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D2.14 Public report on improved initial conditions for Harmonic Balance in solving free oscillatory problems

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Contents

1 Introduction

Distortion Analysis deals with the study how nonlinearity affects harmonics of the solution. For a driven problem one studies how the harmonics of a source function are mapped to the solution of the nonlinear problem. A driven problem is well posed. It can be solved by Newton Raphson procedures using Harmonic Balance in the frequency domain. In Tasks T2.1 and T2.2 special variants have been studied that addressed efficiency and robustness, see the Deliverables D2.3 and D2.5 and the Public Reports D2.10, D2.11 and D2.12.
An autonomous problem introduces an additional problem. A free running oscillator has a non-trivial time Periodic Steady-State (PSS) solution, which is different from the DC-solution. The DC-solution is unstable when performing normal transient analysis and thus it provides a way to ultimately approximate the PSS solution, as will be exploited later on. Contrarely, in a Harmonic Balance setting the DC solution is a normal solution for the Newton Raphson procedure. Hence one should provide good initial estimates for the unknown oscillation frequency and for the solution of the circuit. In practise we see that with increase of the oscillation frequency the need for accurate initial estimates becomes more dominant. Without them the Newton Raphson method will not converge, or "at best" converge to the DC-solution in which one is not interested. It also may prevent to find the solution within an optimization approach.

Task description Task T2.3 of WP2
Task T2.3 of WP2 dealt with "Improved initial conditions for Harmonic Balance", i.e. finding robust initial estimates for the final solution of free-running oscillators, determined by Harmonic Balance.

New algorithms to find the operating frequency of a free-running oscillator will be developed that (drastically) improve the speed and robustness of harmonic balance analysis for these cases. Proposed alternatives were:

- Pole-zero analysis methods to determine the dominant poles of the system and hence find a good initial estimate for the operating frequency.
- Find an initial frequency estimate from optimization techniques.

We exploit techniques from transient analysis to obtain good initial estimates for the oscillation frequency and for the circuit solution to start the HB-based oscillator analysis. The developed techniques were implemented in the APLAC simulator and have been thoroughly tested. Significant speed-up was obtained, while also the robustness was increased. We also describe how we can use modern subspace techniques that allow for extrapolation within an iterative framework. New techniques from bordered matrices and eigenvalue methods led to improved Newton methods for Finite Difference in the time domain as well as for Harmonic Balance and for improving methods based on optimization. The method gauges the phase shift automatically. No assumption about the range of values of the PSS solution is needed.
Both the theoretical background and simulation results are presented. Parts of this report have been presented at the ECMI-2010 (European Consortium for Mathematics in Industry) and SCEE-2010 (Scientific Computing in Electrical Engineering) conferences. Full papers [6, 13, 16] have been submitted to the post-conference proceedings.

2 Methods in use

This section reviews several approaches found in literature. These techniques cover time-domain start-ups, homotopy methods (f.i. using an artificial voltage source), direct methods, etc.

- **Pure long-range time integration** is robust. It exploits the fact that the DC-solution is an unstable Periodic Steady State (PSS) solution for the time integration process. However the integration may take a long time.
  This approach does not easily deal with frequency domain defined elements (using S-parameters). S-Parameter blocks should be interpolated using rational functions after which a synthesis to an RCL block can be made (with added constraint as being passive). The approximation is valid for some range of frequencies.
  The combination with (time-dependent) sources in the initial startup usually can be formally blocked.

- A first modification is to cover time integration as a first step over some specified time interval. Based on this one can apply a **(windowed) DFT** to get an impression of the harmonics involved.

- In Spectre[1] the initial time integration is followed by a **shooting method**. Here one iteratively improves the initial value, from which started, transient simulation will provide a PSS solution.

- A **Finite-Difference method** (FD) in the time domain needs a Newton method to solve the system. The most notable difference to time integration is that the DC solution is a stable PSS solution for the FD method. Hence measures should be taken to prevent convergence to the DC solution.
  We assume $N+1$ discretization points $t_0, t_1, \ldots, t_N$, where $t_i = T\, s_i$, with $s_i \in [0,1]$. The unknowns in the system are: $\mathbf{x}_i = \mathbf{x}(t_i)$; we may choose f as additional unknown. We denote $\mathbf{x} = (\mathbf{x}_0^T, \ldots, \mathbf{x}_N^T)^T$.
  The Jacobian matrix $\mathbf{M}$ for the system $\mathbf{x}, f$ looks like

$$\mathbf{M} \;=\; \begin{bmatrix} \mathbf{A} & \mathbf{b} \\ \mathbf{c}^T & \delta \end{bmatrix} \tag{1}$$

  for suitable vectors $\mathbf{b}$ and $\mathbf{c}$ and (scalar) value δ. The matrix $\mathbf{A}$ has the pencil form $\mathbf{A} = f\,\mathbf{C} + \mathbf{G}$. The matrix $\mathbf{C}$ contains contributions due to capacitors and inductors; $\mathbf{G}$ contains contributions due to resistors and inductors and the effect of the periodicity equation. The vector $\mathbf{c}$ is needed to gauge the solution.
  Some observations can be made:

  – The matrix $\mathbf{A}$ becomes badly conditioned when the Newton process converges. This is 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 $\mathbf{A}$.

[1] Spectre is the analogue circuit simulator provided by Cadence Design Systems, Inc., San Jose, CA.

  - Due to this conditioning problem the vectors **b** and **c** and (scalar) value δ are really needed to make the matrix **M** non-singular. If **A** is non-singular one can apply a block Gaussian elimination using $\mathbf{A}^{-1}$.

  The Newton systems clearly have to be enlarged to a matrix **M** to get a non-singular matrix and to prevent convergence to the DC solution. Here the choice of the additional unknown may look natural, but the equation for this additional unknown is rather arbitrarily. Also, Newton solves, at each iteration, a perturbed system of equations. It is remarkable that one changes the Newton matrix for another one when performing phase noise analysis.

- **Waveform Newton** linearizes the differential-algebraic circuit equations around a previous time waveform and integrates these in time [8]. Assuming that the previous waveform was periodic in time, one determines by a shooting method an initial value at which one obtains a new periodic waveform. Note that the whole step requires only the solution of a linear system. If one uses the same discretization points as in the FD method and the same integration method the results are identical to those generated by the FD method at each iteration. However, Waveform Newton offers adaptivity of the discretization points.

- **Harmonic Balance** (HB) is a nonlinear method in the frequency domain in which one decomposes the solution in Fourier components. The system for the Fourier coefficients looks similar to the one obtained by the FD method (sparse matrix techniques involving matrix vector multiplications can efficiently be combined with the DFT and its inverse - hence one does not need to determine the matrix completely in advance). The Newton process to solve the HB-system has similar characteristics as the process to solve the FD-problem.
  HB and FD may converge faster to the PSS solution of a free oscillator than the transient analysis. However, HB and FD have one common problem. That is that one usually is able to provide a good initial solution for the oscillation frequency f, but a good initial circuit solution is lacking: providing only two harmonics [DC+AC] is, in general, not enough. To enhance convergence one either modifies the HB or FD equations or one applies excitation at an artificial source element (also called a probe element).

3 Initialization of APLAC HB Oscillator Analysis by using transient data

A common way to solve free-running oscillator problems with the Harmonic Balance (HB) method is to use single, multiple, or multi-harmonic probes [1]. In the APLAC simulator [2] the probe element is called OscAProbe, which is actually a voltage source in series with a non-zero resistor, and it is usually connected to the output of an oscillator circuit.

The HB oscillator problem is solved by optimization. The optimization variables are the value of the probe voltage source at the fundamental frequency, V_{osc}, and the HB analysis fundamental frequency f_{osc}. The goal of the optimization is to have the HB fundamental spectral voltage over the probe element equal to V_{osc}, i.e., the current through the probe element is equal to zero.

The user is required to set initial values for V_{osc} and f_{osc}. A poor initial frequency or amplitude value can lead to unsuccessful optimization or will at least require a large number of optimization cycles to succeed. Therefore algorithms have been developed to provide better initial estimates for V_{osc} and f_{osc}.

3.1 Setting Initial Conditions for HB Analysis

Two separate methods were developed to improve the initialization of HB analysis, namely an FFT-based method ("FFT") and a zero-crossing method ("ZeroC") [6, 16]. Each method can be used to initialize both the oscillation frequency f_{osc} and the oscillation amplitude V_{osc} of the probe element. The main steps are:

- Run an initial transient analysis over some specified interval.
- Collect time-domain waveform data, i.e., the voltage over the probe element.
- Extract improved values for V_{osc} and f_{osc} from the data using the two new implemented methods called "FFT" and "ZeroC",
  - "FFT": apply a FFT and search for the location (frequency) and value of the maximum amplitude peak and improve this estimate by parabolic interpolation.
  - "ZeroC": estimate the frequency based on zero-crossings (after removal of the average), and oscillation amplitude based on half of the maximum swing.
- Start the HB analysis based oscillator optimization using these improved values.

The algorithms have been implemented in the APLAC simulator. There are several parameters which can be used to control initial transient analysis and/or how the estimation of V_{osc} and f_{osc} is done.

3.2 Simulation Results

The following figures show the transient start-up and the HB waveform (result of the HB analysis based oscillator analysis) of two test circuits, Colpitts (Fig. 1) and vcoBi (Fig. 2).

Table 1 shows more detailed analysis results for Colpitts, vcoBi, Pierce and VHF oscillator circuits. Columns "Circuit", "Method", "HBITER", "CPU", and "Speedup" show the name of the circuit, the used analysis method (algorithm), the total number of HB iterations, CPU-time in seconds, and the speed-up factor, respectively. A HB iteration in the APLAC simulator involves steps in an optimization loop: solve a driven oscillator problem by Newton Raphson, and update V_{osc} and f_{osc} for the next optimization loop. The analysis algorithm "old" refers to the default settings of the simulator, and "FFT" and "ZeroC" refer to the new implemented methods. The speedup factor has been computed are a ratio of the CPU-times of the simulated case and the reference simulation – faster simulation than the reference simulation gives a speedup factor higher than one. In case of "FFT" and "ZeroC" methods, the CPU-time includes also the time of the initial transient simulation.

In general, the usage of either "FFT" or "ZeroC" based estimate for the initial values improve the efficiency and enhance the robustness of the oscillator optimization analysis. Results have been reported in [6, 16]. Optimization methods are, however, quite sensitive to the initial values, and depending on the values of analysis and/or optimization parameters, the optimization algorithm does not always benefit for the improved initial values. This is partly due to the nonlinear behaviour of the current through the probe element as a function of the supplied voltage (see Lampe [9–11]). Also the number of zero crossings needed to estimate the frequency can

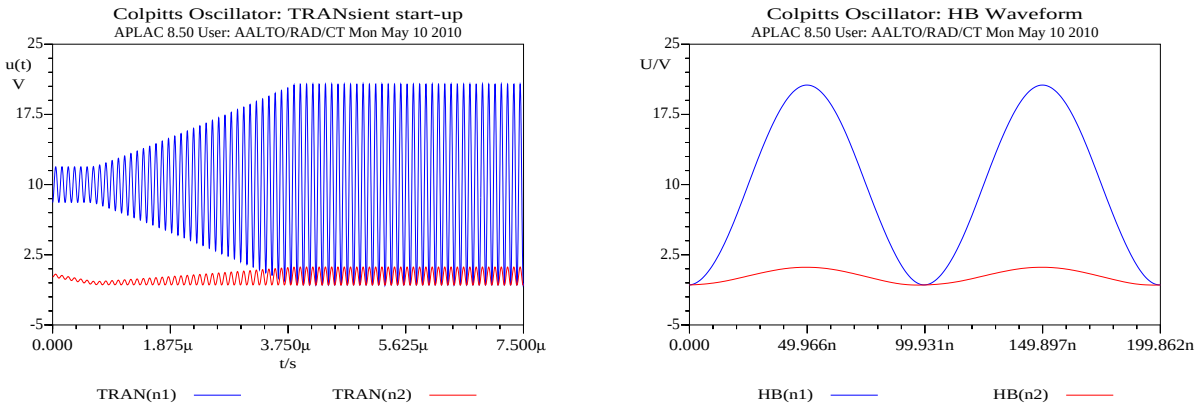

Figure 1: Colpitts Oscillator: Transient start-up (left) and HB waveform (right)

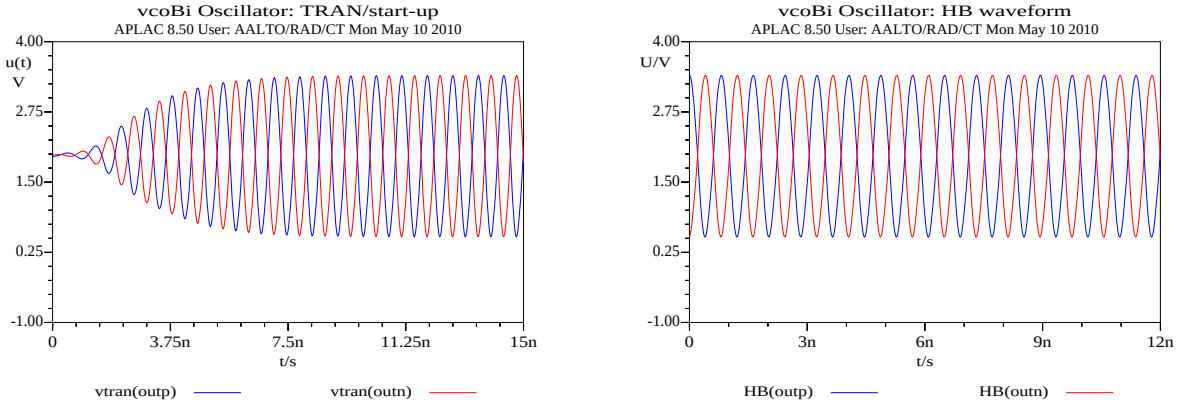

Figure 2: vcoBi Oscillator: Transient start-up (left) and HB waveform (right)

Circuit	Method	HBITER	CPU	Speedup
Colpitts	old	1756	0.58	1.0
	FFT	1529	0.54	1.1
	ZeroC	1153	0.38	1.5
vcoBi	old	738	1.98	1.0
	FFT	312	0.80	2.5
	ZeroC	31	0.08	24.8
Pierce	old	779	0.27	1.0
	FFT	593	0.22	1.2
	ZeroC	452	0.14	1.9
VHF	old	50	0.01	1.0
	FFT	43	0.02	0.5
	ZeroC	31	0.02	0.5

Table 1: Detailed analysis results in case of Colpitts, vcoBi, Pierce and VHF oscillator circuits

be higher than 2. The first item can be improved by applying vector extrapolation techniques before completing the actual zero-crossing process. An example of such a method is shown in the next section.

4 Vector extrapolation applied to the Poincaré method

The Zero Crossing method that was introduced in the previous section can be seen as one step in a Poincaré method. In [4, 5] the free oscillator problem is solved by applying vector extrapolation to a Poincaré method. In essence this is a matrix free method and thus it is easy to combine this with ordinary transient integration. The method requires a 'phase'-condition (which might require a condition at a specific node in the circuit) and generates approximations for the PSS-solution and for the period T. The method may converge on its own, but after a limited number of extrapolations one can use the approximations as initialisation for the Finite Difference (FD) approach in the time domain, or, as initialisation for the Harmonic Balance (HB) method, after applying an FFT. Note that this also provides some feeling for the range of the values of the PSS-solution.
Finally, we remark that actually the vector extrapolation only affects the circuit solution. The period T is derived as a secondary result.
Given $\boldsymbol{x}_0$, the ordinary Poincaré-map method generates a vector function $\boldsymbol{F}(\boldsymbol{x})$ and successive approximations satisfying the recursion:

$$\boldsymbol{x}_{n+1} = \boldsymbol{F}(\boldsymbol{x}_n) \tag{2}$$

Suppose that this sequence converges linearly to some fixed point $\tilde{\boldsymbol{x}}$ of $\boldsymbol{F}$. Convergence might be slow. Hence we are interested in accelerating convergence using an acceleration method.

4.1 Accelerated Poincaré-map method

An acceleration method operates on the first k vectors of a sequence $\{\boldsymbol{x}_n\}$, and produces an approximation $\boldsymbol{y}$ to the limit of $\{\boldsymbol{x}_n\}$. This approximation can then be used to restart (2) and generate the beginning of a new sequence $\boldsymbol{y}_0, \boldsymbol{y}_1, \boldsymbol{y}_2, \ldots$. Again, the acceleration method can be applied to this new sequence, resulting in a new approximation $\boldsymbol{z}$ of the limit. The idea is that the sequence $\boldsymbol{x}, \boldsymbol{y}, \boldsymbol{z}, \ldots$ converges much faster to the limit of $\{\boldsymbol{x}_n\}$ than the sequence $\{\boldsymbol{x}_n\}$ itself. Typically, if $\{\boldsymbol{x}_n\}$ converges linearly, then $\{\boldsymbol{x}, \boldsymbol{y}, \boldsymbol{z}, \ldots\}$ converges super-linearly.

In [5] the accelerated Poincaré-map method is based on the well-known Minimal Polynomial Extrapolation (MPE) method [7, 15]. The method can be proven to be equivalent to Reduced Rank Extrapolation.

With MPE one determines the best approximation for the successive corrections in a subspace that is built similarly as in Arnoldi methods for solving systems. We use the (unaccelerated) Poincaré-map algorithm to produce a sequence of approximations from which the subspace spanned by the corrections is built. It is assumed that all these approximations have an error that is bounded by the error of the first one. When the subspace is large enough we can define a best approximation (a mean value) that has an accuracy that is the square of the starting one. Using this new approximation a restart means that we accelerate the Poincaré-map method.
When the subspace spanned by the corrections is large enough the next correction can be viewed

to be within this subspace. Then we have a linear combination of corrections that is zero due to linear dependency. This linear combination has a crucial application. If we express the corrections in terms of lower and higher order effects we observe that the sum of the lower order effects nearly cancels [15].
The weighted mean of the last approximations using the weights in this linear combination provides the higher accurate extrapolation.

4.2 Simulation result

We applied the Accelerated Poincaré method to a Colpitts oscillator[2]. This gave three outer iterations with 4, 3, 2 inner iterations, repspectively, to build each time a subspace in which extrapolation leads to a new estimate for the initial value for the circuit solution and for its period. Fig. 3 shows the errors made in the extrapolation and in the following inner unaccelerated Poincaré iterations (all compared to the last solution). This clearly shows the superlinear convergence of the extrapolation.

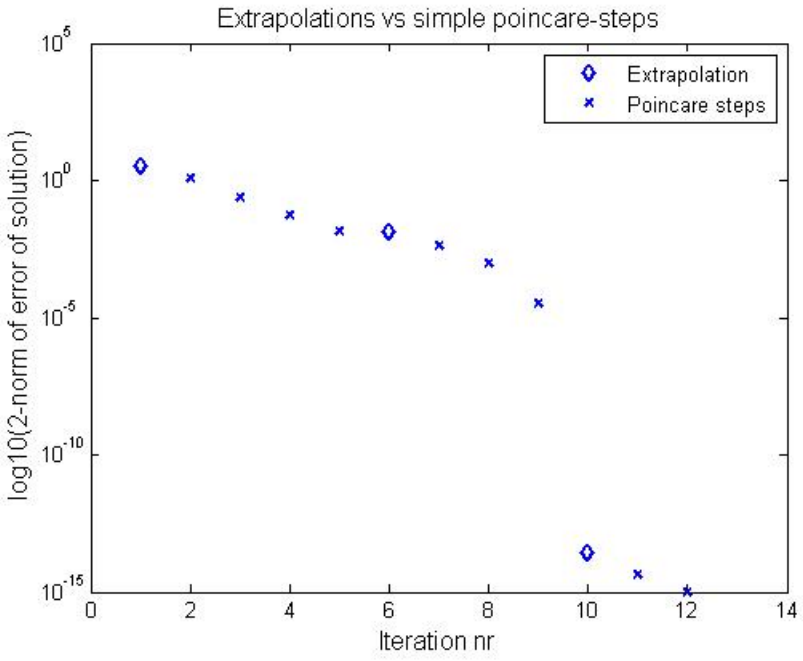

Figure 3: Accelerated Poincaré (outer loop) provides each time a new initial value to which the unaccelerated Poincaré is applied that provides new updates of the initial value. Here we plot the errors compared to the last solution. Each time we check if the subspace is large enough to make an extrapolation.

5 PSS-methods based on generalized eigenvectors

We studied bordered matrices [3, 12] to get an idea how to gauge the Harmonic Balance Jacobian matrix with an extra equation for the additional unknown f. The block part $\mathbf{A}$ belonging

[2]The method has been implemented in Pstar, the in-house analog circuit simulator of NXP Semiconductors

to the driven Harmonic Balance problem becomes badly conditioned when the Newton iterands converge. This is due to the fact that the time derivative of the PSS solution solves the linearized homogeneous circuit equations when being linearized at the PSS solution. Hence when the discretization is exact this time derivative of the ultimate PSS is in the kernel of this block matrix. For the extended, bordered matrix **M** choices of the additional column and of the extra row that are related to the kernel of the Harmonic Balance block matrix and to its transpose generate the most simple expressions for the generalized inverse. However there also is robustness in the sense that if we have other choices then the bordered matrix may still be non-singular. The additional column naturally comes from the partial differentiation with respect to the chosen additional unknown f. The choice of the additional row depends on the "gauge" equation that we add to the system. A choice for a generalized eigenvector (the block matrix actually is a matrix pencil) is best here. As equation we prefer the bi-orthogonality equation. This prevents all problems with determining the location of the oscillation and the range of values of the PSS solution.
Generalized eigenvalue methods for matrix pencils are good candidates for obtaining a dynamic row vector to make the bordered matrix non-singular. Generalized eigenvalue methods are provided by the DPA (Dominant Pole Algorithm) and RQI (Raleigh Quotient Iteration) [14]. We used a combination of these methods (SARQI) to obtain a good accuracy and convergence rate and to select the proper vectors. We approximate the bi-orthogonality relation by replacing one eigenvector by the time derivative of the circuit solution (Newton iterand). First results have been published in [13, 16]. Fig. 4 shows typical results where the new dynamic equation provides automatically a good gauging, while the existing phase equations assume knowledge of the solution (range of values, location in the circuit). A wrong value may even prevent convergence.

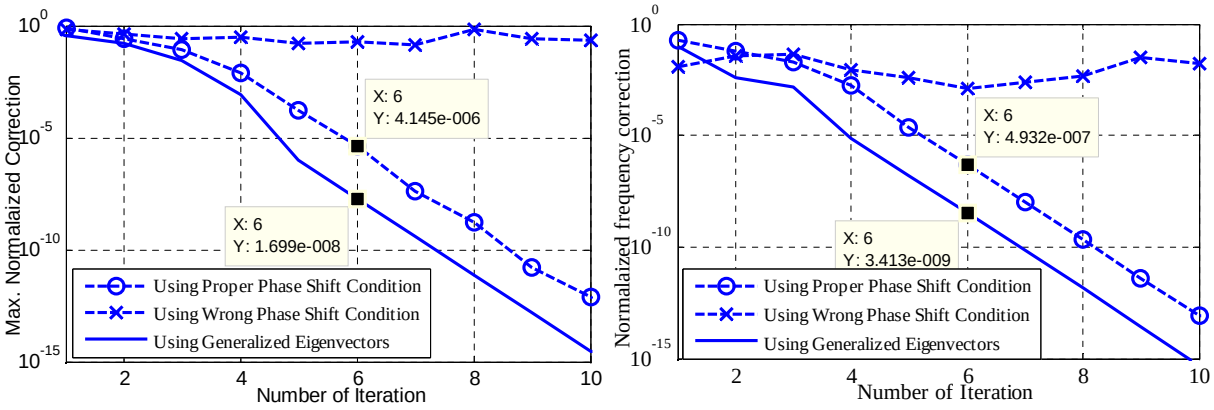

Figure 4: Maximum of the normalized correction and normalized frequency correction for each iteration for different methods.

6 Conclusions

The purpose of the task T2.3 was to obtain initial estimates for Harmonic Balance for free-running, autonomous, oscillators. We exploited techniques from transient analysis to obtain good initial estimates for the oscillation frequency and for the circuit solution to start the HB-

based oscillator analysis. The developed techniques, called "FFT" and "ZeroC", have been implemented in the industrial, commercially available APLAC simulator during H1/2010 and will later be available to designers using AWR (and APLAC) software. These new features have been tested on a large set of industrial problems, and the results have been good: faster convergence and improved robustness of the new approaches are greatly improving the quality of the HB based oscillator analysis. The methods implemented during this project also enable further research and improvements for the algorithms once we have more feedback based on real design problems.

Some cases showed that even more accurate estimates are necessary while also the robustness of the Newton method must be increased. Hence as first step we next described how modern subspace techniques can be used that allow for vector extrapolation within an iterative framework. This was demonstrated by the Accelerated Poincaré-map Method. By this we can improve the accuracy of the initial estimates.

To address the robustness of the Newton method we studied new techniques from bordered matrices and eigenvalue methods to improve Newton methods for Finite Difference in the time domain as well as for Harmonic Balance and for improving methods based on optimization. The new method gauges the phase shift automatically. No assumption about the range of values of the PSS solution is needed. Both the theoretical background and some early simulation results have been presented.

Parts of this report have been presented at the ECMI-2010 (European Consortium for Mathematics in Industry) and SCEE-2010 (Scientific Computing in Electrical Engineering) conferences. Full papers [6, 13, 16] have been submitted to the post-conference proceedings.

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