INVESTIGATION OF THE TIME-SAMPLE SELECTION FOR MULTITONE HARMONIC BALANCE SIMULATION

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Abstract The selection of time samples for multitone harmonic balance (HB) simulation is investigated in this report. An approach proposed by Kundert, Sorkin and Sangiovanni-Vincentelli, a gradient-based optimization selection approach and a Monte Carlo selection approach are discussed in detail. These approaches are demonstrated in a numerical example. The example exposes their advantages and disadvantages.

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I. INTRODUCTION

The harmonic balance (HB) technique has been widely accepted as an efficient tool for nonlinear microwave circuit simulation [1]. Most of the HB applications so far are in single tone situations. Multitone HB simulation is not usually an easy extension of the single tone case, since the normal discrete Fourier transformation (DFT) used in single tone HB simulation can not be applied directly to multitone cases.

Kundert, Sorkin and Sangiovanni-Vincentelli [2] recently proposed an approach to selecting time-sample points for the Fourier transformation (FT) suitable in multitone HB simulation. The KSSV approach exploits the relationship between the orthogonality and the condition number of a matrix, and can substantially improve the condition of the FT matrix while requiring theoretically a minimal number of the time samples. For K frequencies in the HB equation (including 0) only 2K-1 time samples are needed for FT.

In this report, we investigate the numerical behaviour of the KSSV approach. We will compare KSSV with two other approaches: a gradient-based optimization approach and a Monte Carlo approach which is a modified form of KSSV. Our numerical example presents the average condition numbers of the FT coefficient matrices, standard deviations of the condition numbers, CPU time, etc.

II. MULTITONE FOURIER TRANSFORMATION

Following the KSSV notation [2], let λ_i, i=1, .., d, be the fundamental frequencies of the circuit to be simulated. The actual frequencies ω_0, ω_1, ..., ω_{K-1} included in the HB equation can be determined either by

$$\{\omega \mid \omega = k_1\lambda_1 + k_2\lambda_2 + \ldots + k_d\lambda_d,\ k_j = 0, \pm 1, .., \pm H, \text{ for } j=1, \ldots, d\} \tag{1}$$

or,

$$\{\omega \mid \omega = k_1\lambda_1 + k_2\lambda_2 + \ldots + k_d\lambda_d,\ \sum_{j=1}^{d} |k_j| = 0, \pm 1, .., \pm H, \text{ for } j=1, \ldots, d\} \tag{2}$$

which correspond to the two truncation methods in [2]. We organize the frequencies such that

$\omega_0=0$, and $0<\omega_1< \ldots <\omega_{K-1}$.

Denote Γ^{-1} to be the IFT (inverse FT) coefficient matrix. It is shown in [2] that a minimal number of S=2K-1 time samples are needed to form Γ^{-1}, i.e.,

$$\Gamma^{-1} = \begin{bmatrix} 1 & \cos\omega_1 t_1 & \sin\omega_1 t_1 & \ldots & \cos\omega_{K-1} t_1 & \sin\omega_{K-1} t_1 \\ 1 & \cos\omega_1 t_2 & \sin\omega_1 t_2 & \ldots & \cos\omega_{K-1} t_2 & \sin\omega_{K-1} t_2 \\ 1 & \cos\omega_1 t_3 & \sin\omega_1 t_3 & \ldots & \cos\omega_{K-1} t_3 & \sin\omega_{K-1} t_3 \\ \ldots & \ldots & \ldots & \ldots & \ldots & \ldots \\ 1 & \cos\omega_1 t_S & \sin\omega_1 t_S & \ldots & \cos\omega_{K-1} t_S & \sin\omega_{K-1} t_S \end{bmatrix}$$

or

$$\Gamma^{-1} = [\mathbf{a}_1 \ \mathbf{a}_2 \ \ldots \ \mathbf{a}_S]^T \tag{3}$$

where

$$\mathbf{a}_j = [1 \quad \cos\omega_1 t_j \quad \sin\omega_1 t_j \quad \ldots \quad \cos\omega_{K-1} t_j \quad \sin\omega_{K-1} t_j]^T \tag{4}$$

with $K=\mathbf{a}_j^T\mathbf{a}_j$. The FT coefficient matrix Γ can be uniquely determined if S time samples are chosen such that Γ^{-1} is nonsingular.

The multitone HB simulation can be performed with FT and IFT as

$$\Gamma \mathbf{x} = \mathbf{X}$$

and

$$\Gamma^{-1} \mathbf{X} = \mathbf{x}$$

where

$$\mathbf{X} = [X_0 \quad X_1^C \quad X_1^S \ \ldots \ X^C_{K-1} \quad X^S_{K-1}]^T,$$

$$\mathbf{x} = [x(t_1) \quad x(t_2) \ \ldots \ x(t_S)]^T$$

represent frequency domain and time domain variables, respecitively, superscripts C and S denote the real and imaginary parts, respectively, and t_j, j=1, ..., S, are time samples.

Define the ℓ_∞ norm of a N×N matrix B to be [3]

$$\| B \|_\infty = \max_i \{ \sum_{j=1}^{N} | b_{ij} | \ \}$$

The condition of B can be determined by the condition number

$$\kappa(B) = \| B \|_\infty \| B^{-1} \|_\infty. \tag{5}$$

Obviously the accuracy of FT and IFT depends mostly on the conditioning of the coefficient matrices. But in multitone HB simulation, unfortunately, $\kappa(\Gamma^{-1})$ varies widely with different time sample selection strategies. The evenly spaced time sample selection common to DFT generally results in a very ill-conditioned Γ^{-1}. Numerical errors then dominate the HB simulation. A time sample selection approach is desirable which lowers $\kappa(\Gamma^{-1})$ as much as possible.

III. THE KSSV APPROACH [2]

Consider Γ^{-1} as an S-dimensional linear space spanned by $\{\mathbf{a}_1, \mathbf{a}_2, ..., \mathbf{a}_S\}$. A set of orthogonal base vectors $\{\bar{\mathbf{a}}_1, \bar{\mathbf{a}}_2, ..., \bar{\mathbf{a}}_S\}$ can be formed by

$$\bar{\mathbf{a}}_j = \mathbf{a}_j - \sum_{k=1}^{j-1} \frac{\mathbf{a}_j^T \bar{\mathbf{a}}_k}{\bar{\mathbf{a}}_k^T \bar{\mathbf{a}}_k} \bar{\mathbf{a}}_k \quad \text{for } j=1, ..., S. \tag{6}$$

It is shown in [2] that the upper bound of $\kappa(\Gamma^{-1})$ is S^2/α, where $\alpha=\min\{\|\bar{\mathbf{a}}_j\|_2/\sqrt{K},\ j=1,...,S\}$ and $\|\bullet\|_2$ denotes the Euclidean norm. The KSSV approach is an algorithm which selects S time samples from M=2S random samples uniformly distributed between $(0, 6\pi/\omega_1]$, such that α is as large as possible.

Algorithm

for (s ← 1, ..., M)
{ **random** () returns numbers uniformly distributed between 0 and 1.
$t_s \leftarrow (6\pi/\omega_1)$**random** ()
$\mathbf{a}_s \leftarrow [1 \quad \cos\omega_1 t_s \quad \sin\omega_1 t_s \quad ... \quad \cos\omega_{K-1} t_s \quad \sin\omega_{K-1} t_s]^T$
}
for (s ← 1, ..., M)
{ $\bar{\mathbf{a}}_s \leftarrow \mathbf{a}_s$
}
for (r ← 1, ..., S)
{ **argmax**() returns the index of the largest member of a set.

k = **argmax**($\{\| \bar{\mathbf{a}}_s \| : r \le s \le M\}$)

swap($\mathbf{a}_r, \mathbf{a}_k$)

swap($\bar{\mathbf{a}}_r, \bar{\mathbf{a}}_k$)

swap(t_r, t_k)

for ($s \leftarrow r+1, \ldots, M$)

$$\bar{\mathbf{a}}_s \leftarrow \bar{\mathbf{a}}_s - \frac{\mathbf{a}_s^T \bar{\mathbf{a}}_r}{\bar{\mathbf{a}}_r^T \bar{\mathbf{a}}_r} \bar{\mathbf{a}}_r$$

}

The KSSV algorithm for time sample selection is simple and elegant. It can drastically reduce $\kappa(\Gamma^{-1})$ compared with evenly spaced time sample selection.

IV. GRADIENT-BASED OPTIMIZATION APPROACH

Employing the theoretical principle of KSSV, we could use gradient-based optimization to minimize the upper bound of $\kappa(\Gamma^{-1})$. Specifically, we can formulate the time sample selection problem as the following minimax optimization problem

$$\min_{\mathbf{t}} \max_{j \in J} \{ K - \bar{\mathbf{a}}_j^T \bar{\mathbf{a}}_j \} \tag{7}$$

where

$$\mathbf{t} = [t_1 \; t_2 \; \ldots \; t_S]^T$$

$$J = \{2, \ldots, S\}.$$

Notice that in (7) we take $\mathbf{a}_1$ as a reference vector, $\bar{\mathbf{a}}_j$ is a function of t_k, $k=1, \ldots, j$, and $K=\mathbf{a}_j^T \mathbf{a}_j$, $j=1, \ldots, S$. The minimum possible objective function value zero can only be obtained if $\mathbf{a}_i$ and $\mathbf{a}_j$ are orthogonal, for $i, j=1, \ldots, S$ and $i \neq j$.

The analytical gradient of the individual functions in (7)

$$K - \bar{\mathbf{a}}_j^T \bar{\mathbf{a}}_j, \text{ for } j = 2, \ldots, S$$

can be easily derived. The analytical form of the gradient calculation is not only efficient compared with the perturbation method, but also crucial to the success of (7) in situations when

two or more fundamental frequencies are located closely. For instance, in a two tone situation with $\omega_1 = \lambda_2 - \lambda_1$, the time sample t_j changing on the order of ω_1/λ_1 can significantly affect $\mathbf{a}_j$. The optimization steps for time samples are expected to be on the order of ω_1/λ_1, therefore making the accuracy of the gradient very important when ω_1/λ_1 is very small.

Compared with KSSV, this optimization approach should theoretically be better because of its feature of continuous optimization, or "fine tuning". However, due to the nature of Γ^{-1}, the objective function in (7) suffers seriously from local minima. Besides, it requires much more memory, especially for the implementation of the analytical gradient. The computational effort is also far greater than what is needed for KSSV.

V. MONTE CARLO APPROACH

It is intuitive from KSSV that if we increase the number of base sample points, i.e., increase the size of M, a better result should be reached, provided that the physically allowed memory size is large enough and available. When limited by memory, we can modify KSSV to accommodate iterative the Monte Carlo approach. The algorithm is as follows.

Algorithm

loop:

{ **if** (first iteration)

{ **for** ($s \leftarrow 1, \ldots, M$)

{ **random** () returns numbers uniformly distributed between 0 and 1.

$t_s \leftarrow (6\pi/\omega_1)$ **random** ()

$\mathbf{a}_s \leftarrow [1 \quad \cos\omega_1 t_s \quad \sin\omega_1 t_s \quad \ldots \quad \cos\omega_{K-1} t_s \quad \sin\omega_{K-1} t_s]^T$

}

select ()

$\bar{a}_{min} \leftarrow \bar{\mathbf{a}}_S{}^T \bar{\mathbf{a}}_S$

$\bar{a}_{max} \leftarrow \bar{a}_{min}$

copy ($\mathbf{a}_j \rightarrow \mathbf{a}_{j\ back}$, for j=1, ..., S)

copy ($t_j \rightarrow t_{j\ back}$, for j=1, ..., S)

}

else

{ **for** ($s \leftarrow S+1, \ldots, M$)

{ **random** () returns numbers uniformly distributed between 0 and 1.

$t_s \leftarrow (6\pi/\omega_1)$ **random** ()

$\mathbf{a}_s \leftarrow [1 \quad \cos\omega_1 t_s \quad \sin\omega_1 t_s \quad \ldots \quad \cos\omega_{K-1} t_s \quad \sin\omega_{K-1} t_s]^T$

}

select ()

$\bar{a}_{min} \leftarrow \bar{\mathbf{a}}_S{}^T \bar{\mathbf{a}}_S$

if ($\bar{a}_{max} < \bar{a}_{min}$)

{ $\bar{a}_{max} \leftarrow \bar{a}_{min}$

copy ($\mathbf{a}_j \rightarrow \mathbf{a}_{j\ back}$, for j=1, ..., S)

copy ($t_j \rightarrow t_{j\ back}$, for j=1, ..., S)

}

else

{ **copy** ($\mathbf{a}_{j\ back} \rightarrow \mathbf{a}_j$, for j=1, ..., S)

copy ($t_{j\ back} \rightarrow t_j$, for j=1, ..., S)

}

} **until** ($\bar{a}_{max} \geq$ *goal*) or (specified maximum number of iteration has been reached)

{ **copy** ($\mathbf{a}_{j\ back} \rightarrow \mathbf{a}_j$, for j=1, ..., S)

copy ($t_{j\ back} \rightarrow t_j$, for j=1, ..., S)

}

where the procedure **select**() is defined as

select ()

{ **for** ($s \leftarrow 1, \ldots, M$)

{ $\bar{\mathbf{a}}_s \leftarrow \mathbf{a}_s$

}

for ($r \leftarrow 1, \ldots, S$)

{ **argmax**() returns the index of the largest member of a set.

$k =$ **argmax**($\{\| \bar{\mathbf{a}}_s \| : r \leq s \leq M\}$)

swap($\mathbf{a}_r, \mathbf{a}_k$)

swap($\bar{\mathbf{a}}_r, \bar{\mathbf{a}}_k$)

swap(t_r, t_k)

for ($s \leftarrow r+1, \ldots, M$)

$$\bar{a}_s \leftarrow \bar{a}_s - \frac{\bar{a}_s^T \bar{a}_r}{\bar{a}_r^T \bar{a}_r} \bar{a}_r$$

}

}.

The foregoing Monte Carlo approach is more objective and efficient than simply repeating the basic KSSV approach, since it employs random optimization concept and utilizes the time samples in a wider combination. Compared with gradient-based optimization, it does not have the local minimum problem, needs much less memory and much less CPU time.

VI. NUMERICAL EXAMPLE

In this example, we select time samples for Γ^{-1} as follows: equally spaced, randomly chosen, time samples obtained by KSSV, gradient-based optimization (GBO), and a Monte Carlo method (MC). The condition number $\kappa(\Gamma^{-1})$ and its statistics are demonstrated.

For simplicity, we consider a two-tone situation with λ_1=10GHz and λ_2=10.001GHz. The actual frequencies taken in the HB equation are determined by (2) in Section II. Except for evenly spaced time sampling, each approach is applied ten times to generate approximate statistics. M=2S and 3S are used for KSSV and MC. To reduce the chance of a large local minimum, GBO takes the solution of KSSV (with M=2S) as a starting point, and due to excessive CPU time and memory size, GBO is not applied when H>6. The iteration limit is fifteen for GBO and six for MC when M=2S and M=3S, respectively. All the computations are done on a VAX 6420 machine using double precision.

Tables I to V show the results. The following observations can be made.

(1) Evenly spaced time samples used in DFT is not suitable for multitone HB simulation. Simple random time sample selection generates much better conditioned Γ^{-1} than evenly spaced time sampling.

(2) When M=2S, KSSV significantly improves the condition of Γ^{-1} over evenly spaced or

random time sample selection.

(The foregoing observations are consistent with the results of Kundert et al. [2].)

(3) Obvious improvement is achieved for KSSV when M is increase from 2S to 3S.

(4) MC provides much better and, more importantly, consistent results than KSSV, though it needs extra CPU time.

(5) GBO improves the results of KSSV when M=2S. However, due to the local minimum problem, the overall performance is similar to KSSV when M=3S, but worse than MC. Its CPU time requirement makes it unacceptable when H>4.

VII. CONCLUSIONS

In this report, time sample selection for multitone harmonic balance (HB) simulation has been investigated. Besides the approach of Kundert, Sorkin and Sangiovanni-Vincentelli (KSSV), gradient-based optimization selection (GBO) and Monte Carlo selection (MC) have been presented. A numerical example verifies that KSSV is quite feasible, and MC can further improve the conditioning of Γ^{-1} and can provide more consistent results than KSSV at the cost of increased CPU time.

REFERENCES

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TABLE I

AVERAGE CONDITION NUMBER OF Γ^{-1}

H	EVEN	RANDOM	KSSV M=2S	GBO	MC M=2S	KSSV M=3S	MC M=3S
1	6.1×10^{16}	34	10	7	6	8	6
2	9.6×10^{8}	629	29	18	17	22	16
3	5.4×10^{26}	2.8×10^{3}	69	43	37	46	32
4	6.6×10^{12}	4.0×10^{3}	111	96	65	96	54
5	4.5×10^{11}	6.8×10^{3}	194	142	95	133	88
6	5.8×10^{14}	1.2×10^{5}	324	217	151	192	127
7	1.1×10^{20}	2.0×10^{5}	423	N/A	203	246	181
8	7.0×10^{14}	2.0×10^{5}	644	N/A	250	390	229

TABLE II

STANDARD DEVIATION OF
THE CONDITION NUMBER OF Γ^{-1}

H	EVEN	RANDOM	KSSV M=2S	GBO	MC M=2S	KSSV M=3S	MC M=3S
1	0	20	3	1	1	2	0
2	0	688	8	3	1	5	1
3	0	4.7×10^{3}	18	13	7	14	4
4	0	5.1×10^{3}	27	21	10	30	6
5	0	3.6×10^{3}	38	12	12	17	10
6	0	2.7×10^{5}	59	34	21	46	18
7	0	2.8×10^{5}	92	N/A	38	33	25
8	0	4.3×10^{5}	140	N/A	31	103	43

TABLE III

CPU TIME FOR OBTAINING Γ^{-1}
(SECOND)

H	EVEN	RANDOM	KSSV M=2S	GBO	MC M=2S	KSSV M=3S	MC M=3S
1	0.00	0.00	0.01	0.09	0.03	0.01	0.03
2	0.01	0.01	0.04	1.01	0.16	0.06	0.25
3	0.05	0.05	0.20	9.17	0.97	0.33	1.60
4	0.17	0.17	0.83	55.8	4.09	1.34	6.96
5	0.51	0.51	2.67	253	12.5	4.12	22.3
6	1.31	1.31	7.32	895	36.1	11.2	60.4
7	3.03	3.03	16.9	N/A	84.1	26.2	142
8	6.25	6.25	35.2	N/A	173	55.1	292

TABLE IV

MINIMUM CONDITION NUMBER OF Γ^{-1}

H	EVEN	RANDOM	KSSV M=2S	GBO	MC M=2S	KSSV M=3S	MC M=3S
1	6.1×10^{16}	11	5	5	5	5	5
2	9.6×10^{8}	72	19	15	15	17	14
3	5.4×10^{26}	299	40	30	27	27	27
4	6.6×10^{12}	813	75	70	50	66	46
5	4.5×10^{11}	1.9×10^{3}	147	124	80	99	76
6	5.8×10^{14}	3.6×10^{3}	226	166	130	141	97
7	1.1×10^{20}	3.0×10^{4}	318	N/A	160	195	148
8	7.0×10^{14}	1.6×10^{4}	500	N/A	208	265	174

TABLE V

MAXIMUM CONDITION NUMBER OF Γ^{-1}

H	EVEN	RANDOM	KSSV M=2S	GBO	MC M=2S	KSSV M=3S	MC M=3S
1	6.1×10^{16}	77	15	10	7	12	7
2	9.6×10^{8}	2.4×10^{3}	43	23	19	35	18
3	5.4×10^{26}	1.6×10^{4}	93	75	49	68	38
4	6.6×10^{12}	1.8×10^{4}	146	136	83	162	65
5	4.5×10^{11}	1.2×10^{4}	250	163	112	155	102
6	5.8×10^{14}	8.9×10^{5}	417	263	192	307	147
7	1.1×10^{20}	9.2×10^{5}	626	N/A	278	314	242
8	7.0×10^{14}	1.4×10^{6}	913	N/A	324	576	310