'A Priori' Knowledge, Non-Orthogonal Basis Functions, and Ill-Conditionned Matrices in Numerical Methods

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Abstract

Many terms and ideas used in numerical methods have their origin in analytical mathematics. Despite the well-known discrepancies between number spaces of computers and those of good old mathematics, the consequences of applying mathematical theorems to numerical methods and the importance of physical reasoning are often underestimated. The objective of this paper is to demonstrate that introducing 'a priori' knowledge of a problem into a numerical code can lead to superior numerical techniques but it may violate analytic dogmas at the same time.

Introduction

It was essential for Isaac Newton to benefit from introducing the infinitesimal calculus into physics. Although Newton himself developed concepts of matter close to post-modern fractals, the infinitesimal calculus forced people to consider space, time, and functions of space and time to be continuous. "Real numbers" that were believed to represent chaos (Johannes Kepler) replaced integers and Euclids geometry. Maxwell theory was the culmination of the idea of continua: Space, time, field, everything was considered to be continuous and extending to infinity. Thus, Maxwell's theory was much more consistent than Newton's theory in which the mass points did not really fit the idea of continuity. Although this convinced Einstein to develop even more powerful field theories, problems soon arose. Integers struck back. This was the beginning of quantum mechanics with its strange finite number spaces and probability concept. Ironically, the computer is unable to directly understand Maxwell theory, the most important theory of electromagnetics that still is essential for the construction of today's computers. Real numbers, infinity, continuity, and random numbers are far away from computer architecture. Thus, one cannot exactly apply most of the well-known theorems in classical mathematics to develop algorithms for computers. Such theorems can even be misleading.

The first mystery in computational mathematics is the following. Analytically one usually works in function spaces with an infinite number of dimensions. The number of dimensions is often uncountable. For computers, this number must be finite and preferably relatively small. I.e., one has to omit an infinite number of dimensions. Nonetheless, one can obtain useful results. For example, the number of basis functions or the dimension of the function space of a Fourier integral is uncountable infinite, whereas the number of basis functions of Fourier series is countable infinite. Obviously, Fourier integrals cannot be evaluated numerically, except when the function behaves well, i.e., is sufficiently simple. At first glance, it seems that nature is so kind with us, that we often can use Fourier

integrals. But in fact, we usually simplify our models of nature to such an extent that our methods work. For example, we know that absolutely flat surfaces do not exist in real world, but we work with such surfaces in most of the numerical models. Again, nature is really kind: We obtain useful results.

If we consider the approximation of continuous functions, flat surfaces, etc. by computers, we find another mystery. The approximations of real numbers, continuous functions, surfaces, etc. made by computers are rough rather than continuous or flat. The situation can be illustrated by Newton's mirror. To obtain a mirror, Newton polished metal. He knew that the surface initially is rough. Thus, the rays of light are reflected in very different directions. He did recognize that polishing made the surface less rough but never eliminated the roughness completely. Thus, the rays of light should always be reflected in very different directions and one should never obtain a mirror. Newton did introduce the concept of a kind of fluid on the surface of the metal. The rays are reflected by this fluid rather than by the surface of the metal. This explained why there are mirrors. Since Maxwell, we "know" that this is the effect of the wavelength. However, the computer approximates flat surfaces in the analytic model by rough surfaces. Although this is an essential discrepancy, we get useful results.

Of course, we cannot do whatever we want for obtaining useful results. Provided that we are not pure mathematicians, the results we are looking for have a certain meaning and usually are compared with measurements. If we consider the huge difference between measurement, analytical model, and numerical computation, the fact that we can get useful results again is a miracle. However, it is very important to note that we often introduce some 'a priori' knowledge in order to obtain useful results. This can be done to discard wrong results like spurious modes but also in the modelling and in the design of codes. For example, all adaptive methods use a certain kind of 'a priori' knowledge, i.e., the data obtained from previous computations. Since it is such a big miracle that we are able to simulate measurements by computations, the 'a priori' knowledge is extremely important. It can even be used for entirely removing the theory, e.g., Maxwell theory, from the code. This is obviously true for heuristic codes, but one can also try to implement codes that directly analyze measurements, find a theory, simulate, and predict measured data. However, the power of 'a priori' knowledge should not be underestimated. Numerical codes that ignore 'a priori' knowledge (some mathematicians might like such codes) turn out to be inefficient in most cases. As people should be able to learn from each other or from previous generations, a numerical code should at least take advantage of some a priori knowledge of its designer or of its user.

In many series expansions, for example, Fourier series, the basis functions are ordered. This is important for counting the basis functions and above all for defining the convergence. It is well known that convergence is important for the efficiency of a numerical method, but the analytic proof of convergence for any series expansion is not sufficient in practice. Instead, we need a sufficiently fast convergence. On the other hand, one can also obtain useful numerical techniques with asymptotic and other series that do not converge at all. When 'a priori' knowledge is considered, one often can eliminate some of the basis functions in ordered series. For example, symmetries often lead to such reduced sets of basis functions. But one can even obtain completely different, somewhat "chaotic" series expansions. For such expansions, the term "convergence" sometimes cannot even be defined. Nonetheless, they can be very powerful.

The basis functions of many series expansions are orthogonal. The orthogonality considerably simplifies the computation of the coefficients of such series. Thus, destroying the orthogonality seems to be a sacrilege. It is important to note that orthogonality always depends on the definition of a scalar product. In computational electromagnetics, the definition of the scalar product depends on the modelling and can be different from the scalar product with respect to that the basis functions are orthogonal. Although the basis functions are orthogonal in a certain sense, they are often non-orthogonal with respect to the scalar product that actually is used*. Orthogonalization procedures are very time consuming. Therefore it is not reasonable to use them. Numerically, working with non-orthogonal functions is quite simple, provided that the functions are not almost linearly dependent. One usually obtains matrix equations that can be solved with many well-known algorithms. Again, analytic mathematics created the term of linear dependence. However, the requirement of linearly independent basis functions in a numerical code is not enough in general. It is quite cumbersome to detect "almost dependent" basis functions. A well-known measure is the condition number of the matrix. A large condition number means that the matrix is ill conditioned, whereas the "optimal" condition number (which is one) can be obtained when orthogonal basis functions are involved. It will be demonstrated in the following sections that one can obtain more accurate results by increasing the condition number. There are two "optimal" condition numbers: one that only considers the matrix and another that considers the results. The latter can be considerably bigger than the former. Thus, improving the condition of a matrix or using even orthogonal functions may have undesired effects.

Intelligent Fourier Analysis

Fourier integrals usually are applied to time-dependent functions defined in the interval $-\infty < t < \infty$. It is considered to be true that the "real" time of our universe has finite upper and lower limits. Every measurement has even much more restrictive upper and lower limits. In such a finite time interval, Fourier integrals can be replaced by the much more simple Fourier series. In fact, the harmonic functions used as basis functions in the Fourier integrals are orthogonal provided that an appropriate scalar product is defined on the interval $-\infty < t < \infty$. On a finite interval, no scalar product can be defined in such a way that all basis functions used in the Fourier integral are orthogonal, whereas it is no problem to find a scalar product that makes the basis functions of the Fourier series

* For example, the functions $r^n \cos n\varphi$ and $r^n \sin n\varphi$, where $r\varphi$ are polar coordinates and n is an integer number, are orthogonal if the scalar product is defined as $(f,g) = \int_{r=0}^{\infty} \int_{\varphi=0}^{2\pi} fgr\mathrm{d}r\mathrm{d}\varphi$. The functions $r^n \cos n\varphi$ and $r^n \sin n\varphi$ can be used for solving the Dirichlet problem in a bounded 2D domain D. Depending on the numerical method, a scalar product is applied that is defined either on the domain D or on its boundary ∂D. For example, $(f,g) = \int_{\partial D} fg\mathrm{d}s$. With respect to such a scalar product, the functions are non-orthogonal, except when ∂D has a very special shape.

orthogonal*. Obviously, the basis of Fourier series is obtained from the basis of Fourier integrals by erasing most of the basis functions, i.e., the biggest part of the spectrum in such a way that a discrete spectrum is obtained. Thus, one has the same effect as when one takes very high symmetries (symmetry groups with an infinite dimension) into account for any series expansion.

It is obvious that the numerical computation of Fourier series is much simpler than the one of Fourier integrals. There seems to be no reason for Fourier integrals since neither "real" time nor the time intervals of measurements are infinite. But if one considers the spectra of practical functions, one often finds a behavior that can much better be approximated by Fourier integrals (with a practically limited spectral domain). Thus, the approximation of functions in a finite time interval by functions defined on an infinite time interval often is reasonable.

Let us now assume that a function f is defined in the interval $-\infty < t < \infty$ and f can be expanded by a Fourier integral with a finite spectrum. If this function is measured in a time interval $0 < t < T$, it can be expanded by a Fourier series. If we assume that the measured function f^0 is known exactly in every point of the interval, the spectrum of the Fourier series turns out to be discrete and infinite, i.e., the spectra of f and f^0 turn out to be completely different. If we compute the Fourier series of f^0 outside the interval $0 < t < T$, we find that this is a periodic function with the period T. Thus, the "true" function f and the expansion of the measured function f^0 are completely different outside the interval $0 < t < T$ even in the best case, where the measurement of f^0 is exact in the entire interval. As a consequence, the Fourier series cannot be used to predict the behavior of f for $t > T$ even when t is not much bigger than T, as the following discussion illustrates.

For reasons of simplicity, we now assume that f simply consists of two harmonic functions, for example,

$$f = A \cos \omega_A t + B \cos \omega_B t.$$

(See figure 1.) Note that f is not periodic at all when ω_A/ω_B is irrational. If we measure f in a finite number of points $k\Delta t$, $k = 1, 2, ...K$, we easily can approximate it by a Fourier series. Usually, we will not be so lucky that both frequencies ω_A and ω_B are in the discrete spectrum of the Fourier series. Nonetheless, from a pure mathematical point of view, everything is fine: 1) The basis functions of the Fourier series are orthogonal with respect to an appropriate scalar product defined on the interval $0 < t < T$. 2) The condition number of the corresponding matrix is one. 3) The system of equations can be solved with any algorithm. 4) Iterative matrix solvers converge in only one step, and so on. But there are two important drawbacks: 1) The convergence is quite bad in most cases. 2) The prediction of f outside the interval of the measurement is completely useless. Figure 2 illlustrates this.

* This is quite clear because the number of independent basis functions is infinite but countable – otherwise, the set of basis functions of the Fourier series would be incomplete. Since the number of basis functions of a Fourier integral is incountably infinite, there must be incountably many dependent functions, and dependent functions never are orthogonal.

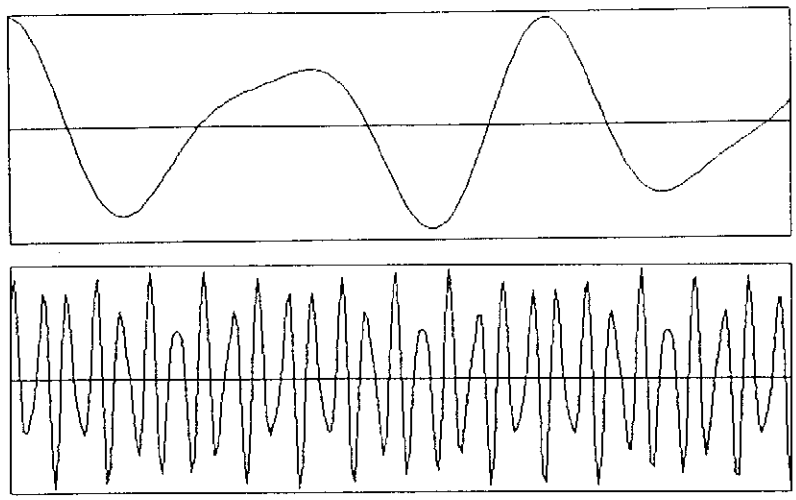

Figure 1 Function $f(t) = \cos(18\pi t) + 0.4\cos(28\pi t)$. Top: in the interval $t = 0...2$ used for sampling and expanding it. Bottom: In the time interval $t = 0...20$ used for computing the error function.

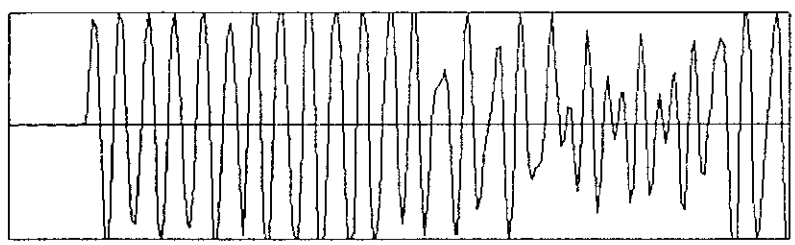

Figure 2 Error obtained when a Fourier series is applied to approximate $f(t) = \cos(18\pi t) + 0.4\cos(28\pi t)$. Note that the condition number of the matrix is one.

If we want to apply Fourier integrals with a finite spectrum to approximate the same function measured in the same points, we recognize that we do not know how to choose the limits of the spectrum. Moreover, the spectral domain needs to be discretized for numerical integration. Finally, the basis functions are no longer orthogonal on the interval $0 < t < T$. Here, some 'a priori' knowledge, for example, an estimation of the limits of the spectrum, can be very helpful.

When we do not have any 'a priori' knowledge or when we are too lazy to care about it, the computer can try to get it from analyzing f^0. An idea how this can be achieved is the following: 1) Assume that f^0 can be approximated by a single harmonic function and compute its amplitude, frequency ω_1, and phase. The computation of the frequency requires a nonlinear optimization. Moreover, a least squares procedure (best fit) is reasonable here. 2) Since the frequency estimated in the previous step probably is inaccurate (this is often typical for 'a priori' knowledge), use now several frequencies ω_{1i} which are close to ω_1. The differences $\omega_{1i} - \omega_1$ depend on the accuracy of the estimation of ω_1. The estimation of this accuracy is another problem that is not considered here. 3) Approximate

f^0 by the series

$$f^1 = \sum_i^I A_{1i} \cos \omega_{1i} t + B_{1i} \sin \omega_{1i} t.$$

Note that the basis functions in this expansion are almost linearly dependent and that the condition number of the matrix to be solved turns out to be very bad when the differences $\omega_{1i} - \omega_1$ are very small. Obviously, the better ω_1 is estimated, the worse the situation becomes, i.e., the more accurate the 'a priori' knowledge, the worse the condition of the matrix. Thus, it is extremely important that the method for computing the unknowns does not fail when the condition is bad. Here, it is strongly recommended to use Generalized (weighted) point matching [1,2] with an overdetermined system of equations that is directely solved with QR decomposition or even singular value decomposition. 4) Compute the error function $e = f^0 - f^1$ and analyze e as you did analyze f^0, i.e., estimate the frequency ω_2, add a set of basis functions $\cos \omega_{2i} t$, $\sin \omega_{2i} t$, compute the parameters in the series expansion. Of course, this procedure can be repeated. Since we only have two harmonics in our original function f, this is not necessary here. The figures 3 and 4 illustrate this for 3, 5, and 7 basis functions per frequency. Note that one can not only analyze the function and errors in the time domain but also the spectrum in the frequency domain. From the latter one often can obtain more accurate estimations of the frequencies which directly leads to an iterative improvement of the results. The biggest advantage of this procedure is the fact that one can predict f outside the interval where it has been measured. Moreover, the number of basis functions required can considerably be reduced and the accuracy of the approximation in the interval $0 < t < T$ is much better than for the Fourier series. Concerning the condition of the matrices, the following behavior is important: when the number of basis functions ω_{ki} per estimated frequency ω_k is increased for a fixed maximal difference $|\omega_{ki} - \omega_k|$, the condition number is increased but the results obtained are at first improved. The point where the results become worse depends on the problem but also on the numerical method used for computing the parameters in the series expansion. At this point the condition can be very bad, when a good numerical technique is applied. Maybe, the badness of the condition is even a measure for the quality of the method.

Note that the function $f(t) = \cos(18\pi t) + 0.4 \cos(28\pi t)$ used for testing the "intelligent" procedure is periodic because 18/28 is rational. Thus, one can apply a Fourier series. This is very sucessful when one knows the actual length of the period T_a. Since T_a is much larger than the interval T where the function is measured, the basis functions of the Fourier series are non-orthogonal with respect to a scalar product defined on the interval $t = 0...T$ and the matrix turns out to be ill-conditioned. Of course, the knowledge of T_a is an 'a priori' knowledge as well.

Computational Electromagnetics with the MMP Code

Computational electromagnetics is a considerably more complex task than the approximation of functions by a series expansion with a given set of basis functions. But essentially most of the codes for computational electromagnetics use either explicitely or implicitly a

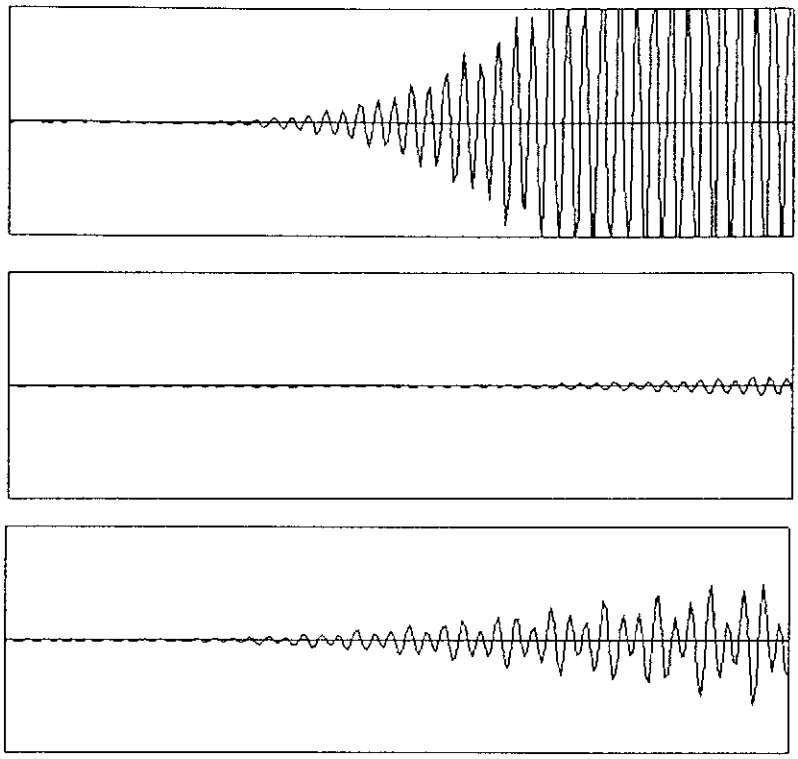

Figure 3 Error obtained when the "intelligent" procedure is applied to approximate $f(t) = \cos(18\pi t) + 0.4\cos(28\pi t)$. Top: Two times three non-orthogonal basis functions. The condition number of the matrix is 425. Middle: Two times five non-orthogonal basis functions. The condition number of the matrix is $9.7E6$. Bottom: Two times seven non-orthogonal basis functions. The condition number of the matrix is $1.0E8$. All computations with single precision.

similar expansion of the electromagnetic field. Thus, one can find similar effects as shown in the previous section.

The MMP code [3,4] is very closely related to analytic solutions of the Maxwell equations. In each domain, the field F is approximated by

$$F = F^0 + \eta = \sum A_i F_i + \eta$$

where η is an unknown error function, A_i are the unknown parameters to be computed, and F_i are known solutions of Maxwell equations in the corresponding domain, playing the role of basis functions. Obviously, the approximated field F^0 automatically fulfills Maxwells equations in the corresponding domain and the parameters A_i have to be computed in such a way that the boundary or continuity conditions are fulfilled numerically. In the MMP code, multipole fields are preferred basis functions F_i but many other functions are available as well. It is well known that the quality of the results depends not only on the basis functions but also on the technique used for computing the parameters.

It is very clear that simple techniques can be applied when the basis functions are orthogonal. Actually, multipole functions are orthogonal when a scalar product is defined

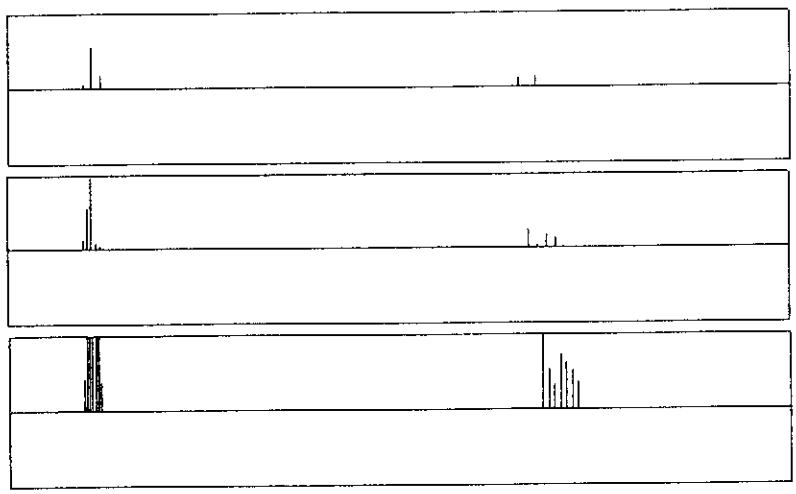

Figure 4 Spectrum obtained when the "intelligent" procedure is applied to approximate $f(t) = \cos(18\pi t) + 0.4\cos(28\pi t)$. Top: Two times three non-orthogonal basis functions. Middle: Two times five non-orthogonal basis functions. Bottom: Two times seven non-orthogonal basis functions. Note that the large amplitudes in the last spectrum indicate that there are severe cancellations in this computation.

everywhere in space. But this not relevant for the numerical computation of the parameters since the boundary conditions do not hold everywhere in space. When a scalar product is defined on the boundaries of the domains, the multipole functions are no longer orthogonal – except for very special and simple cases. Thus, one has to deal with non-orthogonal basis functions anyway. Unfortunately, Simple MultiPole (SMP) expansions that have successfully been used for relatively simple geometries [5] do not converge rapidly in most cases and are useless for more complex geometries. To overcome this drawback, Multiple MultiPole (MMP) expansions have been proposed [6] wherby most of the scientists discarded the SMP approach in favor of the Method of Moments (MoM) [7].

In older codes based on SMP expansions the parameters have been computed using Simple Point Matching SPM on the boundaries. It is very imortant to recognize that SPM is a relatively weak method that does not work unless the matching points are selected appropriately. There seems to be a relatively strict relation between the basis functions and the appropriate locations of the matching points. If SMP expansions are replaced by MMP expansions, it is extremely hard to find appropriate locations for both the multipoles and the matching points. This is a reason for abandoning not only SMP but also SPM and replacing it by defining a scalar product and performing a projection on a certain set of testing functions. People working with MoM have noticed that there is some relation between the numerical computation of the scalar products and the matching

points [2]. When one uses more points to compute the integrals in the scalar products than the number of unknown parameters, one obtains an equivalence with the weighted point matching technique. This technique is essentially the same as the Generalized Point Matching (GPM) that has already been used in the early versions of the MMP code [8] for removing the problems of SPM with MMP expansions. In GPM the numerical equivalence mentioned above has been used for deriving an appropriate geometrical weighting of the equations. In addition, a physical and a user defined weighting is implemented in the MMP code, and continuity equations for all components of the electric and magnetic field are usually imposed.

Although GPM is numerically equivalent to a projection method with trapezoidal numerical integrations and Galerkin's choice of testing functions [1], it is very important to note that the overdetermined system of equations $AP = G$ obtained from GPM is solved directly in the MMP code using a Givens updating based on QR decomposition, whereas the projection method usually applied in MoM codes leads to the square system $A^*AP = A^*G$. Solving $AP = G$ directly is numerically superior to solving $A^*AP = A^*G$. In fact, the latter is useless when the condition of the matrix A is not sufficient. Mathematicians might believe that this is no drawback because ill-conditioned matrices should be avoided anyway. But we did already see in the previous section that one can obtain numerically more accurate results with "worse" matrices with larger condition numbers. Exactly the same effect can be shown using the MMP code.

Actually, the computation of the condition number of a matrix is quite cumbersome. Some algorithms like Cholesky decomposition [9] allow to estimate it but this estimation is very inaccurate and it is always too high. Singular value decomposition can be performed to compute the condition number accurately. This requires the storage of relatively large matrices and is quite time consuming. For these reasons, singular value decomposition is not implemented in the usual version of the MMP code, but it is contained in a testing version of the 2D MMP code. In addition to the singular value decomposition, the columns of the matrix A must be scaled. The column scaling does not affect the results in most cases – in some cases it even leads to slightly worse results because of the additional numerical operations – but it is important for iterative matrix solvers and for the condition number. For example, when the scattering of a plane wave from a circular cylinder is computed with the MMP code, the basis functions are orthogonal and the condition number is one if the columns of the matrix are scaled. Otherwise, a typical condition number is 10000 and depends on the frequency and size of the cylinder.

For demonstrating that the accuracy can be improved when ill-conditioned matrices are used, a 2D counterpart of the famous 3D ACES cylinder [10] has been considered with a vertically incident plane wave. A cylinder with a height of one wavelength and a width of 0.4 wavelengths (see figure 5) has been computed with 2D MMP. The matrix to be solved had 82 rows and 45 columns. I.e., the system was slightly overdetermined. On the long symmetry axis of the cylinder, M multipoles were set with equal distances between their origins, according to the MMP rules discussed in [1]. When an SMP expansion, i.e., only one multipole, was used, the result turned out to be completely wrong because of the "wrong" locations of the matching points. But for more multipoles, useful results have been obtained (see table). Note that the orders used for the different multipoles have been varied in such a way that always 45 unknowns have been obtained. Of course, both the condition number and the error depend on the distribution of the orders of the poles but this problem is not considered here. In the computation of the example, the horizontal

symmetry axis has been used for reducing the computation time. One multipole has always been set in the center. Because of the symmetry operations one effectively has $2M - 1$ multipoles when one sets M multipoles with one multipole on the axis. This explains why only odd numbers are contained in the table below. The error number is computed by the MMP code and contains the mismatching of all field components on the boundary. It is a relatively reliable measure and usually turns out to be considerably higher than the error estimated by other codes, for example, [11].

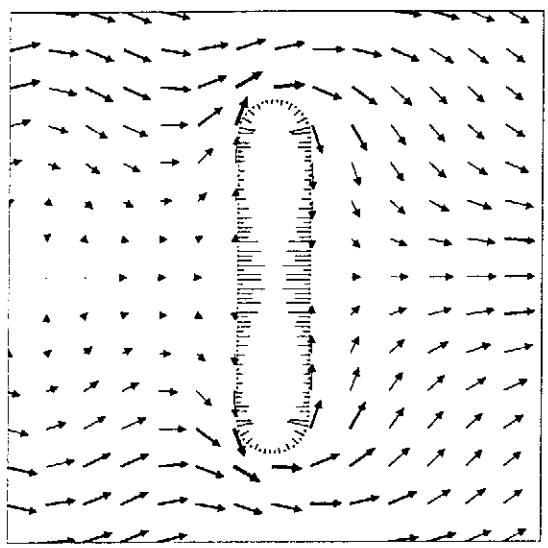

Figure 5 Scattering at a 2D "ACES-shape" cylinder used as an example to test the condition numbers and the MMP errors for different MMP expansions. Time average of the Poynting vector field and error distribution in the matching points for a total number of 11 multipoles. The condition number $5.5E5$ is already quite high but obviously the results are very accurate. Computation with double precision.

Condition Number and Error in Function of Multipoles
for a 2D Conducting ACES-Shape Cylinder

Multipoles	Condition Number	MMP Error
3	2.6E2	5.4E-1
5	7.8E2	9.3E-3
7	1.3E4	5.2E-3
9	1.3E5	2.2E-3
11	5.5E5	2.9E-3
13	2.4E6	3.7E-3

If one considers the table above, one will recognize that the optimal result is obtained with 9 multipoles where the condition is already quite bad. Since the condition number is considerably increased between 5 and 7 multipoles, a code that is not able to handle ill-conditioned matrices might lead to optimal results when only 5 multipoles are used. Since the example is very simple, the condition numbers remain moderate. For more complex applications, very high condition numbers can be obtained. In this case, even QR and singular value decomposition fail. But good results have been obtained with block-iterative matrix solvers [12].

Note that 'a priori' knowledge is very important in the MMP code. 1) Some 'a priori' knowledge is used in the modelling, where the user defines the matching points. The GPM in the MMP code allows to set much higher matching point densities near critical points, i.e., points where the user assumes 'a priori' that the field varies considerably. This would not be possible or at least not to same extent with SPM. 2) The setting of the multipoles can be done with 'a priori' knowledge. Many simple rules have been established for this purpose and the graphic MMP editors contain semi-automatic procedures for the pole setting. 3) When a rough model has already been computed, one can use a lot of 'a priori' knowledge for improving the model. In this case, the MMP code even allow to introduce the field computed from a previous run (eventually with a different model) as a new basis function called "connection" [13,1]. Connections can lead to excellent results with ill-conditioned matrices.

Conclusion

It has been demonstrated that terms known from analytic considerations and goals like orthogonal basis functions and small condition numbers of matrices can be misleading and prevent engineers from designing useful codes for computational electromagnetics and similar tasks. Introducing 'a priori' knowledge in numerical codes requires open structures and often leads to ill-conditioned matrices. Thus, it is important to develop and apply methods for handling such matrices, for example, the generalized point matching used in the MMP code instead of the projection technique used in many MoM codes.

Mathematicians usually derive theorems and algorithms for certain classes of functions. For them, all possible solutions are of the same interest. Engineers often look for very special, physically meaningful soltions. Although algorithms able to approximate any solution can naturally be used for approximating special solutions, they are inefficient compared with more specialized or more intelligent algorithms. Similarly, mathematical theorems can be useless for engineers. An engineer who wants to simulate, for example, the scattered field for a certain geometry and for a given incident wave, has to find a relatively small set of basis functions allowing to approximate the solution with the desired accuracy. A mathematical proof of the completeness of a certain set of infinitely many basis functions allowing to approximate, for example, all regular solutions for any incident wave and for any geometry is neither necessary nor helpful. The important question "how many basis functions are required to solve a given problem with the desired accuracy?" is never answered by mathematicians. This big discrepancy between classical mathematics and

engineering forces us to invent new, efficient, and intelligent codes that are not based on a "solid" mathematical foundation.

Design of intelligent codes does not only mean to gather a lot of knowledge from books and papers but also to violate analytic dogmas for testing whether they still hold in the age of computers.

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