

Letters

Comments on "Comparison of the FFT Conjugate Gradient Method and the Finite-Difference Time Domain Method for the 2-D Absorption Problem"

TAPAN K. SARKAR

The objective of this letter is to point out certain wrong assumptions that the authors¹ have made about the FFT conjugate gradient method. Based on these erroneous assumptions, they made certain statements which are quite meaningless. Perhaps the statements made come from lack of acquaintance with recent publications on the conjugate gradient method (CGM). There are four specific comments.

1) Borup *et al.* claim that "...FFT-CGM is nothing more than an efficient means of solving PM-MOM linear system..." This statement is wrong. The fundamental misconception that the authors have is the assumption that the conjugate gradient method is only applicable to matrix equations and that it is too specialized for a pulse expansion and point matching. The following explanation illustrates why it is not so.

The application of the conjugate gradient method to solve a matrix equation is just a special case of the application of the conjugate gradient method to solve an operator equation. This is because, when one applies the conjugate gradient method to solve a matrix equation, the expansion and weighting functions have already been preselected. For the problem that Borup *et al.* have solved, the expansion and weighting functions were pulse expansion and point matching; however, in general, this need not be the case [2]. They solved the resulting matrix equation by the conjugate gradient method.

Now if one follows the procedure [3], [4] of applying the conjugate gradient method directly to the operator equation, the first difference that one observes is that the expansion and weighting functions evolve during the iteration and they are quite different from the previous case. The expansion functions in this implementation are a function of the initial guess made for the unknown solution. If the initial guess is assumed to be zero, then the expansion functions that evolve during the iterative solution of $AX = Y$ are, respectively, A^*Y ; $(A^*A)A^*Y$; $(A^*A)^2A^*Y$; and so on. The weighting functions are AA^*Y ; $A(A^*A)^2A^*Y \dots$. Here A^* is the adjoint matrix or operator. For a more detailed description and a better appreciation and basic understanding of the conjugate gradient method, the authors may like to read the tutorial paper [5]. Also, the approach just described is similar to those of [6] and [7]. It is also interesting to point out that the conjugate gradient method is sometimes called the method of moments, as the expansion functions are the generalized moments of Y for a self-adjoint operator A [7]. It is established now, beyond a reasonable doubt, that CGM can exist in various forms. The basic difference in the exact solution of a matrix equation and an approximate solution of an operator equation can be found in [23] and [20].

Now let us look at the numerical implementation. In the conventional pulse expansion utilized in the matrix methods, the kernel is integrated over the domain of existence of the basis function. In the numerical implementation of the FFT and the conjugate gradient method [4], the functions are sampled at N equidistant points and they are assumed to have the sampled value over each FFT bin. This is what a MOM practitioner would term a delta function expansion. Regarding the weighting functions, the weighting functions are approximated in a similar fashion; hence it is a sort of point matching. So from a philosophical point of view, most numerical methods programmed on a computer perform some form of point matching; hence to conclude from that that all forms of the conjugate gradient method are simply pulse expansion and point matching does not make any sense!

Finally, in order to conclude that the conjugate gradient method does not converge, that the rate of convergence is very slow for the solution of a matrix equation, or that it produces unstable results, one has to demonstrate that another method, such as Gaussian elimination or the nonconvergent spectral iterative method, yields the correct solution. This Borup *et al.* have not done. Therefore, it puzzles me on what grounds they conclude that the conjugate gradient method yields unstable results. It is my conjecture that had they used Gaussian elimination instead of the conjugate gradient method, they would have obtained identical unstable results. Therefore, to put the blame on a method rather than on an incorrect choice of expansion and weighting functions really does not make any sense.

It is important to point out that in the solution of very large problems with over 10000 unknowns the conjugate gradient method produced quite reliable results [4], [8]. So the fundamental problem lies in the choice of basis functions and not with FFTCGM. One can use FFTCGM without pulse expansion and point matching as described in [4].

2) By solving the matrix equation by FFT and CG, the full potential of the FFT is not utilized. In implementation of the FFT and the conjugate gradient method in [4], the FFT is utilized not only to compute the convolution between the Green's function and the other functions, but also to compute the derivative operation that exist in the charge term of the electric field. The derivative operation is converted to a multiplication in the transformed domain; hence the error incurred in the finite difference approximations for the electric field operator is minimized, particularly for the solution of the current on electrically small bodies. Hence what is known as FFT CGM does not fit the description of Borup *et al.* Any example presented to show that the matrix implementation is similar to the operator implementation should deal with the TE case and not the TM case.

3) The authors' claim that they developed the FFT-CGM perhaps arises from the lack of knowledge of published literature in other areas such as signal processing. For example, the application of FFT and CGM can be found in the works of Fineup [9], where they applied the FFT-CGM to solve a matrix equation.

4) Borup *et al.* also state (p. 385) that "CGM is a popular means for solving linear systems encountered in application of MOM..." Again, this statement is incorrect. The CGM has been applied in [2]–[6] directly to the solution of operator equations and hence one need not form or even store any matrices.

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The author is with the Department of Electrical Engineering, Syracuse University, Syracuse, NY 13244-1240

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Also, for MOM no mathematical proof is readily available that states as the number of expansion and weighting functions approaches infinity (pulse basis and point matching or for any other expansion functions) one obtains an exact solution. However the monotonic convergence of the solution (case B[3]) or of the residuals (case A[3]) is guaranteed for CGM. There is no equivalence of case B of CGM [3] for matrix methods.

In summary, what Borup *et al.* have shown is that for 2-D biological problems the pulse expansion point matching method in the frequency domain is inferior to the finite difference time-domain method. However to conclude that time domain methods are more accurate or that the FFT CGM does not work would be totally nonsensical.

It is important to point out that pulse expansion point matching does provide excellent results for the TE case if it is implemented intelligently (i.e., how the source integration points and the field matching points are chosen). Several papers and reports are available in the antennas and propagation literature that actually implement it.

There are other problems with the ordinary conjugate gradient method, such as squaring of the condition number and hence slower convergence, which can be partially corrected as outlined in [10]. However, when the conjugate gradient method is applied intelligently and programmed correctly on a computer having enough bits of information to represent the problem, the method works without any problem and provides accurate results for both frequency-domain and time-domain [11], [12] problems.

Reply² by D. T. Borup and O. P. Gandhi³

Many of the comments made by Sarkar above may also be found in his response to our comments [13] concerning his paper [4]. Unfortunately we were not allowed to reply at that time and so we gratefully welcome this opportunity.

Our response is divided into two parts. First, we would like to point out several conclusions that Sarkar attributes to us that do not appear in our paper. These misrepresentations of our work are particularly troubling and indicate either that he does not understand our paper or that he did not read it carefully. Then we would like to consider more carefully the amazing claim that his algorithm described in [3] and [4] is the solution of an operator equation rather than a matrix equation. This statement is quite meaningless of course since all finite-dimensional linear operator equations are equivalent to some finite-dimensional matrix equation. Obviously, the computer cannot perform operations in an infinite-dimensional space and so there is no distinction between a linear operator and a matrix as far as the computer is concerned. We will show that this misunderstanding is due to the way in which Sarkar derives his algorithm. In [3] and [4], the effect of the approximation of the continuous Fourier transform with the discrete Fourier transform is not discussed adequately. This clever derivation avoids explicitly stating the basis and testing functions that arise in the discretization process, giving the illusion that the continuous operator equation is being solved. In fact, Sarkar's method is just another example of a matrix moment method. It results from the expansion of the unknown wire current with a finite, periodic basis followed by point matching. The resulting matrix equation is then solved

by the CG method. The Toeplitz form of the matrix is exploited by the use of the FFT algorithm and the discrete convolution theorem to provide an efficient means of computing the matrix products needed during the CG iterations. Thus, there is no philosophical difference between Sarkar's algorithm and our approach [1]. They differ only in the selection of the basis functions.

The following is a list of claims that Sarkar incorrectly attributes to our work along with a description of our actual conclusions.

1) In the second paragraph Sarkar quotes from our paper that the "...FFT-CGM is nothing more than an efficient means of solving the [pulse basis method of moments (PB-MOM)] linear system..." from which he concludes that we are asserting that the CG method is only applicable to linear systems obtained from the PB-MOM. If we actually held this belief our understanding of the CG method would be poor indeed and Sarkar would be quite correct in suggesting that we read his tutorial paper. Actually the statement is taken out of context. If this statement is read in context, it is quite clear that our intent was to stress the fact that, in our method, the FFT-CGM is nothing more than an efficient means of solving the matrix that we obtain via the PB-MOM. From this we conclude that the errors we observed in the transverse electric (TE) cylinder solutions cannot be attributed to the FFT-CGM and that any fundamental problem with the pulse basis formulation will also plague our solutions.

2) In paragraph six, we are accused of putting the "...blame on a method [the CG method] rather than on an incorrect choice of expansion and weighting functions..." This comment is particularly unsettling since the main conclusion of our paper is that the discontinuities introduced by the pulse basis produce fictitious charge sources that degrade the accuracy of the numerical solution for the TE illumination of dielectric cylinders. In other words, we quite clearly put all the blame on the basis functions. The only observation that we make concerning the CG method is that the rate of convergence can be quite slow for the matrix obtained from the PB-MOM for the TE polarization. This is in contrast to the transverse magnetic (TM) polarization for which adequate convergence is obtained in a number of iterations far less than the number of unknowns. This is an important consideration in the comparison of the relative efficiency of our FFT-CG method and the finite-difference time-domain (FD-TD) method. Recently, we have found that this problem can be alleviated by replacing the pulse basis with the sinc basis to be described shortly. Apparently, use of the sinc basis results in a matrix with clustered eigenvalues and a smaller condition number. This results in rapid convergence of the CG iterations for both the 2-D TE and 3-D dielectric scattering problems. Further gains in numerical efficiency can be obtained by using the biconjugate gradient method [14] as suggested by Sarkar.

3) The statement in paragraph six that our results would be unchanged if Gaussian elimination were used was already acknowledged by us. We quite clearly stated that "...this method of solving [the PB-MOM linear system] introduces no additional error over more traditional methods such as LU decomposition..."

4) In comment 3, Dr. Sarkar states that we claim to be the originators of the FFT-CG method. The fact is that the first application of this combination to electromagnetic scattering problems that we are aware of is [15]. However, we have never claimed any special monopoly on the idea. The only place we find the claim of novelty is in the first paragraph of Sarkar *et al.* [4].

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³The authors are with the Department of Electrical Engineering, University of Utah, Salt Lake City, UT 84112
IEEE Log Number 8717911

Most of Sarkar's remaining comments concern his distinction between operator equations and matrix equations. In the next section we will demonstrate that the method in [3] and [4] is a matrix moment method in the sense that basis and testing functions are preselected and employed to reduce the integral equation to a matrix equation. The only role that the CG method plays in Sarkar's algorithm is to solve this matrix equation. The solution obtained would be unchanged if another method such as Gaussian elimination were used.

Consider the Fredholm integral equation of the first kind with shift invariant kernel

$$y(x) = \int_{-L/2}^{L/2} f(x') g(x-x') dx', \quad -\frac{L}{2} \leq x \leq \frac{L}{2}. \quad (1)$$

For the wire antenna problem, f is the unknown wire current, y is the incident field excitation, g is the Green's function, and L is the wire length.

Because we seek a solution with finite support on $[-L/2, L/2]$, the limits of integration can be extended to $\pm\infty$. Introducing the support function

$$t(x) = \begin{cases} 1 & -\frac{L}{2} \leq x \leq \frac{L}{2} \\ 0 & \text{otherwise} \end{cases}$$

we get the following problem: Find $f(x)$ with support on $[-L/2, L/2]$ that solves

$$y(x) = t(x) \int_{-\infty}^{\infty} f(x') g(x-x') dx'. \quad (2)$$

The procedure for solving (2) by the moment method begins by expanding $f(x)$ in a finite-dimensional basis. The finite support constraint on the solution can be enforced at this point by selecting a finite support basis expansion (e.g., piecewise constant, piecewise linear, etc.); however, in order to arrive at Sarkar's algorithm, we introduce the grid nodes illustrated in Fig. 1 and use the basis expansion

$$f(x') \approx \hat{f}(x') = \frac{1}{2M-1} \sum_{m=-M+1}^{M-1} t_m f_m \frac{\sin\left[\frac{\pi}{\Delta}(x' - m\Delta)\right]}{\sin\left[\frac{\pi}{\Delta} \frac{(x' - m\Delta)}{2M-1}\right]} \quad (3)$$

where the constraint $f_m = 0$ for $N-1 < |m| < M$ has been enforced by defining the support sequence $t_m = t(m\Delta)$. Notice, however, that (3) is periodic with period $(2M-1)\Delta$. Thus, the use of (3) introduces fictitious copies of the wire current. However, as M becomes large, the coupling between these copies is reduced due to the decay of the Green's function. Sarkar suggests the arbitrary choice, $M = 2N$. A means of eliminating these fictitious copies altogether will be described shortly.

By a trivial step

$$\begin{aligned} \hat{f}(x') &= \frac{1}{2M-1} \sum_{k=-M+1}^{M-1} \sum_{m=-M+1}^{M-1} t_m f_m e^{-i(2\pi mk)/(2M-1)} \\ &\quad \cdot e^{i(2\pi k x')/(\Delta(2M-1))} \\ &= \frac{1}{2M-1} \sum_{k=-M+1}^{M-1} \tilde{f}_k e^{i(2\pi k x')/(\Delta(2M-1))} \end{aligned} \quad (4)$$

where \tilde{f}_k is the discrete Fourier transform (DFT) of the zero

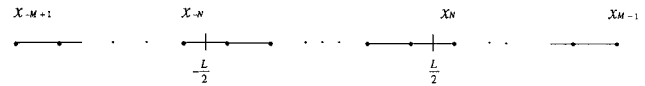


Fig. 1 Geometry of the equally spaced sample points used to define the basis expansion, eq. (3) $x_n = n\Delta$, $\Delta = L/(2N-1)$.

padded array f_m defined as

$$\text{DFT}\{f_m\}_k = \tilde{f}_k = \sum_{m=-M+1}^{M-1} t_m f_m e^{-i(2\pi mk)/(2M-1)}, \quad -M+1 \leq k \leq M-1. \quad (5)$$

Inserting (4) into (2) gives

$$\begin{aligned} y(x) &\approx \frac{t(x)}{2M-1} \int_{-\infty}^{\infty} \sum_{k=-M+1}^{M-1} \tilde{f}_k e^{i(2\pi k x')/(\Delta(2M-1))} g(x-x') dx' \\ &= \frac{t(x)}{2M-1} \sum_{k=-M+1}^{M-1} \tilde{f}_k e^{i(2\pi k x')/(\Delta(2M-1))} \tilde{g}_k \end{aligned} \quad (6)$$

where \tilde{g}_k equals the continuous Fourier transform of $g(x)$ sampled at $2\pi k/(\Delta(2M-1))$.

To complete the numerical solution, the equality of (6) is enforced at the grid nodes (point matching) to give the matrix equation

$$y_n = \frac{t_n}{2M-1} \sum_{k=-M+1}^{M-1} \tilde{f}_k \tilde{g}_k e^{-i(2\pi nk)/(2M-1)} \quad (7)$$

or

$$y_n = t_n \text{DFT}^{-1}\{\text{DFT}\{t_m f_m\}_k \tilde{g}_k\}_n. \quad (8)$$

Equation (8) defines the algorithm used by Sarkar to compute the matrix products needed in the implementation of the CG iterations. In order to find an simplified expression for the matrix equation implicit in (7), substitute (3) into (7) to get

$$y_n = \frac{t_n}{2M-1} \sum_{k=-M+1}^{M-1} \sum_{m=-M+1}^{M-1} t_m f_m \tilde{g}_k e^{i(2\pi k(n-m))/(2M-1)} \quad (9)$$

or simply

$$y_n = \sum_{m=-N+1}^{N-1} f_m g_{n-m}, \quad -M+1 \leq n \leq M-1 \quad (10)$$

where g_n is the discrete kernel

$$g_n = \frac{1}{2M-1} \sum_{k=-M+1}^{M-1} \tilde{g}_k e^{i(2\pi nk)/(2M-1)}. \quad (11)$$

Equation (10) is then the matrix equivalent of the algorithm defined in (8). In Sarkar's algorithm, the matrix equation (10) is now solved iteratively by the conjugate gradient method. Rather than explicitly forming the Toeplitz matrix (10), the FFT algorithm is used to rapidly compute the matrix products needed during the CG iterations by utilizing the algorithm defined in (8). The adjoint matrix products, which are also needed to implement CG, can also be computed by simply replacing \tilde{g}_k with its complex conjugate in (8).

We have now shown that Sarkar's algorithm can be derived by applying the method of moments to (2) using the basis defined in (3) and point matching to reduce the integral equation to a matrix equation. In Sarkar's approach, the CG method is used only as a means of solving the matrix equation (10). The same result would be obtained if another method were used such as Gaussian elimination. The advantage of using the CG method is that only matrix products are needed in its implementation. This

allows the use of the FFT by algorithm and obviates the storage of the matrix.

From the following development it should now be clear that Sarkar's distinction between using the CG method to solve an matrix equation versus an operator equation is meaningless. Also, his claim that the basis is not preselected but evolves during the iteration process is incorrect. It is true that at the k th step of the CG method the iterate f^k is found by minimizing the residual error

$$\|r^k\|_2^2 = \|Af^k - y\|_2^2$$

over the Krylov set (see for example Axelsson [16])

$$S_k = \{A^*y, (A^*A)A^*y, \dots, (A^*A)^k A^*y\}.$$

However, this has nothing to do with the basis functions used to discretize the integral equation into a matrix equation. As we have shown, the preselected basis set used implicitly in Sarkar's approach is exactly that given in (3). This fact is obscured in his development.

In [3] and [4], the claim is made that proof of the convergence of the CG method is somehow a proof of the convergence of the numerical solution. This would certainly be true if the CG method were applied directly to the continuous integral equation without the intermediate step of discretization. Unfortunately this is not possible and so the only alternative is to discretize the continuous integral operator into a finite-dimensional matrix. Proofs concerning the convergence of the numerical solution must certainly consider how well the basis expansion approximates the unknown solution in the limit as the sample interval, Δ , goes to zero. An example of such a proof can be found in [17].

An important additional point needs to be made. If Sarkar had noticed that his formulation (8) can be reduced to (10), he would have realized that, in effect, the zero pad length M can be limited to infinity. Since (10) is in the form of a discrete convolution on $[-N+1, N-1]$, it can be solved by the FFT-CG method using FFT's of length $4N-1$ with no wraparound aliasing for arbitrarily large M . The calculation of the discrete kernel g_n need be computed only once using a single $2M-1$ point FFT prior to the iterative solution of (10). This allows the periodic copies of the current to be separated by an arbitrarily large distance without increasing the FFT length needed during the CG iterations.

Now consider what happens if we take the limit $M \rightarrow \infty$. Equation (3) then becomes

$$\hat{f}(x') = \sum_{m=-N+1}^{N-1} t_m f_m \frac{\sin\left[\frac{\pi}{\Delta}(x' - m\Delta)\right]}{\frac{\pi}{\Delta}(x' - m\Delta)} \quad (12)$$

which is the well-known sinc basis expansion. The advantages of sinc basis methods versus polynomial methods are discussed by Stenger in [18]. In this monogram, Stenger derives a class of sinc-based numerical methods for problems ranging from interpolation and quadrature to the solution of partial differential equations and integral equations. The utility of the sinc basis for the solution of scattering integral equations is further supported by the work of Johnson *et al.* [19], in which the sinc basis and FFT are used to solve the acoustic scattering integral equations that arise in ultrasound imaging.

The formula for the discrete kernel (11) limits to

$$g_n = \frac{\Delta}{2\pi} \int_{-\pi/\Delta}^{\pi/\Delta} \tilde{g}(\omega) e^{i\omega n\Delta} d\omega = g(x) * \frac{\sin\left(\frac{\pi}{\Delta}x\right)}{\frac{\pi}{\Delta}x} \quad (13)$$

where the $*$ denotes the convolution operation. Thus, the use of (10) with the kernel defined in (13) is equivalent to limiting M to infinity, which removes the fictitious copies of the current. Equation (10) can then be solved with no wraparound aliasing using $4N-1$ point FFT's and the CG method.

An important limitation of Sarkar's algorithm occurs in the 2-D and 3-D electric field integral equation cases for which $\tilde{g}(k)$, the spatial Fourier transform of the Green's function, is singular on the Ewald surface, $|k| = k_0$. This causes problems in the evaluation of (11). It has been suggested that this problem can be obviated by adding a small imaginary part to k_0 [13], [20]. Our numerical experiments indicate that this is a highly unsatisfactory remedy. In particular, solutions obtained in this way for the 2-D circular cylinder problem do not agree at all with analytic solutions. The importance of correctly including the contribution of the scattered field due to this singularity is obvious in the light of the well-known fact that the externally scattered field is completely determined by the transform of the current on the Ewald surface [21]. The problem with using (11) is that it consists of a mid-point rule approximation of the continuous integral (13) which has a singular integrand (for the 2-D and 3-D Green's functions). The slow convergence of the approximation (11) as M goes to infinity means that very high resolution grids must be used to obtain an accurate quadrature. It is indeed fortuitous that Sarkar chose the wire antenna problem for his test case for which such singularities do not exist. Fortunately, the sinc basis method does not suffer from this problem since the singularity is integrated analytically in (13). We have derived analytic expressions for the 2-D and 3-D equivalents of (13) and have implemented this approach for calculating scattering and absorption by arbitrarily inhomogeneous lossy dielectrics. Comparison with analytic solutions for concentrically layered spheres of biological tissues exposed to a plane wave have verified the accuracy of the method. We have also successfully solved inhomogeneous man models embedded in a $72 \times 24 \times 12$ grid. Of these 20000 grid nodes, 6000 define the inhomogeneous man models. The remaining points are in air and fill out the cuboid grid on which the 3-D FFT operates. This then results in 18000 unknown electric field values. Typical run times for this model are between 7 to 14 minutes on the Cray-2 supercomputer at the University of Minnesota. A complete description of the algorithm and results is in preparation for publication [22].

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Comments on "A Method for Measurement of Losses in the Noise-Matching Microwave Network While Measuring Transistor Noise Parameters"

MARIAN W. POSPIESZALSKI

In the above¹ paper, expressions (1), (2), and (3) appear to be correct only if the physical temperature T_a of the tuner is equal to the standard temperature $T_0 = 290$ K. The expression (1) for $T_a \neq T_0 = 290$ K should read

$$F_m(\Gamma_n) = \frac{T_a}{T_0} \left[\alpha_{\Gamma_n}(\Gamma_n) - 1 \right] + 1 + \alpha_{\Gamma_n}(\Gamma_n) \left[F(\Gamma_n) - 1 + \frac{F(S'_{22}) - 1}{G_a(\Gamma_n)} \right] \quad (1)$$

using the notation of the paper. Generally valid versions of expressions (2) and (3) follow in a straightforward manner. The

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The author is with the National Radio Astronomy Observatory, Charlottesville, VA 22903.

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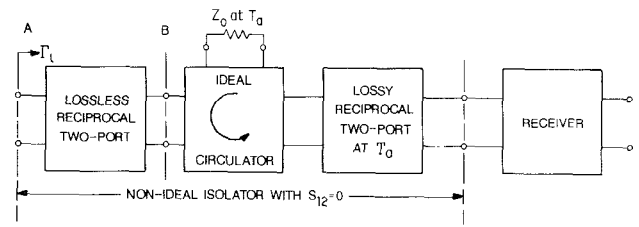


Fig. 1 Equivalent circuit of a receiver with nonideal isolator at its input.

error caused by the limited validity of expressions (1), (2), and (3) in the subject paper may be quite significant, even for room temperature measurement. For instance, for the tuner losses of 1.5 dB (worst case in the example discussed), each kelvin of a difference between physical temperature of a tuner and standard temperature T_0 will contribute 0.4 K of an error.

Also, the remaining nonreferenced expressions in the subject paper (i.e., (5) through (9)), which deal with the noise temperature of a receiver with isolator at the input, are derived in the Appendix ((A1) through (A14)) in an unnecessarily complicated way. In order to demonstrate this point, let us refer to the equivalent circuit of Fig. 1. This equivalent circuit is valid for a receiver preceded by an isolator having $S_{12} = 0$ and a physical temperature T_a . In this case, a nonideal isolator is modeled by a cascade connection of lossless reciprocal two-port, followed by an ideal isolator and lossy reciprocal two-port.

It has been brought to the attention of the authors of the subject paper [1] and also discussed in some greater detail in [2] that at plane B (refer to Fig. 1), the noise parameters of such a system are

$$T_{\min} = T_R^B(\Gamma_g = 0), \quad \Gamma_{\text{opt}} = 0, \quad N = \frac{T_a + T_{\min}}{4T_0}. \quad (2)$$

It follows immediately from the invariant properties of T_{\min} and N [3] that at plane A the noise parameters are

$$T_{\min} = T_R^A(\Gamma_g = \Gamma_i^*) = T_R^B(\Gamma_g = 0), \quad \Gamma_{\text{opt}} = \Gamma_i^*, \quad N = \frac{T_a + T_{\min}}{4T_0}. \quad (3)$$

The relations (2) and (3) follow in a straightforward manner from those published many years ago [4], [5]. The expressions (5), (7), and (8) in the subject paper can be easily obtained by substitution of noise parameters given by (3) into standard expression for equivalent noise temperature (noise figure).

The relations (3) also clearly demonstrate why, for a full noise description of a receiver with isolator ($S_{12} = 0$) at the input, only single noise measurement will suffice if the input reflection coefficient Γ_i and physical temperature of the isolator are known.

Reply² by G. Martinez and M. Sannino³

I. PREMISE

Before replying in detail to the above comments, we would like to reassure experimenters working in the field of transistor noise measurements that the questions raised do not affect to any

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³The authors are with the Dipartimento di Ingegneria Elettrica, Università di Palermo, Viale delle Scienze, 90128 Palermo, Italy.
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