A Broad-Band Adaptive-Frequency-Sampling Approach for Microwave-Circuit EM Simulation Exploiting Stoer–Bulirsch Algorithm

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***Abstract*—In traditional adaptive frequency sampling (AFS) techniques, it is inevitable to invert an $N \times N$ matrix in order to solve for the coefficients of targeted rational interpolation functions, where N is the number of samples. The ill-conditioned matrix of a large N restricts traditional AFS techniques to an electromagnetic simulation accelerator for a circuit with few poles or narrow bandwidth responses. In this paper, the general Stoer–Bulirsch (S–B) algorithm is employed in developing a new AFS scheme (S–B AFS). Since the S–B algorithm is a recursive tabular method and requires no matrix inversion, it can process a large number of sampling data for obtaining a rational interpolation function without suffering from singularity problems. This attribute virtually leads the proposed AFS approach to an ultra broad-band interpolation with a single rational function. The new proposed approach greatly improves the efficiency of the traditional AFS techniques and simplifies the AFS process. In order to enable the S–B algorithm to be used in the proposed S–B AFS approach, three legitimate grid paths for constructing two pairs of complementary rational models are being proposed in this paper for modeling a general microwave circuit. Four practical broad-band examples are given to demonstrate the effectiveness of the S–B AFS, including waveguide harmonic filters, a waveguide diplexer, and a broad-band microstrip diplexer.**

***Index Terms*—Adaptive frequency sampling (AFS), Cauchy method, electromagnetic (EM) simulation, Stoer–Bulirsch (S–B) algorithm.**

I. Introduction

WITH THE increase of complexity and scale of microwave circuits to be simulated by computer, electromagnetic (EM) simulation is never fast enough to meet the tight design schedule. This situation becomes even more severe when details of a broad-band response of a microwave circuit need to be understood, for which hundreds or even thousands of EM simulation sampling data are required. One effective method that alleviates the predicament is to interpolate the required data by analytic model-based functions [1]. Among them, it has been practically proven that the rational function is versatile, effective, and apposite for being used as the fitting model (FM) for microwave-circuit EM simulation.

Various methods have been proposed to determine the orders and coefficients of an appropriate rational function for a given microwave circuit. When the derivative information of a given expansion point is available, the Padé method [2] can be used to do the rational function interpolation and extrapolation. The Cauchy method [3]–[10] is another popular method for rational function interpolation. It is derivative free and is, therefore, more applicable to those general-purpose EM simulation tools. Lehmensiek and Meyer proposed a rational interpolation models for microwave circuits by using a Thiele-type branched continued fraction and extended this method to multi-dimensional cases [6].

How to effectively and accurately estimate the orders of the required rational function and determine its coefficients has drawn a great deal of attention from researchers. Adaptive frequency sampling (AFS) is an effective technique to do the work by adaptively selecting EM sampling points [11]. One of the desired features of an AFS technique is to obtain the desired rational function with the least EM simulation overhead. Several possible AFS strategies were introduced in [5]. In practice, there are two approximate rational function models required in each of iterative steps. The two different models can be constructed either by using different analytical functions with the same set of samples or by using different samples with the same function. With the increase of the number of samples, the difference between the two models will decrease. When a termination criterion is satisfied, any one of the two approximate models can be used as the interpolation model. Theoretically, convergence of this iterative process is guaranteed provided that both of these two approximate models will be close to the desired curve as much as expected. However, numerical error always arises with the increase of the number of samples because of the resultant ill-conditioned matrix whose inverse needs to be calculated.

Singular value decomposition (SVD) is used to obtain the coefficients and estimate the orders of the polynomials by solving the matrix inversion directly [4]. In practice, when the total number of samples is large, the rational function model directly

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solved becomes unreliable because of the likely independence of a large number of samples. The sub-zoning technique [5], [7], [9] is a remedy to such an over-sampling problem. In this technique, the whole frequency range is divided into multiple sub-zones so that the number of samples required in each of sub-zones can be kept small. The adjacent sub-zones can also be overlapped [11] to ensure the continuity of derivatives. Nevertheless, it is always highly desired that there is a truly broad-band AFS method that is singularity worry free. Strictly speaking, a truly broad-band AFS method should possess the following two attributes: 1) the information of each of the function samples should contribute to the rational function model of the entire frequency range, no matter how broad the frequency range is (in other words, all samples should be global and there is only one rational function model within the frequency range of interest) and 2) the method is singularity free and requires no matrix inversion such that virtually unlimited number of function samplings can be incorporated in the model.

In this paper, the Stoer–Bulirsch (S–B) algorithm for rational interpolation is employed to develop a new AFS approach (hereafter referred to as the S–B AFS) for accelerating full-wave EM simulation of a microwave circuit. Since the S–B algorithm is a recursive tabular method and requires no matrix inversion, it can process a large number of samples to obtain a rational interpolation function without suffering from singularity problems. As a result, the S–B AFS can virtually lead to a broad-band rational interpolation by a single FM. This unique feature greatly improves the efficiency of existing AFS schemes and simplifies the AFS process. The most attractive feature of the S–B algorithm is its flexibility in constructing a large range of rational functions with polynomials of any order. It is this feature that enables construction of the proposed S–B AFS scheme, in which two different rational function models are required to check the convergence. It will be shown in this paper that the diagonal rational recursive interpolation algorithm mentioned in [9] is only one of the special cases of the S–B algorithm. In order to effectively apply the S–B algorithm to the proposed AFS scheme, three legitimate grid paths that correspond to two pairs of complementary rational function models are being proposed in this paper for modeling a general microwave circuit.

Four representative and practical examples of microwave circuits are presented in this paper to demonstrate the effectiveness and strength of the proposed S–B AFS algorithm, emphasizing the broad-band applications. It will be shown that the new S–B AFS algorithm can greatly reduce the effort of a full-wave EM simulation by up to a order of magnitude and improve the efficiency of existing AFS-like interpolation schemes by over 30% for a typical broad-band EM simulation, as far as the responses of a fine resolution are concerned.

II. Theory of the S–B AFS Technique

A rational function can be defined as a ratio of two polynomials $A(f)$ and $B(f)$ by

$$R(f) = \frac{A(f)}{B(f)} = \frac{\sum_{i=0}^{p} a_i f^i}{1 + \sum_{j=1}^{q} b_j f^j} = \frac{\mathrm{Deg}(p)}{\mathrm{Deg}(q)} \tag{1}$$

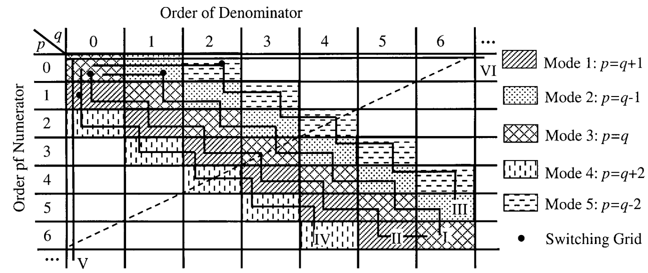


Fig. 1. Grid paths of possible rational functions of FMs.

where $\mathrm{Deg(N)}$ represents a polynomial of order N. Theoretically, for given orders of p and q, the coefficients $\{a_i; i = 0, \ldots, p\}$ and $\{b_j; j = 1, \ldots, q\}$ can be determined from $p + q + 1$ samples of $R(f)$ by solving a set of linear equations.

A. FMs

In this paper, rational functions with different orders of p and q are investigated as FMs. In Fig. 1, each grid represents a rational function, whose orders of denominator and numerator are given by the values in the first row (q) and the first column (p), respectively. For example, the grids locate on the back diagonal dash line in Fig. 1 denote all the possible FMs with $p + q + 1$ equals to 7.

If the number of samples is given, there are a number of possible FMs as long as the sum of p and q is less than the number of samples by one. However, the best FM that characterizes the objective response in physics will be with the least number of samples. Hence, the first step of an AFS scheme is to select the FM that can best present the objective system.

The frequency response of a linear circuit is basically determined by its system zeros and poles. It can be shown that the impedance (or admittance) transfer functions of a passive linear circuit can be characterized by a partial fraction expansion [14]. Each term of the expansion represents the behavior of the system transfer impedance (or admittance) function at a system pole, which may be the pole at the zero frequency, the infinite frequency, or an intermediate pole.

In light of the above-mentioned fact, the frequency response of a passive microwave circuit can most likely be approached by three models: *model 1*, in which $p = q + 1$, *model 2*, in which $p = q - 1$, and *model 3*, in which $p = q$. Other two potential usable models that are close to the three models are *model 4*, in which $p = q + 2$, and *model 5*, in which $p = q - 2$. Different models are represented by grids with different hatch pattern in Fig. 1. Obviously, model 3 is the closest FM to both model 1 and model 2 because it lies between the two models. It is not necessary to constrain the FM being positive real since the fitting-model function is only valid within a limited frequency band.

To check the convergence, an AFS process needs to have two distinct FMs for a given set of samples. The pair of FMs should be close to each other at the end of the whole AFS process. Therefore, when the number of samples is even, model 1 and model 2 can be served as a pair of models because the two models appear on every back diagonal line of even sampling points. By the same token, when the number of samples is odd, model 3 and model 5 are used as a pair of models in the proposed

AFS. When the samples are sufficient, all these four models tend to be converged.

B. Paths of S–B Algorithm in S–B AFS

With the progressive increase of sampling points, a prescribed FM is developed while creeping along a zigzag (or straight) path in Fig. 1. In order to conduct a rational interpolation using the S–B algorithm, a legitimate path needs to be defined. To be discussed below, a path represents a certain combination of different recursive formulas in association with certain step sequences. A path in the proposed S–B AFS must be stipulated by the following two rules.

Rule 1) The number of samples along a path at one grid must be less than that at the next grid by one, which means the trace can only be extended either horizontally or vertically.

Rule 2) Commencing from the switching grid, the main body of a path must be developed in a zigzag manner. It means that the orders of denominator and numerator must be increased by one in turn.

It is apparent that a path must pass through more than two models. For example, path I of Fig. 1 goes through model 2 and model 3; path II passes through model 1 and model 3.

To comply with the stipulations and to incorporate the models in a prescribed recursive fashion, a preparation section of either a horizontal line or a vertical line needs to be developed first. Afterwards, the main body of each of the zigzag paths has to commence from a *switching grid* and goes through two different FMs alternatively. For example, P_1 is the switching grid of path I and P_3 is the switching grid of path III. For path II, its preparation section is zero length. The *terminating grid* of a path corresponds to the final rational function of interpolation.

Stoer and Bulirsch gave a recursive algorithm to conduct interpolation of a rational function of form (1) [12]. This algorithm performs rational interpolation on tabulated data in a recursive manner. The basic theory of the S–B algorithm is outlined here for the sake of completeness.

Suppose that there are a group of samples $\{(f_i, P(f_i), i = 1, \ldots, k\}$ available for obtaining a rational function interpolation of function value $P(f)$ at any $f \in (f_1, f_2)$, whereas the explicit expression of this rational function is unknown. A triangle table shown in Fig. 2 illustrates the recursive process of the S–B algorithm. The recursive algorithm starts with the initial condition

$$R_{i,1} = P(f_i), \qquad i = 1, \ldots, k$$

which constructs the first column of the triangle table. Starting from the second column, all the elements are obtained using a recursive formula associated with two or three elements in the preceding columns. The S–B algorithm provides two "triangle rules"

$$R_{j,k} = \frac{(f - f_j)R_{j+1,k-1} + (f_{j+k} - f)R_{j,k-1}}{f_{j+k} - f_j} \tag{2}$$

and

$$R_{j,k} = \frac{f_{j+k} - f_j}{\dfrac{f - f_j}{R_{j+1,k-1}} + \dfrac{f_{j+k} - f}{R_{j,k-1}}} \tag{3}$$

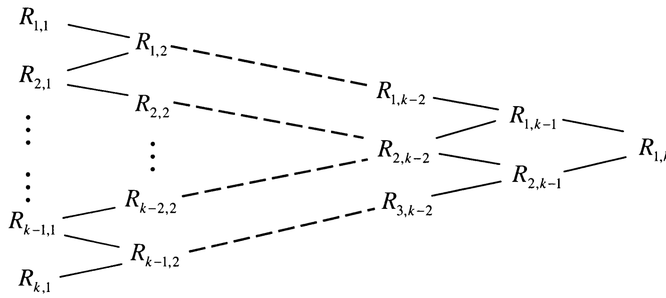


Fig. 2. Tabular chart of the S–B algorithm for rational interpolation.

and one "rhombus rule"

$$R_{j,k} = R_{j+1,k-2} + \frac{f_{j+k} - f_j}{\dfrac{f - f_j}{R_{j+1,k-1} - R_{j+1,k-2}} + \dfrac{f_{j+k} - f}{R_{j,k-1} - R_{j+1,k-2}}}. \tag{4}$$

It can be observed that each element in Fig. 2, except those in the first column, is an interpolated value of a rational function. The order of such a rational function is determined by the number of samples, whereas its coefficients are determined by the value of the samples. Therefore, the elements in the same column represent a group of rational functions of the same order of denominators and numerators.

A complex-coefficient rational interpolation along a path is implemented by using a distinct combination of the above three recursive rules in association with a step sequence. Equations (2) and (3) are used to determine the position of the switching grid of a path. Equation (2), which represents a polynomial interpolation, is used to extend a trace vertically until the switching grid of a model path is reached. On the other hand, (3), which represents an inverse polynomial interpolation, is used to extend a trace horizontally. In this case, only the order of denominator increases. After each of the prescribed paths reaches to the switching grid of its main body, (4) will be used to zigzag along a designated path. Since the switching grid of each path is different, although (4) is used for all the paths, except path V and path VI, the resultant rational function models are different. Three special paths are paths II, V, and VI. There is only one governing equation for each of these paths: (4) for path II, (2) for path V, and (3) for path VI. It's obvious that the diagonal rational interpolation used in [11] only matches to path II and is one of the special cases of the S–B algorithm and path V corresponds to Neville interpolation scheme.

Take path III as an example to illustrate how to use Figs. 1 and 2 and (2) –(4) to construct a recursive algorithm. Since P_3 is the switching grid of path III and its preparation section is a horizontal line, (3) is used first to calculate each of the elements in the second column using two elements in the first column. All the rest of the elements on path III are then calculated using (4).

During the AFS process, the cost of evaluating one interpolation point grows in proportion to $O(N'^2)$, where N' is the number of samples used by an intermediate FM. The whole computational time for establishing the final FM is approximately $O(F \times N^3/6)$, where N is the total number of frequency samples and F is the number of points to evaluate the updated FM.

C. Definitions of Error for the AFS Algorithm

There are two basic problems that need to be addressed in the AFS approach. One is how to keep the iterative process going on and another is when to stop the process. In AFS, both of these problems are controlled by error. There are two types of error that need to be defined in AFS. The error for judging whether or not more samples are required is called convergence error. The error used to locate the next possible sample is called FM error, which ensures a successively adaptive process. A set of testing points is defined in AFS, which is scattered all over the whole frequency band of interest with a sufficiently fine space. The frequency responses of the two FMs are compared at these testing points at each iterative step. The testing point at which the maximum FM error occurs is used as the next sample.

A good definition of the FM error will lead to less required samples. A pertinent definition of the convergence error is a prerequisite for an AFS process since it can avoid the possibilities of under- or over-sampling. Some possible choices for the convergence error area are as follows.

1) Using the FM error as the convergence error.
2) Using the FM error of path II at different iteration steps as the convergence error.
3) Defining a surrogate model error as the convergence error. The surrogate model error is defined by the difference between the rational function value of path I and the actual sampling value from EM simulation at the next possible sample.

The surrogate model error has been practically proven to be a good choice by our numerical experiments. The only payoff of this definition is that it requires one extra sample on top of the maximum number of samples required in the AFS process. Usually, there are more than one complex parameters needed to be modeled for a microwave circuit, such as insertion and return losses. Any one of them can be used to carry out the S–B AFS. After the sampling process ends, all the other parameters can be recovered using the same set of samples.

D. Main Steps for Implementing the S–B AFS Algorithm

It is assumed that the whole frequency band is defined from f_1 to f_2. The FMs corresponding to paths I–III are $P_1(f), P_2(f)$, and $P_3(f)$, respectively. A testing point within the frequency band of interest is f_t and a sample for an FM is f_s. The sampling value from EM simulation or from experiment is $\mathrm{EM}(f_s)$.

Step 1) Setting $f_{s1} = f_1$ and $f_{s2} = f_2$, and acquiring $\mathrm{EM}(f_{s1})$ and $\mathrm{EM}(f_{s2})$.

Step 2) Selecting path I and path II as the FMs and finding the point at which the maximum FM error occurs, say, at point f_{s3}, such that

$$\left|P_1(f_{s3}) - P_2(f_{s3})\right| = \max_i \left(\left|P_1(f_{ti}) - P_2(f_{ti})\right|\right).$$

Step 3) Conducting $\mathrm{EM}(f_{s3})$. If a given error tolerance, which is denoted as EPS, is larger than the FM error in step 2, i.e., $|P_1(f_{s3}) - P_2(f_{s3})| < \mathrm{EPS}$, the process switches to step 6 for termination; otherwise, adds the sample of $\{f_{s3}, \mathrm{EM}(f_{s3})\}$ into the sample collection and goes to next step for finding the next samples.

Step 4) Selecting path I and path III as FMs, comparing the FM values at all testing points, and finding the point at which the maximum FM error occurs, say, at point f_{s4}, such that

$$\left|P_1(f_{s4}) - P_3(f_{s4})\right| = \max_i \left(\left|P_1(f_{ti}) - P_3(f_{ti})\right|\right).$$

Step 5) Having had $\mathrm{EM}(f_{s4})$, if $|P_1(f_{s4}) - P_3(f_{s4})| < \mathrm{EPS}$, which means that the samples obtained are enough for the FM along path I, the process goes to step 6; otherwise, adds the point $\{f_{s4}, \mathrm{EM}(f_{s4})\}$ into the sample collection and goes back to step 2 to find the next samples.

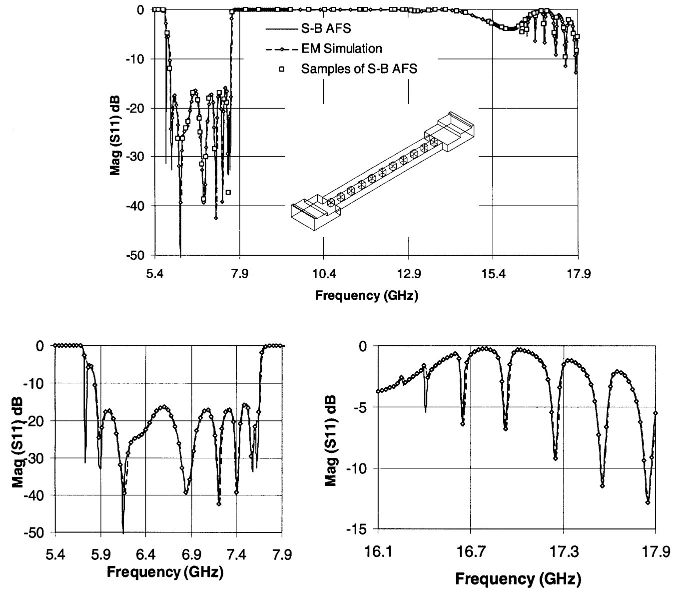
Step 6) Sufficient samples have been acquired for FMs I–III. Saving the sample collection $\{f_{si}, \mathrm{EM}(f_{si}), i = 1, \ldots, N\}$, which is the only required knowledge for rational function interpolation. Note that N is the number of samples in the last step of the AFS.

After an iterative AFS process terminates, three FMs, i.e., paths I–III, should be sufficiently close to each other. In this study, path I is used for interpolating frequency response at any given frequency f.

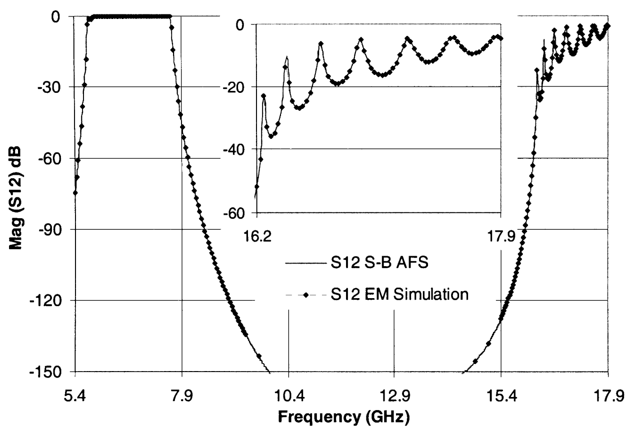
III. Numerical Examples

An 11-pole ridged waveguide filter is investigated as the first example. The response of the filter spans passband, rejection band, and the harmonic passband of the TE_{30} mode. By using the S–B AFS algorithm presented in this paper, only 74 samples are required to establish a single FM of the filter with error tolerance of -80 dB. Notice that the sampling points are selected adaptively across the entire frequency band of interest and that heavier sampling activities happen in the dominant and harmonic passbands. It is interesting to see that, if the frequency range is divided into three, no overlapped sub-zones, i.e., 5.4–7.9, 7.9–15.7, and 15.7–17.9 GHz, the required total number of samples for each sub-zone is 38, 28, and 28, respectively. More than 27% of the sampling points are redundant due to the sub-zoning. The full-wave EM response of 501 samples of equal space is superposed to the response from the S–B AFS FM in Fig. 3(a)–(c), in which very good correlation can be observed. A distinct convergence cutoff point can be observed in the convergence behavior shown in Fig. 4.

The second example is a three-port waveguide diplexer, as shown in Fig. 5. The diplexer consists of two five-pole bandpass filters at the Tx and Rx channels. There are only 33 samples needed to obtain the S–B AFS FM of the scattering transfer function with error tolerance of -60 dB. The magnitude of interpolated frequency responses from the S–B AFS FM are compared with those of the original EM model with 501 equal spaced samples. As shown in Fig. 6, the responses of the two models match very well. The behavior of error convergence of the AFS modeling is given in Fig. 7.



(a)



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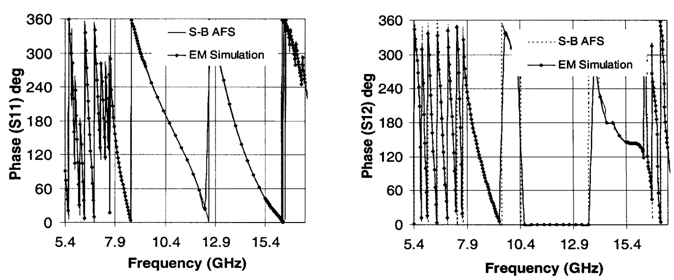

(c)

Fig. 3. (a) Magnitude of $S11$ of an 11-pole waveguide filter calculated by S–B AFS and full-wave EM simulation with 501 samples. (b) Magnitude of $S12$ of an 11-pole waveguide filter calculated by S–B AFS and full-wave EM simulation with 501 samples. (c) Phase of an 11-pole waveguide filter calculated by S–B AFS and full-wave EM simulation with 501 samples.

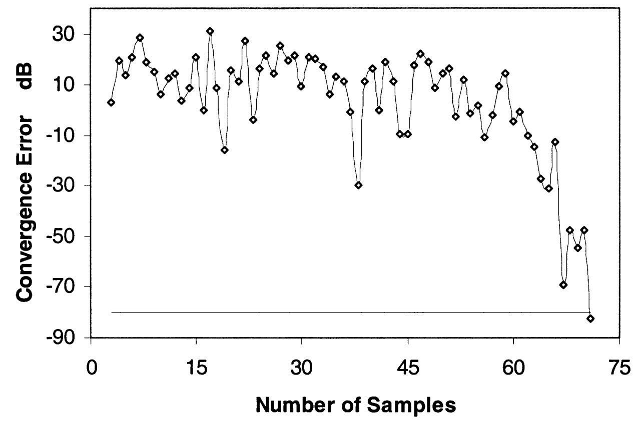

Fig. 4. Convergence error of the S–B AFS for an 11-pole waveguide filter.

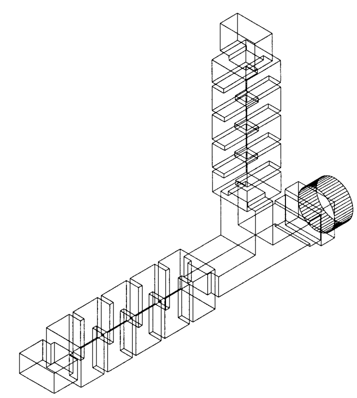

Fig. 5. Waveguide diplexer with two five-pole bandpass filters at Tx and Rx channels and a rectangular-to-circular waveguide transition at the common port.

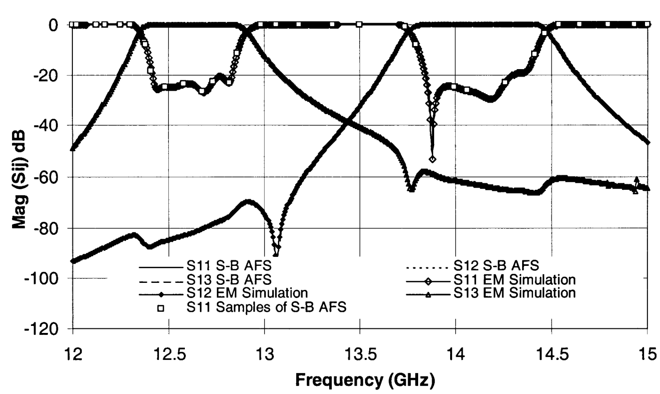

Fig. 6. Magnitude of S-parameters of a waveguide diplexer calculated by the S–B AFS and full-wave EM simulation with 501 samples.

An effective simulation scheme was introduced in [15] to predict hidden spurious harmonic modes of corrugated low-pass waveguide filter. The hidden ansymmetric harmonic modes can be excited by placing an H-plane waveguide bent at both the input and output ports. In practical application, people need to accurately know the level and locations of spikes of the harmonic modes. The application of an effective AFS modeling can greatly reduce the overhead of a full-wave EM simulation that requires more than 1000 sampling points to identify the spikes. As shown in Fig. 8, with the S–B AFS introduced in this paper, the response across the whole frequency band can be interpolated by only one rational function with 314 sampling points. It would be very difficult for any one of the traditional AFS algorithms to model such a broad-band response with only one FM since an inversion of a severe ill-conditioned matrix is inevitable. A quantitative description is given in Fig. 9 to present the error of the example between the EM model and the FM recovered by the S–B AFS. The maximum error of the FM is below 0.08 (absolute value of S-parameters). It is found that

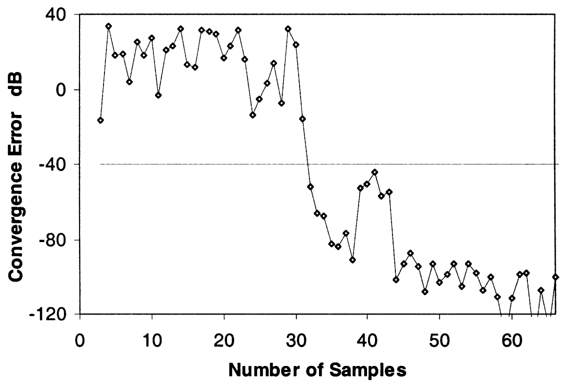

Fig. 7. Convergence error of the S–B AFS for the waveguide diplexer.

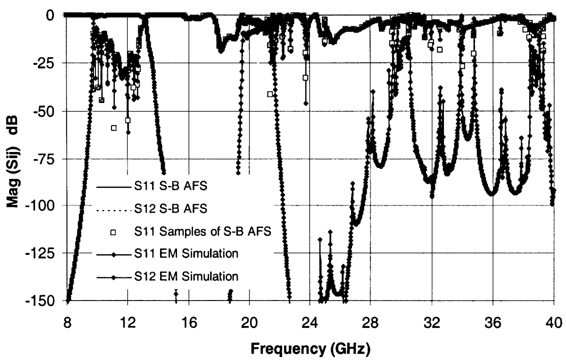

Fig. 8. S-parameters of hidden spurious harmonic modes of a low-pass corrugated waveguide filter calculated by the S–B AFS and full-wave EM simulation with 2001 samples.

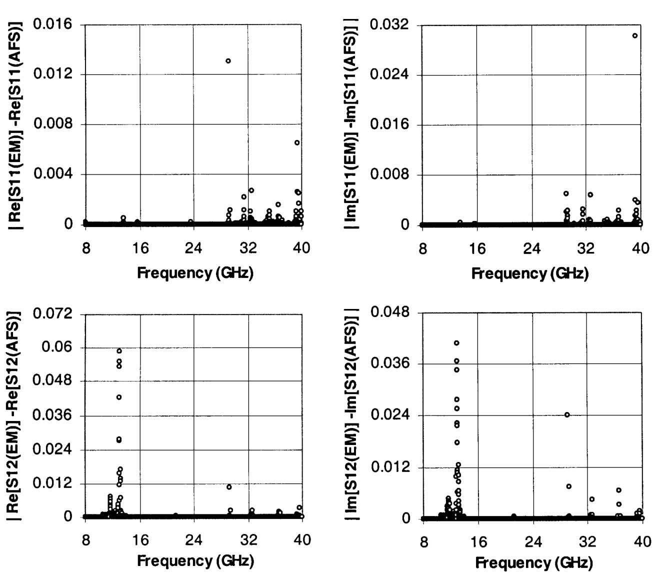

Fig. 9. Error of the FMs of the low-pass corrugated waveguide filter.

the greatest error happened at the spikes of the EM model and usually the value is not well defined.

The last example is a three-port microstrip multifrequency band diplexer, as shown in Fig. 10. It was used in a phased-array transceiver system to separate a broad-band signal to 10- and 19-GHz bands at port 1 and 12 and 21-GHz bands at port 3 [16]. Therefore, the response from 9 to 22 GHz needs to be

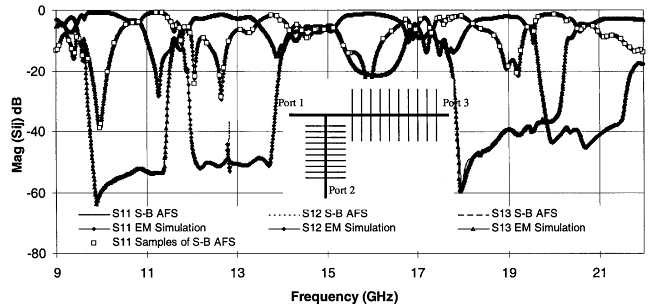

Fig. 10. Magnitude of S-parameters of a microstrip broad-band diplexer obtained by the S–B AFS and direct EM simulation with 1001 sampling points of equal space.

TABLE I
COMPARISION OF THE NUMBER OF EM SAMPLES REQUIRED BY DIFFERENT INTERPOLATION SCHEMES

Software	S-B AFS	EM package 1	EM package 2	EM package 3
Number of Samples	103	156	152	152

investigated. For this microstrip example, a commercial planar circuit EM simulation software is used as the original full-wave EM simulator to obtain the S–B AFS rational FM. Fig. 10 shows the magnitude of S-parameters interpolated by the S–B AFS and those obtained directly by the full-wave EM simulator. The direct EM responses are smoothed with 1001 sampling points of equal space, whereas the responses of the S–B AFS are interpolated by a single rational FM obtained only by 103 EM simulation samples. In order to demonstrate the strength of the proposed S–B AFS, the AFS-like interpolation features of three most popular commercial full-wave EM packages for planar RF circuits are used to study this broad-band diplexer circuit. Each of the commercial EM packages has its built-in interpolation scheme. The comparison of the required number of EM sampling points of the three EM packages with that of the proposed S–B AFS is summarized in Table I. It needs to be mentioned that the maximum error across the band for the S–B AFS is 0.3645 dB, whereas the other three packages are 0.367, 3.38, and 18.85 dB, respectively. This example shows that the S–B AFS can save over 30% of extra computation effort over existing AFS-like interpolation accelerators for this particular example.

IV. CONCLUSIONS AND DISCUSSIONS

This paper has introduced a new AFS approach by exploiting the S–B algorithm for modeling the frequency-domain response of a microwave circuit. Using the proposed approach, the frequency-domain response can be modeled by only one rational function with virtually the least number of sampling points of EM simulation. Since the S–B algorithm is a recursive tabular rational interpolation, there is no matrix inverse required. In addition, the algorithm provides a great flexibility to construct various models of rational functions. This feature makes the proposed adaptive derivation of the required FM possible. The derived FM can be applicable in a very broad frequency band, regardless of the orders of the poles and zeros that a circuit response corresponds to.

The rapid convergence feature in the proposed AFS schemes partially attributed to the designated development paths. It is the legitimate paths that enable the S–B algorithm to be fully used as a systematic AFS approach for EM simulation of microwave circuits. The approach also provides a systematic framework for adaptive rational interpolations for the physical phenomena of other disciplines.

Various microwave-circuit applications have been investigated in this paper to demonstrate the validation, effectiveness, and strength of the proposed S–B AFS approach. An expensive EM simulation load can be reduced by an order of magnitude in general by using the proposed S–B AFS approach as an accelerator to any frequency-domain EM simulator. This approach can be combined with a sub-zone technique to balance the EM simulation time and the time for establishing the FM model if too many sampling points are required.

Further developments of this study include optimal zigzag grid paths for different applications, legitimate strategy to adaptively search for an optimal grid path during the AFS process, and extension to multidimensional applications.

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