MMP-CG-PET: THE PARAMETER ESTIMATION TECHNIQUE APPLIED TO THE MMP CODE WITH THE METHOD OF CONJUGATE GRADIENTS

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Abstract

The Parameter Estimation Technique (PET) is presented as a new technique that can be applied to numerical codes based on dense matrices as a power booster for the computation of frequency plots, etc. In this paper it is applied to the Multiple Multipole Program (MMP) in conjunction with the method of Conjugate Gradients (CG) for iteratively and efficiently solving the rectangular MMP matrix. The PET takes advantage of the a priori knowledge obtained from previous computations and allows to a dramatic reduction of the computation time in various situations. It is demonstrated that one of the most important drawbacks in the use of frequency domain methods based on dense matrices as opposed to time domain methods based on iterative techniques can be eliminated using PET.

1. Introduction

One of the most important benefits of time domain methods such as the Finite Difference Time Domain (FDTD) technique [1] comes from the fact that the information on the EM field of the previous time steps can be used as a starting value for the computation of the actual EM field. This rigid use of the a priori knowledge [2,3] allows one to iteratively compute the EM field in each time step with typically one iteration only - provided that the time step is sufficiently small. As a consequence, the method is extremely efficient and fast.

Today, iterative matrix solvers such as the method of Conjugate Gradients (CG) are most frequently applied to large sparse matrices although the CG algorithm was originally designed for small, dense matrices [4]. Variants of the CG have also been applied to the Method of Moments (MoM) and other integral methods [5]. Although CG is very helpful in many situations it has important drawbacks: Its convergence depends to a great extent on the choice of the preconditioner and of the starting values. Moreover, CG is often either robust or efficient rather than robust and efficient as desired.

The MMP codes [6-8] are based on an overdetermined system of equations characterized by a dense, rectangular matrix. The condition number of the MMP matrix is often very high. Therefore, many of the simple matrix solvers cannot successfully be applied - except for almost trivial problems [9]. This is the most important reason why the CG matrix solver in the 2D MMP code [10] and the Choleski matrix solver in the 3D MMP code were rarely used in the past. It is important to note that the bad condition of the matrix does not cause inaccurate results. It has been shown [2,3] that the accuracy of the results can often be increased by increasing the condition number of the matrix. Moreover, ill-conditioned matrices simplify the modeling and are important for the user-friendliness of the code.

For the reasons outlined above, iterative MMP matrix solvers were discarded [10] and Block-Iterative Techniques (BIT) [11] were preferred for computing large MMP models. Since the performance of block-iterative techniques is usually not high at all, the 3D MMP features required for easily applying such techniques were not implemented. Instead, the 3D MMP user applies the "connection" feature of the 3D MMP code. He has to copy and edit MMP data files for each iteration, whereas the MMP code performs only one iteration in one run. I.e., the BIT is rather performed by the 3D MMP user than by the code. This explains why block-iterative techniques were only used by 3D MMP experts in complicated situations when the direct MMP matrix solution failed. Since the implementation of the 2D MMP "connection" feature and the 2D MMP file handling are much simpler, the BIT was also applied to less complicated 2D MMP models [8].

It is very important to recognize that CG and other iterative matrix solvers can handle ill-conditioned matrices. The main problem for the efficient use of such techniques is a sufficiently accurate estimation of the initial values. FTDT codes usually start with zero fields which allows one to exactly set the initial values.

Obviously, finding appropriate starting values for MMP and other frequency domain codes is much less trivial. The key to good starting values can only be some a priori knowledge [2,3]. A priori knowledge can be some knowledge of the user but it also can be the knowledge obtained from previous computations. In many situations one is not only interested in the EM field for a well defined model at exactly one frequency but also in the frequency dependence of the EM field and of quantities derived from the EM field or in the dependence of these quantities on other variables such as the angle of incidence of the incident wave, material properties, or geometric data. As soon as the EM field has been computed for one set of variables, one has some a priori knowledge for computations with slightly modified variables. This knowledge should be recycled rather than wasted. The main idea of the Parameter Estimation Technique (PET) is the recycling of knowledge. This technique is explained in the following sections.

The second problem for iterative techniques is the stopping criterium. In FDTD codes, this problem is avoided by a sufficiently small time step that guarantees a convergence with one iteration. When one is solving square matrices, CG algorithms converge toward the exact solution within at least N iterations, where N denotes the number of unknowns. This does not cause problems in finding an appropriate stopping criterium. Unfortunately, the convergence of the CG algorithm applied to overdetermined systems of equations shows a staircase behavior and the maximum number of iterations required is not known in advance. It is shown in this paper that the PET provides not only an appropriate estimation of the starting values for iterative techniques but also an appropriate stopping criterium.

2. Some important MMP features

In MMP and other matrix methods, the EM field is defined by a series expansion of the form

$$Field = \sum_{k=1}^{K} A_k \, Basis_k + Error \qquad (1)$$

MMP provides a large library of basis functions. Since MMP is based on a boundary method, the basis functions are analytic solutions of Maxwell's equations inside the domain where they are applied to approximate the EM field. Multipole expansions are most frequently used due to their local behavior and efficient recursive computation [6-8]. In the test example considered in the following section and in most applications, plane waves are assumed to be the incident EM field. Plane waves can also be applied to simulate a part of the scattered EM field of large bodies [12] and many other expansions can be helpful in special situations. Since this has no influence on the application of the PET, we only consider multipole expansions and a plane wave excitation.

The parameters A_k of the MMP expansion (1) are determined by the Generalized Point Matching (GPM) technique [8]. This technique is relatively simple. It leads to an overdetermined system of equations that is solved in the least squares sense. Since the different equations are weighted, this method is also called the method of weighted residuals. The GPM implicitly minimizes an error function defined along the boundaries of all domains and has interesting advantages when the condition number of the matrix is large. In the MMP codes, large condition numbers, i.e., ill-conditioned matrices, are tolerated because this considerably increases the freedom in setting multipole expansions and makes it possible to obtain more accurate results as we will see in the following.

The GPM allows one to easily validate the results. It provides several measures for the accuracy. First of all, the sum of the squares of the weighted residuals is a scalar value that is small when the accuracy is high. This provides a simple and quick hint. More detailed information is obtained from the mismatching along the boundaries. When the MMP matrix is sufficiently overdetermined, the mismatching in the matching points is comparable with the mismatching between them. Therefore, it is sufficient to compute the residuals in the matching points. The peak errors of MMP computations are typically located on the boundaries and rapidly decay with distance from the boundaries [13]. Therefore, the analysis of the residuals is a reliable measure.

The MMP codes offer several methods for solving the matrix equations. Givens updating (QR decomposition), Householder transformations (another QR decomposition) and Cholesky factorization are available in the 3D MMP code, whereas the 2D MMP code offers Givens updating, Singular Value Decomposition (SVD) and iterative matrix solvers like CG and Gauss-Seidel. Although SVD is optimal for ill-conditioned matrices, this technique is rarely applied because it is very time- and memory consuming. In the following, SVD has only

been used for computing the condition numbers. Householder transformations are more memory consuming, not much faster, and have more problems with ill-conditioned matrices than Givens updating. This algorithm has only been used in conjunction with a Finite Element (FE) code [14]. The Cholesky factorization is faster than the Givens updating but it is useless, except when the condition number is relatively small. Therefore, this technique has only been used in simple benchmark cases [9]. Among the iterative matrix solvers, CG seems to be most appropriate. This is the first choice in conjunction with the PET.

3. The Test Example

In [10] the EM scattering of a plane wave at a cylindrical, perfectly conducting plate with the cross section shown in Figure 1 has been considered for testing the performance of the CG algorithm in the 2D MMP code. Although this example is very simple, it shows all the main effects. Therefore, it is well suited as a test case for the MMP-CG-PET implementation.

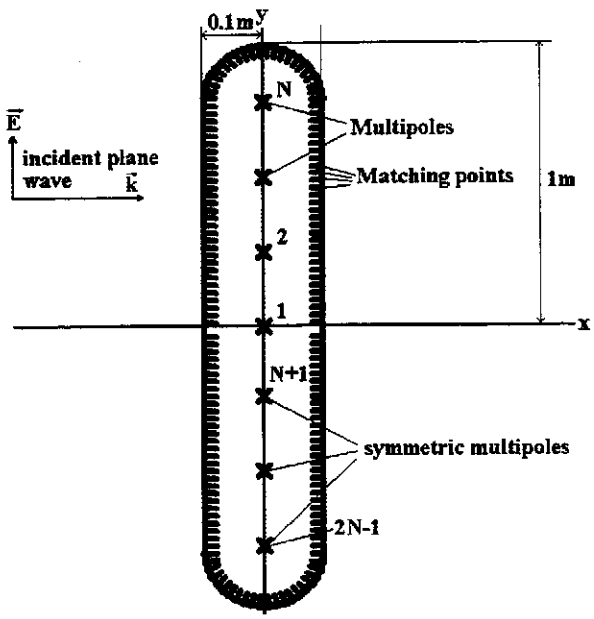

Figure 1: Cross section of the test case. Only the multipoles 1...N need to be defined explicitly. The symmetric counterparts, i.e., the multipoles N+1...2N-1 are automatically generated by the 2D MMP code. Since the first multipole is on the y axis, it has no symmetric counterpart. The incident EM field is a plane wave with wave vector in the x direction and an electric field in the y direction.

It is well known that the number and locations of multipoles used for simulating the scattered EM field is critical for the accuracy. Simple rules for setting the multipoles and automatic pole setting procedures are described in [8,15]. For our test example, a uniform distribution of multipoles seems to be most reasonable. It has been shown in [13] that the critical points of a model such as our test example are at the connection of straight lines and circles and that the efficiency and accuracy can considerably be increased when more sophisticated MMP expansions are applied. Such expansions should have multipoles in the vicinity of the critical points. Since the aim of our test example is the exploration of the relation between the condition numbers and the accuracy obtained with different MMP expansions, uniform multipole distributions on the y axis are appropriate.

In order to obtain a fair comparison of the different MMP expansions, we keep the size of the MMP matrix, i.e., total number of unknowns and of matching points, fixed. The multipole on top covers much more matching points than all the other multipoles. Therefore, this multipole must have higher orders than all the other multipoles. Moreover, the multipole on the x axis has only half as many unknowns as its neighbours because of the symmetry. Thus, the number of orders of the different multipoles, i.e., the number of columns of the MMP matrix corresponding to the different multipoles, is not fixed. The distribution of the orders of the multipoles is not unique and has a considerable influence on the condition number of the MMP matrix and on the accuracy of the results. Instead of exploring this influence in the following, we apply the usual MMP rules [8].

The condition number of the single multipole expansion with only one multipole on the x axis (N=2N-1=1) is 1 if the MMP matrix is appropriately scaled, but this expansion leads to completely wrong results except for very high orders. Since we want to perform a large number of computations, we have to keep the computation time, i.e., the number of unknowns, relatively small. Therefore, we will not consider the single multipole expansion here. The MMP matrix of all computations in this paper has 82 rows and 44 columns. A symmetry decomposition of the incident wave and of the matrix would allow us to obtain two 41*22 matrices but this has not been done here for reasons of simplicity. Figure 2 illustrates a typical MMP matrix for N=4.

It has been stated in [2,3] that the condition number of the MMP matrix considerably increases with the number N of multipoles. Figure 3 shows that this statement holds for different frequencies.

From Figure 4 one can recognize that more accurate results can be obtained with larger numbers N and that this statement is also true for different frequencies. The best results are obtained with 9 multipoles for all frequencies. Models with less than 5 multipoles are characterized by a good condition of the matrix but the residuals obtained are considerably higher. Therefore, it is not reasonable to use less than 5 multipoles. When more than 9 multipoles on the y axis are applied, the condition number becomes so large that even the Givens algorithm inaccurately computes the parameters. Note that 5 multipoles would be optimal for a matrix solver that cannot handle large condition numbers. Such an algorithm would force the user to guess the optimal number and distribution of multipoles. The Givens procedure gives much more freedom because it produces acceptable results even for 13 multipoles.

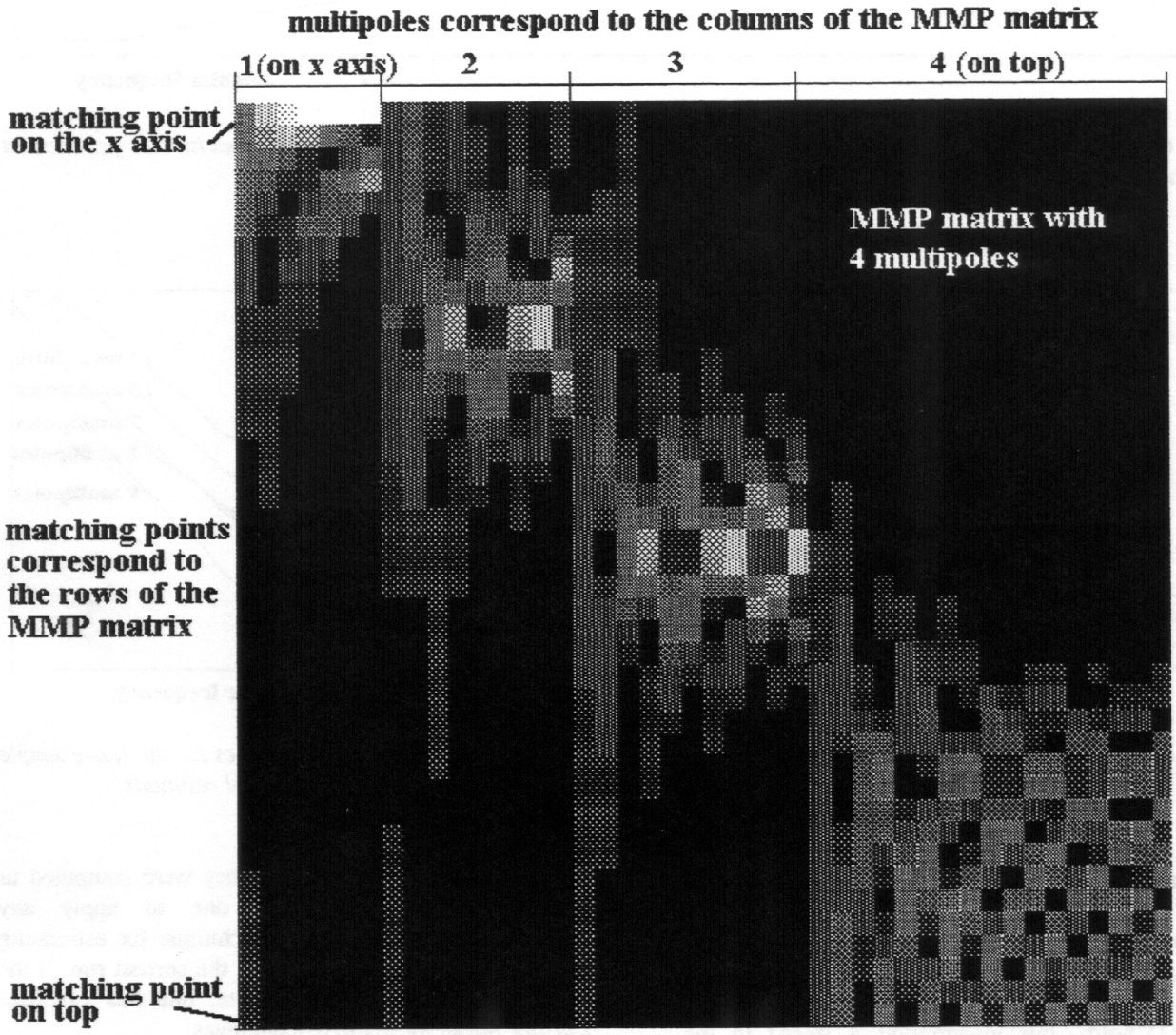

Figure 2: Typical MMP matrix for the test example with 2N-1=7 multipoles. Only the upper half of the matrix is shown because of its symmetry. The intensity corresponds to the size of the matrix elements.

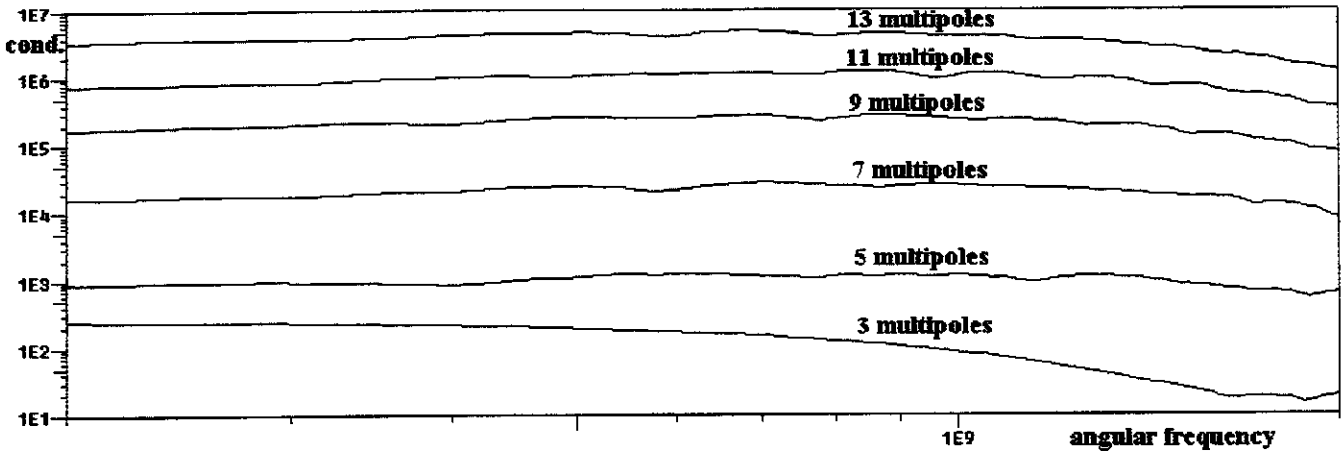

Figure 3: Condition number of the MMP matrix versus frequency for different total numbers of multipoles for the test example shown in Fig. 1.

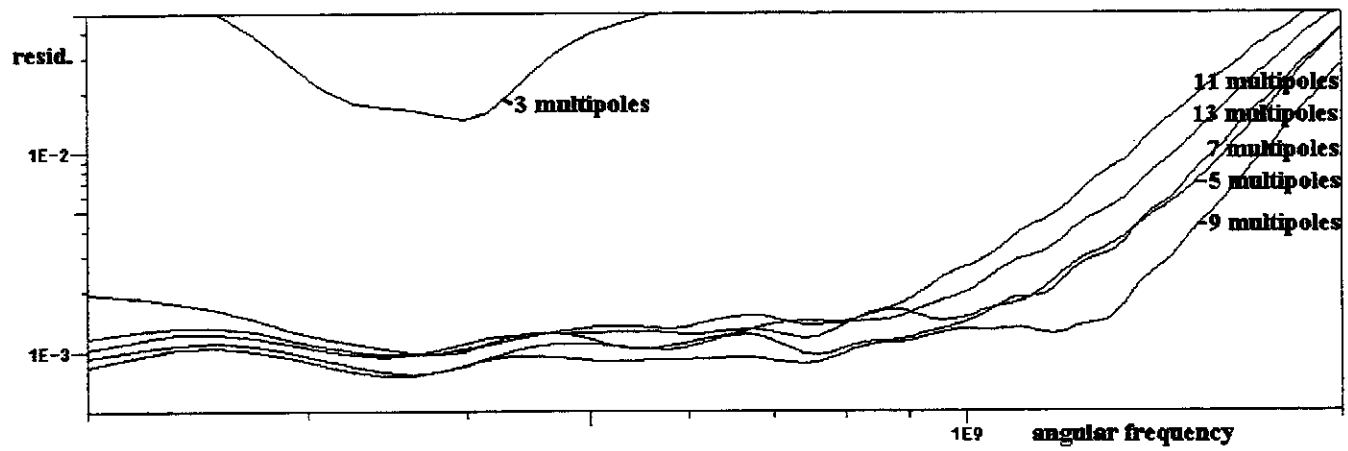

Figure 4: Residual of MMP computations versus frequency for different total numbers of multipoles for the test example shown in Fig. 1. The residual shown here is the square root of the sum of the squares of the weighted residuals.

3. Parameter Estimation Technique (PET)

The Parameter Estimation Technique (PET) is based on the concept of recycling the information obtained from previous computations of a given problem. When equation (1) holds, this information is stored in the parameters A_k, in the basis functions $Basis_k$, and in derived quantities. When the basis functions are kept unchanged during several computations, the parameters A_k (and all derived quantities) are functions of the variables of the computations. These functions are known in all the points where they were computed in previous runs. This allows one to apply any extrapolation or interpolation technique for estimating the parameters to be computed in the current run. If the estimation is sufficiently accurate, one has excellent starting values for iterative techniques.

Although the PET can be applied to any variable, we consider the frequency as a single variable for reasons of simplicity. When we compute the frequency dependence of our test model, we have 44 parameters, i.e., 44

functions of the frequency. If we consider the frequency dependence of these parameters in an interesting area where one observes resonances of the structure, we observe a very strong variation of all the parameters.

Figure 5 shows the logarithm of the absolute values of the parameters obtained from the Givens matrix solver.

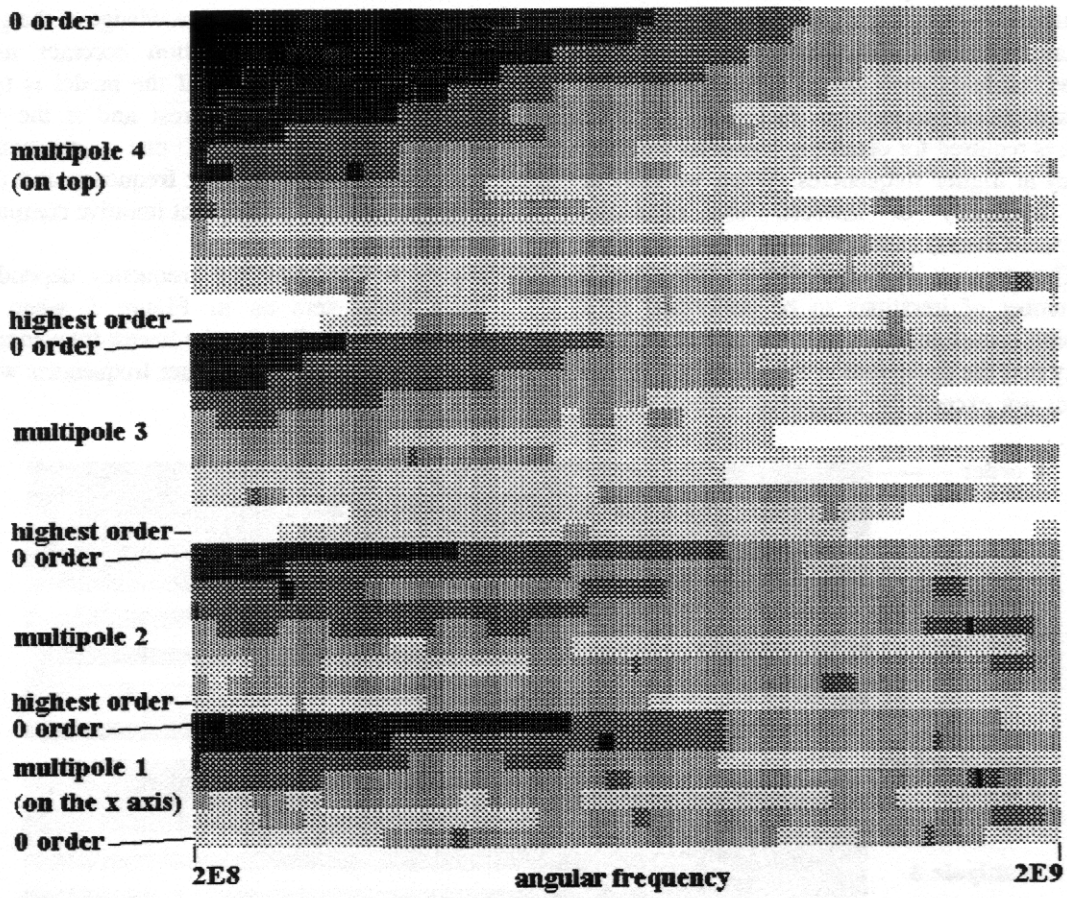

Figure 5: Frequency dependence of the parameters of the test model obtained with the Givens updating procedure. Dark areas indicate large values. A logarithmic scale has been used because the range of parameter values is very great. Therefore, this representation is useful for a quick overview, but it does not show the frequency dependence in detail. The number of multipoles shown here is 4. The total number of multipoles is 7. The parameters of the symmetric multipoles are not explicitly shown.

Despite the strong variation of the parameters, we can assume that the parameter set of a given frequency provides a useful starting value for the iterative computation of the parameter set at a slightly higher or lower frequency.

Before we can apply an iterative technique, we have to solve the problem of the stopping criterium. From an initial computation with a direct matrix solver (in the MMP code this usually is the Givens algorithm) we know not only the parameter set, but also the residual (more precisely, the square root of the sum of the squares of the weighted residuals). The residual obtained by the Givens algorithm is the smallest residual that might be obtained with an iterative matrix solver. It typically does not vary rapidly when the frequency is increased. Therefore, we can multiply the residual *res(Givens)* with a factor *fac*<1 to obtain a stopping criterium for the iterative matrix solver, i.e., the iterative matrix solver is stopped as soon as the condition *res(iter)<fac*res(Givens)* is met. The residual *res(Givens)* is obtained from an initial MMP

computation of the parameters with the Givens algorithm. The larger we set the factor *fac*, the lower the accuracy will be, and the fewer iterations will be required for computing the new parameter set.

As one can see from Figure 4, the residuals of all reasonable models (with 5 and more multipoles) are almost constant up to a certain frequency. Above this frequency, the residuals grow almost linearly. This can easily be understood from the fact that a finer discretization is required for obtaining solutions with the same accuracy at higher frequencies. When we start at the lowest frequency of interest, the condition *res(iter)<fac*res(Givens)* cannot be met above a critical frequency. Therefore, it is reasonable to introduce a maximum number of iterations to be performed as a second stopping criterium. This number can be defined in such a way that the computation time required for all iterations does not exceed the computation time for the Givens algorithm (which is another type of a priori knowledge). When *fac* is reasonably large (>2), the second stopping criterium indicates that the actual model is not fine enough. This means that the set of basis functions and matching points should be improved. If the basis functions are modified, the parameter set is entirely changed and the knowledge of the parameter set of the previous computation becomes useless. Such problems can be avoided if the model is tested for the highest frequency of interest and if the frequency is traced backwards, i.e., if one starts with a Givens computation at the highest frequency and decreases the frequency for the subsequent iterative computations.

Figure 6 illustrates the frequency dependence of the same parameters as in Figure 5 when the Givens algorithm is applied for the lowest frequency and the CG algorithm is used for all other frequencies with *fac*=10.

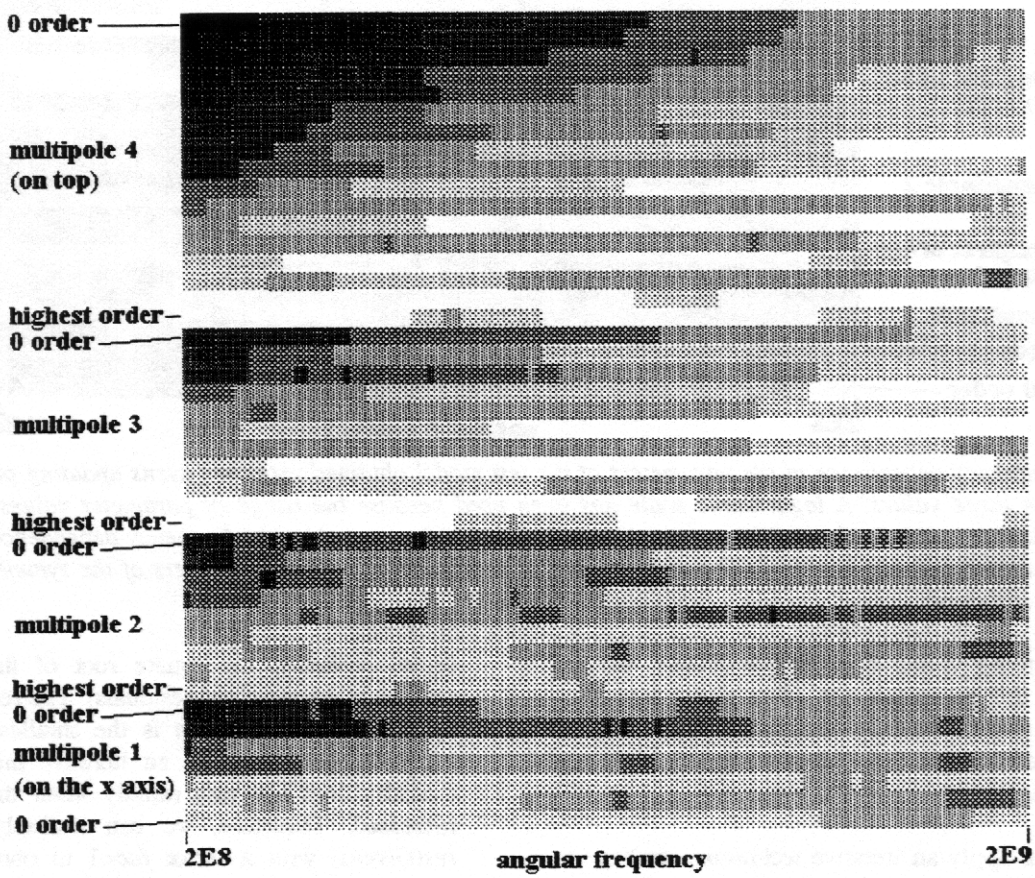

Figure 6: *Frequency dependence of the parameters of the test model with 7 multipoles obtained with the iterative CG procedure. Dark areas indicate large values. The same scale as in Figure 5 has been used. The computation is started at the lowest frequency with the parameters known from the Givens solution (see Fig. 5). The factor fac of the stopping criterium is 10, the frequency scale is linear. The parameters of the symmetric multipoles are not shown explicitly.*

As one can see, the parameters obtained with the CG algorithms (Fig.6) are far away from the parameters obtained with the Givens algorithm (Fig.5). The same has been found with a smaller factor *fac*=3, with different frequency steps, negative frequency steps (starting at the highest frequency) and logarithmic instead of linear frequency scales. The parameters obtained for one frequency with the CG procedure with fixed stopping criteria depend to a considerable degree on the starting values obtained from the previous computations. This is an effect of the large condition number of the MMP matrix. It does not mean that the results are completely different. When the first stopping criterium is met, one has the same accuracy of the results although the parameter sets are different.

Figure 7 gives some more precise information on the frequency dependence of the first MMP parameter. Note that this parameter corresponds to the zero order of the first multipole. Zero orders typically have relatively large parameters with a smooth frequency dependence. As one can see, the Givens and the CG procedures already lead to different parameters at relatively low frequencies. At sufficiently high frequencies one cannot observe any correlation between the different functions. Obviously, there is a stronger correlation for the parameters of the first model with 5 multipoles than for the parameters of the second model with 7 multipoles. This effect is caused by the larger condition number of the matrix of the second model. As one can see from Figure 8, the residuals of the CG computations of the two models remain almost constant even at frequencies where the corresponding parameters are completely different. One can also recognize that the large condition number of the second model causes problems for the CG computation at high frequencies. For a third model with 9 multipoles, the condition number is so high, that the second stopping criterium of the CG algorithm is already met at relatively low frequencies.

Figure 9 illustrates that there is a good correlation between the residual and the average of the error along the boundary. In Figure 9 one can see the same effects as in Figure 8.

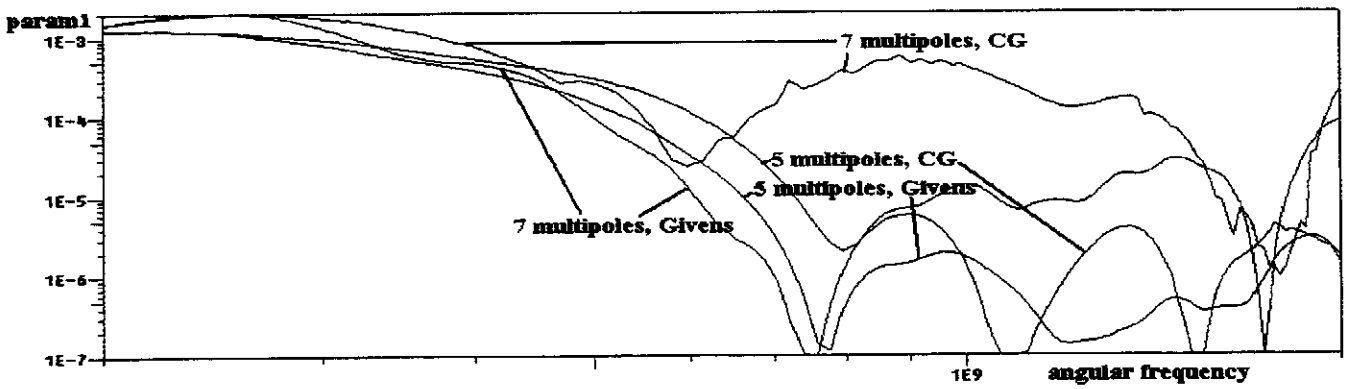

Figure 7: Frequency dependence of the first parameter of the MMP expansion, i.e., the zero order of the first multipoles located on the x axis. The parameter obtained with two different models (5 and 7 multipoles) and with two different methods (direct Givens matrix solver and iterative CG matrix solver with the same stopping criterium as in Figure 6) is shown.

The parameter estimation that has been used up to now is simple and crude. The parameter set of the previous computation is used as a starting value. This corresponds to a zero order extrapolation. Of course, one can expect more accurate parameter estimations from extrapolations with higher order power series approximations of the functions A_k (f). For an n-th order extrapolation at least n+1 values $A_k(f_i)$ must be stored. Since the computation time required for the parameter extrapolation is small, this seems to be reasonable. As one can see from Figure 10 and from Table 1, the first order PET allows one to considerably reduce the number of CG iterations, but the second order PET is much worse. Note that an average of less than two iterations is obtained for the models with 5 and 7 multipoles when a first order PET is applied.

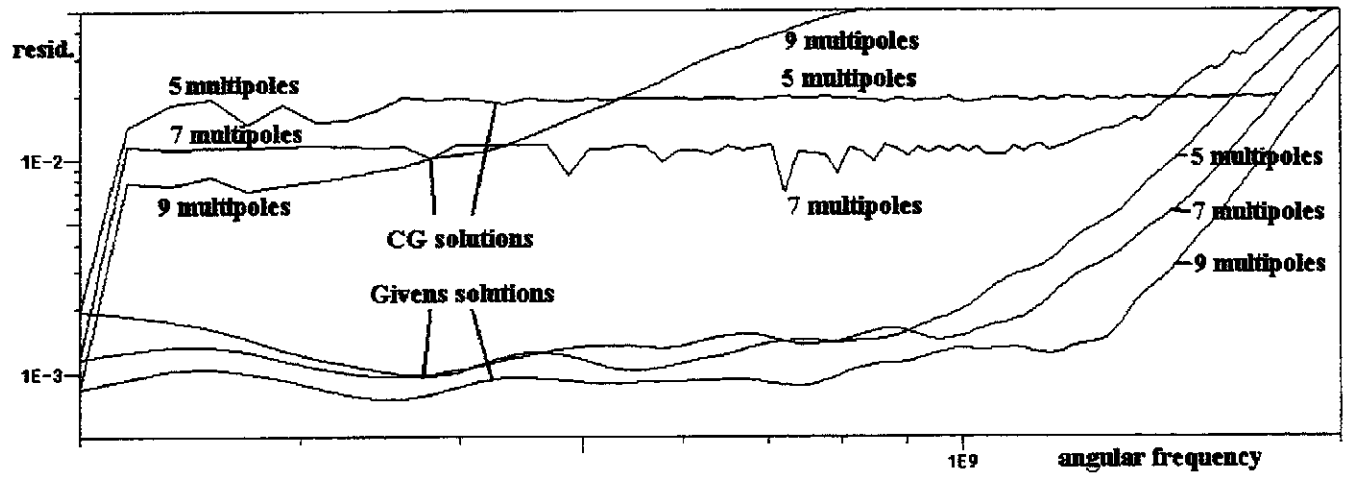

Figure 8: Frequency dependence of the residual (square root of the sum of the squares of the weighted residuals) of the test example, obtained with three models (5, 7, 9 multipoles) and two different methods (direct Givens matrix solver and iterative CG matrix solver with the same stopping criterium as in Figure 6). The residual of the CG computation with 5 multipoles is almost constant (slightly below the value of the first stopping criterium) up to the critical frequency where the first stopping criterium can no longer be met. Above this frequency, the CG and Givens residuals are almost identical. The residuals of the CG computations with more than 5 multipoles already increase before the critical frequency is met. This effect is caused by the large condition numbers of the corresponding matrices.

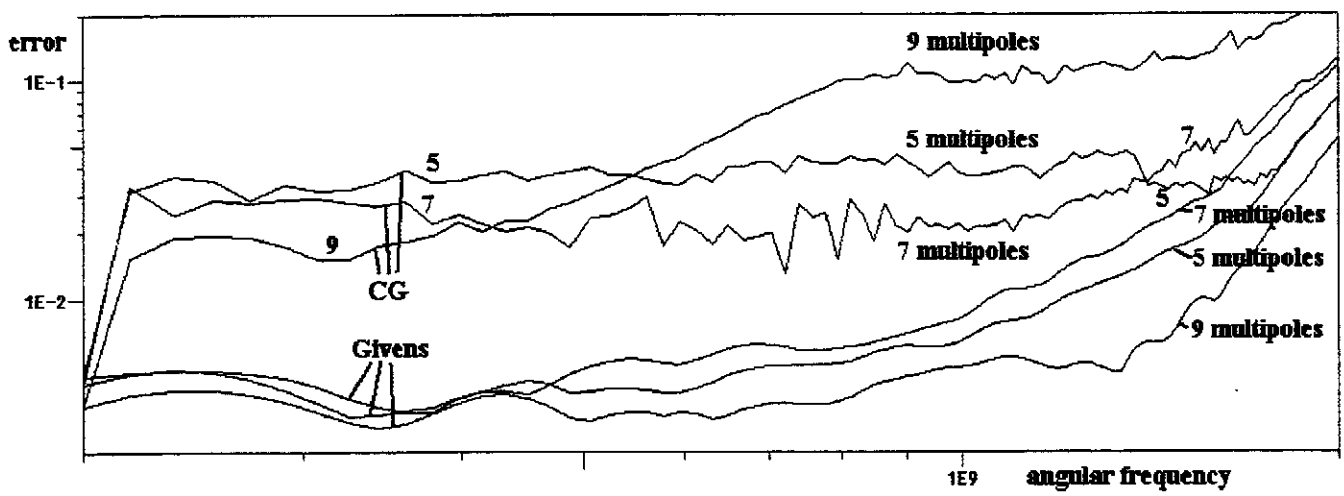

Figure 9: Frequency dependence of the average of the error (mismatching) along the boundary of the test example for the same computations as in Figure 8.

It is important to note that the computation time required for performing a few CG iterations is far below the computation time for the elements of the MMP matrix. Therefore, it is reasonable to increase the frequency steps. One might expect that the number of iterations required for one frequency step is at least proportional to the size of the frequency step. As one can see from Table 2, fewer iterations are required. Therefore, the total number of iterations can even be reduced when the frequency step is increased.

It is hard to estimate the optimal length of a frequency step because it depends on various parameters. At low frequencies, the frequency dependence of all parameters is very smooth and very large steps can easily be performed (see Table 3).

PET order	number of multipoles				
	5	7	9	11	13
0	3.4	2.9	5.1	11.5	8.4
1	1.8	1.9	2.5	7.2	4.2
2	24	24	25	29	26

Table 1: Average of the iterations required for the CG algorithm for different MMP models with 5-13 multipoles and for different orders of a PET with power series. The frequency is traced starting at the lowest frequency (3E7 Hz) with a logarithmic frequency scale up to the highest frequency (3E8 Hz). The total number of frequencies shown here is 98. The factor of the first stopping criterium of the CG algorithm has been set to a relatively low value (3) in order to obtain relatively large numbers of iterations.

PET order	number of multipoles				
	5	7	9	11	13
0	11	7.4	18	29	22
1	9.4	7.9	15	28	22
2	14	15	15	32	25

Table 2: Average of the iterations required for the CG algorithm for different MMP models with 5-13 multipoles and for different orders of a PET with power series. Same computation as in table 1 with 10 instead of 98 frequency steps.

multipoles	5	7	9	11	13
iterations	1.8	1.5	1.9	1.8	1.7

Table 3: Average of iterations required for the CG algorithm for different MMP models with 5-13 multipoles, first order PET. Same computation as in table 2, but the frequency is traced from 3kHz up to 30MHz with 10 steps only.

When the frequency step is relatively large, one might wish to know the EM field and derived quantities in between. Instead of setting up the corresponding MMP matrix and computing the corresponding parameters, one can estimate the parameters by an n-th order interpolation. Since interpolations are much more reliable than extrapolations [2,3], the parameters can usually be accurately estimated. Therefore, the matrix setup and solution can be avoided by an appropriate PET. In more complex situations, where the interpolations might be inaccurate, adaptive methods might be applied.

Note that all parameters can simultaneously be estimated with the same expansion functions. This helps to keep the computation time of the PET very small even for relatively large orders.

The disappointing results of higher order PET can be removed by more sophisticated extrapolation techniques as discussed in [2,3]. For example, one can use more than n+1 values of the parameter to be estimated with an n-th order approximation. This requires the introduction of appropriate weight and leads to overdetermined systems of equations that are similar to the matrix equations of the MMP codes. Appropriate weights for third order PET for our test examples have been found that reduce the number of CG iterations to one even for quite large frequency steps. But the optimization of the weights is extremely time consuming and these weights are not appropriate in general. Instead of power series, one can apply other types of expansion functions. However, more sophisticated techniques require more experience and the simple first order PET is already very efficient.

It should be mentioned that the CG procedure has been replaced by other iterative techniques. So far, CG is the most efficient algorithm that has been tested. It is important to note that the CG algorithm has to be applied to the rectangular MMP matrix M rather than to the normal equations with the symmetric matrix M*M because of the large condition number of M. Therefore, most of the available CG algorithms and preconditioners cannot be applied.

Conclusion

The PET presented in this paper is a very powerful and promising new technique that can be applied as a power booster to many numerical codes. It takes advantage of

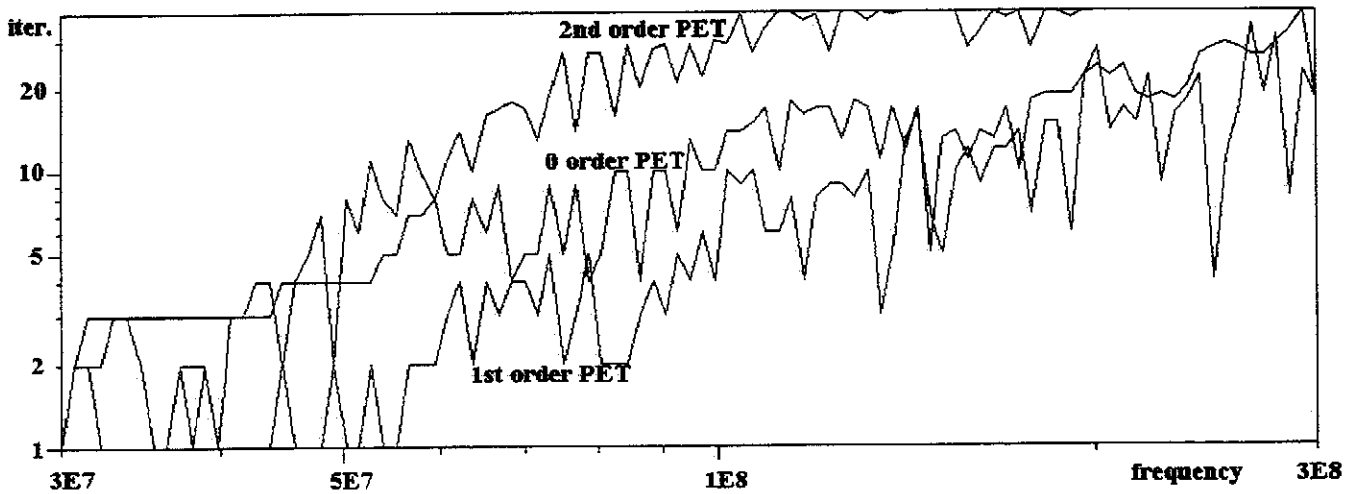

Figure 10: Frequency dependence of the number of iterations required for the CG algorithm when a PET of different order is applied. The frequency is traced from the lowest frequency upward with a logarithmic frequency scale. The total number of frequencies for the entire decade shown here is 98. The factor of the first stopping criterium of the CG algorithm has been set to a relatively low value (3) in order to obtain relatively large numbers of iterations. Moreover, an ill-conditioned model with 11 multipoles has been used.

the a priori knowledge obtained from previous computations and allows one to replace direct matrix solvers by efficient iterative matrix solvers even when the condition of the matrix is so bad that the iterative matrix solvers fail without the PET.

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