n}{\partial \hat{\boldsymbol{X}}_n} = \frac{\partial \hat{\boldsymbol{Y}}_n}{\partial \hat{\boldsymbol{y}}_n}\left(\frac{\partial \hat{\boldsymbol{y}}}{\partial \hat{\boldsymbol{X}}}\right)_n = \frac{\partial \hat{\boldsymbol{Y}}_n}{\partial \hat{\boldsymbol{y}}_n}\left(\frac{\partial \hat{\boldsymbol{y}}}{\partial \hat{\boldsymbol{x}}}\frac{\partial \hat{\boldsymbol{x}}}{\partial \hat{\boldsymbol{X}}}\right)_n \tag{13}$$

and noting that the forward and inverse transform matrices are

constants, we have

$$\frac{\partial \hat{Y}_n}{\partial \hat{y}_n} = \frac{\partial \hat{\Gamma}\hat{y}_n}{\partial \hat{y}_n} = \hat{\Gamma}\frac{\partial \hat{y}_n}{\partial \hat{y}_n} = \hat{\Gamma}\boldsymbol{I} = \hat{\Gamma} \tag{14}$$

where $\boldsymbol{I}$ is the identity matrix. Similarly

$$\frac{\partial \hat{x}_n}{\partial \hat{X}_n} = \hat{\Gamma}^{-1}. \tag{15}$$

If we define $\hat{\beta}_n = [\beta_{pm}]_n = \hat{g}_n\hat{\Gamma}^{-1}$, the operation $\hat{\Gamma}\hat{\beta}_n$ in (13) is nothing more than the Fourier transform of $\hat{\beta}_n$ and the NFFT can be used to efficiently accomplish the transform. We note that a single column, $\hat{\beta}_{m,n}$, of the two-dimensional matrix $\hat{\beta}_n$ is of the same size as the data vector $\hat{y}_n$. So the premultiplication of $\hat{\beta}_{m,n}$ by $\hat{\Gamma}$ in (13) corresponds exactly to the operation in (3), and the same transform and data structure used for the circuit variables can be used in determining the frequency-domain derivatives. Thus (13) is accomplished for the mth frequency of $\boldsymbol{X}_n$ by use of the transform operator

$$\frac{\partial \boldsymbol{Y}_n}{\partial X_{m,n}} = \left[\frac{\partial Y_p}{\partial X}\right]_n = \mathcal{F}(\beta_m)_n \tag{16}$$

where $\partial \boldsymbol{Y}_n/\partial X_{m,n}$ is an N-dimensional matrix from which the elements of the Jacobian can be extracted. Again, the matrix $\beta_{m,n}$ (and thus $\partial \boldsymbol{Y}_n/\partial X_{m,n}$) is the same size as the data matrices $\boldsymbol{x}_n$, $\boldsymbol{X}_n$, $\boldsymbol{y}_n$, and $\boldsymbol{Y}_n$.

When Newton's method is accomplished using strictly real quantities, the following four quantities must be computed:

$$^{RR}j_{m,n} = \frac{\partial \operatorname{Re}(Y_n)}{\partial \operatorname{Re}(X_{m,n})} \tag{17}$$

$$^{RI}j_{m,n} = \frac{\partial \operatorname{Re}(Y_n)}{\partial \operatorname{Im}(X_{m,n})} \tag{18}$$

$$^{IR}j_{m,n} = \frac{\partial \operatorname{Im}(Y_n)}{\partial \operatorname{Re}(X_{m,n})} \tag{19}$$

$$^{II}j_{m,n} = \frac{\partial \operatorname{Im}(Y_n)}{\partial \operatorname{Im}(X_{m,n})} \tag{20}$$

but the procedure (16) produces the quantity

$$\mathcal{F}(\beta_{m,n}) = {}^{RR}j_{m,n} + {}^{II}j_{m,n} + j\left({}^{RI}j_{m,n} + {}^{IR}j_{m,n}\right) \tag{21}$$

and the individual components cannot be recovered. We form ${}^{R}\beta_{m,n} = \operatorname{Re}(\beta_{m,n})$ and ${}^{I}\beta_{m,n} = \operatorname{Im}(\beta_{m,n})$ as

$${}^{R}\beta_{m,n} = g_n \operatorname{Re}\left(\Gamma_m^{-1}\right) \tag{22}$$

and

$${}^{I}\beta_{m,n} = g_n \operatorname{Im}\left(\Gamma_m^{-1}\right). \tag{23}$$

Then following (16) we get

$$\mathcal{F}\left({}^{R}\beta_{m,n}\right) = {}^{RR}j_{m,n} + j^{IR}j_{m,n} \tag{24}$$

$$\mathcal{F}\left({}^{I}\beta_{m,n}\right) = {}^{RI}j_{m,n} + j^{II}j_{m,n} \tag{25}$$

from which the needed derivatives are available.

V. Discussion and Conclusion

Equations (24) and (25) can be efficiently implemented in a circuit simulator since no matrix multiplications are required. The operations in (22) and (23) are *scalar* multiplications. This results from the fact that the nonlinear constitutive relations are algebraic ($\hat{g}_n = \partial \hat{y}_n/\partial \hat{x}_n$ is a diagonal two-dimensional matrix). The γ_{km}^{-1} are constants and need be computed only once per simulation. However, the values of g_n are dependent on the nonlinear constitutive relations and so they change from iteration to iteration. For each iteration they are computed once and are then used in determining all the $\beta_{m,n}$ in β_n. The major operation is the multidimensional Fourier transform, which is performed once at each frequency of $\boldsymbol{X}_n$.

The method presented for evaluating the Jacobian permits the use of the efficient NFFT algorithm in conjunction with Newton's method for the harmonic balance analysis of nonlinear analog circuits. This procedure has been implemented in FREDA, a general nonlinear circuit simulator. The MESFET amplifier circuit of Chang *et al.* [4] was driven by two incommensurate input signals, one at 0 dBm and the other at 5 dBm, and simulated using 14 analysis frequencies. The time-domain element response was oversampled [5] so that the transform contained 26 frequencies. The solution was obtained in 1.1 s after 11 iterations using a modified Sămanskii method on a DEC DS 3100 workstation. The equivalent simulation using a matrix multiplication based transform (APDFT) required 3.8 s.

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Harmonic Balance and Frequency-Domain Simulation of Nonlinear Microwave Circuits Using the Block Newton Method

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***Abstract*—An efficient algorithm using block Newton and chord methods is presented for the iterative minimization of the spectral balance error in the analysis of nonlinear microwave circuits. This algorithm is used in the harmonic balance and frequency-domain spectral balance simulation of a MESFET amplifier with single-tone and two-tone excitation.**

I. Introduction

Methods of nonlinear microwave analog circuit analysis can be classified by the nature of the linear and nonlinear subcircuit calculations: time-domain methods, where all elements are ana-

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