Initial conditions and robust Newton-Raphson for harmonic balance analysis of free-running oscillators

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Abstract Poor initial conditions for Harmonic Balance (HB) analysis of free-running oscillators may lead to divergence of the direct Newton-Raphson method or may prevent to find the solution within an optimization approach. We exploit time integration to obtain estimates for the oscillation frequency and for the oscillator solution. It also provides an initialization of the probe voltage. Next we describe new techniques from bordered matrices and eigenvalue methods to improve Newton methods for Finite Difference techniques in the time domain as well as for Harmonic Balance. The method gauges the phase shift automatically. No assumption about the range of values of the Periodic Steady State solution is needed.

1 Introduction

A free-running oscillator is an autonomous circuit, which has only DC bias sources connected to the circuit and, thus, no periodic excitation. During the time-domain transient analysis of an oscillator, the oscillation starts by itself due to noise or instability. Long start-up time implies long simulation time to get the Periodic

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Steady State (PSS) solution. Harmonic balance (HB) analysis is a frequency-domain PSS method. HB is needed for (phase) noise simulations and is more suitable for frequency-dependent linear devices. It may converge faster to the PSS solution of a free oscillator than the transient analysis. To enhance convergence one either modifies the HB equations or one applies artificial excitation. In addition, the oscillation frequency (the fundamental HB frequency), is unknown and one needs a gauge equation and an initial estimate. Frequency domain methods to estimate these can be found in [1, 3, 6–8] (and their references).
We present two algorithms for oscillation frequency detection from transient data and improve by (vector) extrapolation [10]. The initialization of the probe voltage amplitude and of the HB solution are considered. Finally we describe new techniques from bordered matrices and eigenvalue methods to improve the Newton method for HB analysis.

2 Initializing HB Oscillator Analysis

The oscillator analysis in the APLAC simulator [2] utilizes a probe element and optimization techniques. Inside an optimization loop HB analysis is performed with new values of the optimization variables, being the oscillation frequency, f_{osc}, and the oscillation amplitude, v_{osc}. An artificial excitation probe, being a voltage source in series with a non-zero resistor (to prevent an increase of the DAE-index), is connected to the circuit. The goal of the optimization is to have a zero current through the probe element. For a related procedure see [8]. The initial conditions for the optimization of f_{osc} and v_{osc} are obtained from transient analysis as described next.
Initially a (limited) transient analysis is run, followed by a Fourier transform (FFT) to get an impression of the spectrum of the oscillator and of the solution. A spectral line having the largest magnitude indicates the oscillation frequency. Depending on the sampling rate, the actual oscillation frequency may be situated between the sampled frequency points. Therefore, quadratic interpolation with three frequency points around the maximum is used to determine a more accurate estimate for the

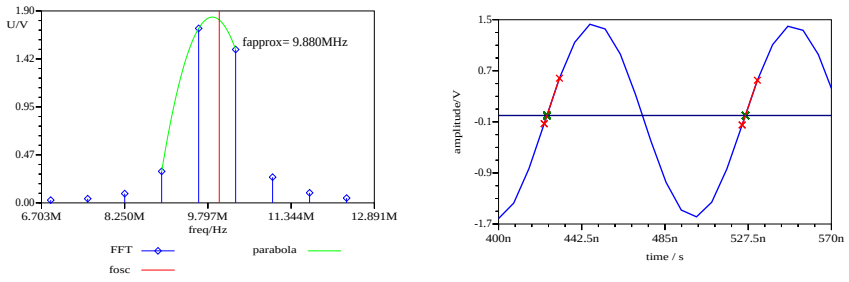

Fig. 1 Left: Quadratic interpolation of the frequency from the spectrum. **Right:** Zero-crossing: the x-markers connected with lines show the points used for interpolation.

oscillation frequency, see Fig. 1 (left). An alternative, zero-crossing, method also applies to transient simulation results. The period is determined from the zero crossings in the waveform with the DC-value. Accuracy of the zero crossings is improved by using linear inverse interpolation, see Fig. 1 (right). This can be generalized to a Poincaré method [4, 5] that determines the next root of a (scalar) phase condition $s(\mathbf{x}(t)) = (\mathbf{x}(t), \mathbf{n}) - \alpha = 0$ (i.e. solve both $\mathbf{x} = \mathbf{x}_\alpha$ [with constraint $d(\mathbf{x}(t), \mathbf{n})/dt > 0$] and $t = t_\alpha$) and restarts the time integration at $t = t_\alpha$ with initial value $\mathbf{x}_\alpha$[1]. The values $\mathbf{x}_{k+1} = \mathbf{F}(\mathbf{x}_k)$ (for some function $\mathbf{F}$ and $k \geq 0$), determined in this way, approximate the boundary value used by the ultimate PSS solution. We accelerate by vector extrapolation. Define recursively $\mathbf{D}_{k+1} = [\mathbf{D}_k \ \mathbf{d}_{k+1}]$, with $\mathbf{D}_0 = \emptyset$ (empty) and $\mathbf{d}_{k+1} = \mathbf{x}_{k+1} - \mathbf{x}_k$. Clearly $\mathbf{D}_k = \mathbf{X}_k \Delta_k$ for $\mathbf{X}_k = [\mathbf{x}_0 \ \mathbf{x}_1 \ \dots \ \mathbf{x}_k]$ and a difference matrix Δ_k. By a QR-decomposition we determine the rank of $\mathbf{D}_{k+1} = \mathbf{Q}_{k+1}\mathbf{R}_{k+1}$, with $\mathbf{Q}_{k+1} = [\mathbf{Q}_k \ \mathbf{q}_{k+1}]$ and $\mathbf{R}_{k+1} = \begin{bmatrix} \mathbf{R}_k & \mathbf{r}_{k+1} \\ 0 & \alpha_{k+1} \end{bmatrix}$. If $|\alpha_{k+1}| \leq \varepsilon$ we assume that $\mathbf{d}_{k+1} \in \text{Span}(\mathbf{Q}_k) = \text{Span}(\mathbf{D}_k)$, i.e. we we can write $\mathbf{d}_{k+1} = \mathbf{Q}_k\mathbf{r}_{k+1} = \mathbf{D}_k\mathbf{R}_k^{-1}\mathbf{r}_{k+1} = \sum_{p=1}^{k} \sigma_p \mathbf{d}_p$ where $\sigma = (\sigma_1, \dots, \sigma_k)^T = \mathbf{R}_k^{-1}\mathbf{r}_{k+1}$. Setting $\sigma_{k+1} = -1$ we thus have $\sum_{p=1}^{k+1} \sigma_p \mathbf{d}_p = \mathbf{0}$. This linear combination has a crucial application. If we express the $\mathbf{d}_n$ in terms of lower and higher order effects we observe that the sum of the lower order effects nearly cancels. We assume that $\sigma_1 \neq 1$, that $\Phi = \partial\mathbf{F}/\partial\mathbf{x}$ is uniformly bounded and that also $(\mathbf{I} - \Phi)^{-1}$ exists and is uniformly bounded. We summarize some basic steps in Alg. 1. Starting with this value $\mathbf{y}$ one generates iterands $\mathbf{y}_k$

Algorithm 1 Algorithmic background for the accelerated Poincaré map method [5].

1: Denote the limit of the recursion $\mathbf{x}_{n+1} = \mathbf{F}(\mathbf{x}_n)$ ($n \geq 0$) by $\tilde{\mathbf{x}} = \lim_n \mathbf{x}_n$.
2: Let $\mathbf{e}_n = \mathbf{x}_n - \tilde{\mathbf{x}}$, then $\mathbf{e}_{n+1} = \Phi\mathbf{e}_n + \mathscr{O}(||\mathbf{e}_n||^2)$. Thus $||\mathbf{e}_{n+1}||^2 = \mathscr{O}(||\mathbf{e}_n||^2) = \mathscr{O}(||\mathbf{e}_0||^2)$.
3: For the $\mathbf{d}_n$ mentioned above we have $\mathbf{d}_{n+1} = \Phi\mathbf{d}_n + \mathscr{O}(||\mathbf{e}_n - \mathbf{e}_{n-1}||^2) = \Phi\mathbf{d}_n + \mathscr{O}(||\mathbf{e}_{n-1}||^2) = \Phi\mathbf{d}_n + \mathscr{O}(||\mathbf{e}_0||^2)$ (for $n \geq 1$). This last 2-terms recursion makes the next steps a bit easier to formulate than the more precise intermediate 3-terms recursion. For $n = 0$ we have $\mathbf{d}_1 = \mathbf{x}_1 - \mathbf{x}_0 = \mathbf{e}_1 - \mathbf{e}_0 = (\Phi - \mathbf{I})\mathbf{e}_0 + \mathscr{O}(||\mathbf{e}_0||^2)$, hence $\mathbf{e}_0 = (\Phi - \mathbf{I})^{-1}\mathbf{d}_1 + \mathscr{O}(||\mathbf{e}_0||^2)$.
4: We have $\mathbf{0} = \sum_{p=1}^{k+1} \sigma_p \mathbf{d}_p = \sum_{p=2}^{k+1} \sigma_p \Phi^{p-1}\mathbf{d}_1 + \sigma_1\mathbf{d}_1 + \mathscr{O}(||\mathbf{e}_0||^2)$, hence $\sum_{p=1}^{k+1} \sigma_p \Phi^{p-1}\mathbf{d}_1 = \mathscr{O}(||\mathbf{e}_0||^2)$.
5: Let $\Xi = (\sum_{p=1}^{k+1} \sigma_p)\tilde{\mathbf{x}}$. We obtain $\sum_{p=1}^{k+1} \sigma_p \mathbf{x}_p = \sum_{p=1}^{k+1} \sigma_p(\tilde{\mathbf{x}} + \mathbf{e}_p) = \Xi + \sum_{p=1}^{k+1} \sigma_p \mathbf{e}_p = \Xi + \sum_1^{p+1} \sigma_p \Phi^{p-1}\mathbf{e}_1 + \mathscr{O}(||\mathbf{e}_1||^2) = \Xi + \sum_1^{p+1} \sigma_p \Phi^p \mathbf{e}_0 + \mathscr{O}(||\mathbf{e}_0||^2) = \Xi + \sum_1^{p+1} \sigma_p \Phi^p (\Phi - \mathbf{I})^{-1}\mathbf{d}_1 + \mathscr{O}(||\mathbf{e}_0||^2) = \Xi + \Phi(\Phi - \mathbf{I})^{-1} \sum_1^{p+1} \sigma_p \Phi^{p-1}\mathbf{d}_1 + \mathscr{O}(||\mathbf{e}_0||^2) = \Xi + \mathscr{O}(||\mathbf{e}_0||^2)$.
6: Finally $\mathbf{y} = \sum_{p=1}^{k+1} \sigma_p \mathbf{x}_p / (\sum_{p=1}^{k+1} \sigma_p)$ is a higher order accurate approximation, with error $\mathscr{O}(||\mathbf{e}_0||^2)$, or, taking the effect ε into account, with error $\mathscr{O}(||\mathbf{e}_0||^2) + \mathscr{O}(\varepsilon)$.

with as next extrapolation $\mathbf{z}$. The row $\mathbf{x}, \mathbf{y}, \mathbf{z}, \dots$ converges super-linearly. Storing the $t_k = t_\alpha$ easily provides the period $T = t_{k+1} - t_k$. A final integration over one period gives a time-domain solution from which an initial HB solution is obtained.
With $\mathbf{n} = \mathbf{e}_k$ one traces a particular unknown (this choice requires knowledge by the designer about the location where the oscillation occurs). The phase condition can be for a difference of a voltage or a zero condition for a current.

[1] This method is used in Pstar, the in-house analog circuit simulator of NXP Semiconductors.

3 VCO oscillator

The methods implemented in APLAC were tested with an industrial VCO circuit that consists of 40 MOSFETS (modelled by BSIM3) and 80 (Juncap) diodes. The expected results based on transient simulation are $f_{\rm osc} = 3.25\,{\rm GHz}$ and $v_{\rm osc} = 1.25\,{\rm V}$, while the initial values for the analysis were: $f_{\rm osc} = 3.0\,{\rm GHz}$ and $v_{\rm osc} = 1.0\,{\rm V}$.
The circuit has been simulated using HB oscillator analysis without initialization (old), and with FFT and zero crossing (ZeroC) initialization. Table 1 summarizes the CPU times and the number of HB iterations obtained to reach the oscillator solution ($f_{\rm osc} = 3.25\,{\rm GHz}$ and $v_{\rm osc} = 1.25\,{\rm V}$) as well as initial values of $f_{\rm osc}$ and $v_{\rm osc}$ for the HB based optimization – with the old method user-specified values are used directly, and improved values are obtained using either FFT or ZeroC method.
A typical result of the Poincaré method for a Colpitts oscillator gives 3 outer iterations (extrapolations) with 4, 3, 2 inner iterations, repectively, to build each time a subspace in which extrapolation leads to an improved initial value for solution and period (final error $< 10^{-16}$). The zero crossing and the Poincaré method assume that two successive crossings determine the period. This excludes situations in which four or more crossings really determine the overall period.

Table 1 Number of HB iterations and CPU times, and user-specified ('old') or improved initial values ('FFT', 'ZeroC') of $f_{\rm osc}$ and $v_{\rm osc}$ of the VCO circuit.

method	HBITER	CPU/s	initial value of $f_{\rm osc}$/GHz	initial value of $v_{\rm osc}$/V
old	2259	110.6	3.0	1.00
FFT	47	6.2	2.7	1.09
ZeroC	31	1.4	3.1	1.17

4 Newton Raphson

The Newton-Raphson method to solve the Harmonic Balance system becomes

$$\mathbf{M}^k \begin{bmatrix} \mathbf{X}^{k+1} - \mathbf{X}^k \\ f^{k+1} - f^k \end{bmatrix} = - \begin{bmatrix} \mathbf{F}(\mathbf{X}^k, f^k) \\ \mathbf{c}^T \mathbf{X}^k - c \end{bmatrix}, \quad \mathbf{M}^k = \begin{bmatrix} \mathbf{A}^k & \mathbf{b}^k \\ \mathbf{c}^T & \delta \end{bmatrix}. \tag{1}$$

Here

$$\mathbf{A}^k = \left.\frac{\partial \mathbf{F}}{\partial \mathbf{x}}\right|_{\mathbf{X}^k, f^k} = \Omega^k \cdot \mathbf{C}^k + \mathbf{G}^k, \quad \mathbf{b}^k = \left.\frac{\partial \mathbf{F}}{\partial f}\right|_{\mathbf{X}^k, f^k}, \tag{2}$$

for suitable matrices $\mathbf{C}$ and $\mathbf{G}$, that are composed by the local Jacobians and (discrete) Fourier Transforms; $\Omega = {\rm diag}(\ldots, i\omega_k, \ldots)$, with $\omega_k = \phi_k(f^k)$ (for some function ϕ_k). The last row in (1) corresponds with the phase equation; usually $\delta = 0$. The matrix $\mathbf{A}$ becomes badly conditioned when the Newton iterands converge. This is

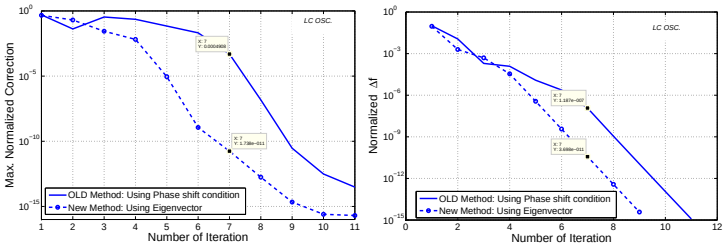

Fig. 2 LC oscillator: normalized corrections for solutions and frequency.

due to the fact that the time derivative of the PSS solution solves the linearized homogeneous circuit equations when linearized at the PSS solution. Hence when the discretization is exact this time derivative of the ultimate PSS is in the kernel of $\mathbf{A}$. This has led to study more carefully bordered matrices [1, 9] and generalized eigenvalue methods. In [9] the eigentriple $(\mathbf{V}, \mathbf{W}, \lambda)$ is determined such that $[\lambda f \mathbf{C} + \mathbf{G}]\mathbf{V} = \mathbf{0}$ and $\mathbf{W}^T[\lambda f \mathbf{C} + \mathbf{G}] = \mathbf{0}$ for the λ closest to 1. We approximate the bi-orthogonality relation between $\mathbf{V}$ and $\mathbf{W}$ by $\mathbf{W}^T \cdot \mathbf{C} \cdot \Omega \cdot \mathbf{X} - 1 = 0$, i.e. in (1) we take $\mathbf{c}^T = \mathbf{W}^T \cdot \mathbf{C} \cdot \Omega$ and $c = 1$. We may even consider $\mathbf{c}^T = \mathbf{V}^T$.

5 LC oscillator

We consider an *LC* tank with a nonlinear resistor that is governed by the following differential equations for the unknowns (v, i) [v being the nodal voltage; i being the inductor current]

$$\begin{bmatrix} C & 0 \\ 0 & L \end{bmatrix} \frac{\mathrm{d}}{\mathrm{d}t} \begin{bmatrix} v(t) \\ i(t) \end{bmatrix} + \begin{bmatrix} \frac{1}{R} & 1 \\ 0 & -1 \end{bmatrix} \begin{bmatrix} v(t) \\ i(t) \end{bmatrix} + \begin{bmatrix} S\tanh(\frac{Gv(t)}{S}) \\ 0 \end{bmatrix} = \mathbf{0} \tag{3}$$

$$v(0) = v_0, \quad i(0) = i_0. \tag{4}$$

where C, L and R are the capacitance, inductance and resistance, respectively. The voltage controlled nonlinear resistor is defined by the S and G parameters. The values $L = 0.53$ nH, $C = 1.33$ pF, $R = 250\ \Omega$, $S = 1/R$, and $G = -1.1/R$ correspond with an oscillation frequency 6 GHz. Starting with initial conditions $T_0 = 1.1 \times 2\pi$, $v_0(t) = \sin(t)$, $i_0(t) = 0.2\sin(t)$, and $N = 101$ (100 actual grid points), the PSS solutions are obtained using the old phase-shift condition method and with the new eigenvector gauge method. For both methods we determine the maximum of the normalized correction of the solution and the normalized frequency correction

$$\Delta \mathbf{X}^k\Big|_{\text{Normalized}} = ||\mathbf{X}^{k+1} - \mathbf{X}^k||_\infty / ||\mathbf{X}^k||_\infty, \qquad \Delta f^k\Big|_{\text{Normalized}} = |f^{k+1} - f^k| / |f^k|$$

during each k-th Newton-Raphson iteration, which are presented in Fig. 2. A wrong value in the old phase shift condition even prevents convergence for this method [9].

6 Conclusion

Time domain initializations have been presented that enhance the convergence options for Harmonic Balance within an outer optimization approach and within a direct Newton-Raphson procedure. One method exploits FFT techniques. A zero-crossing technique was generalized to a Poincaré method. Here speed up by vector extrapolation was based on Minimal Polynomial Extrapolation.
Finally, a new technique for the Newton-Raphson simulation of a free-running oscillator was presented. The generalized eigenvectors for the eigenvalue closest to 1 and the time derivative of the solution provide a robust gauge equation that is dynamically updated within each Newton-Raphson iteration. It was verified that the new method has better convergence properties compared to the popular phase-shift condition method and does not need additional information about the solution.

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