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Method of analytical regularization in computational photonics

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Abstract We discuss the advantages of the conversion of electromagnetic field problems to the Fredholm second-kind integral equations (analytical regularization) and Fredholm second-kind infinite-matrix equations (analytical preconditioning). Special attention is paid to specific features of the characterization of metals and dielectrics in the optical range and their effect on the problem formulation and on the methods applicable to the mentioned conversion.

1. Introduction

Optical antennas, sensors, absorbers, lasers, and other devices of contemporary optics and photonics can possess one or more dimensions comparable with and even smaller than the light wavelength and have to be analyzed in infinite spatial domains. In terms of their modeling, this leads to the so-called exterior problems for the electromagnetic field. Further, by many reasons, the time-harmonic-field simulations ($\sim e^{-ikct}$, k and c being the free-space wave number and light velocity, respectively) give the most important amount of engineering information. This brings us to the analysis, which considers the wave scattering and radiation as phenomena modeled with the aid of the boundary value problems for the time-harmonic Maxwell and Helmholtz equations. Such problems possess a very valuable property: if the scatterer is passive (no active regions), then the uniqueness of their solution is normally guaranteed by a sufficient set of boundary conditions, edge conditions (or, equivalently, local power boundedness condition), and radiation conditions.

Today, there are many ways to look for solutions of Maxwell equations. For instance, one may try to find it by using finite-difference discretizations of the partial differential equations. However, the associated problems of domain truncation, "good" exterior meshing, and solving extremely large matrices block the ways for achieving a high accuracy. To avoid these pitfalls, Green's function methods can be used as explained, for instance, by *Colton and Kress* [1983], leading to various integral-equation (IE) formulations. Of the many advantages of IE approach, two main points have to be emphasized. The first is that the radiation condition is automatically taken into account by the proper choice of the Green's function that enters (generally speaking, together with its derivatives) the kernels of IEs. The second is that only the *finite* domains or their boundaries need to be discretized. Still a direct discretization of IEs usually generates ill-conditioned dense matrices, and so something should be done to adapt these formulations to meeting the combined challenge of high speed (intrinsically, this implies small size of resulting matrices) and high accuracy of computations.

Many textbooks and journal papers on computational electromagnetics deal with IEs for determining the surface or polarization currents of two-dimensional (2-D) and three-dimensional (3-D) metallic or dielectric scatterers, respectively, given the incident field. Such IEs are obtained from the boundary conditions, and many types of them are first-kind IE and always have logarithmic-type or higher singular kernels. In the following discussion, we shall assume that when passing from the boundary value problem to an IE, uniqueness of solution is preserved (some types of IEs lose it on discrete sets of frequencies usually called "spurious eigenvalues"). As a rule, IEs are further discretized for a numerical solution with method of moments (MOM) by using the subdomain (collocations) or the entire-domain basis functions. Although this commonly brings meaningful and useful results, unfortunately, there are no any theorems proving universal MOM convergence or even the existence of an exact solution for such IEs, as noted by *Klien and Mittra* [1973] and *Dudley* [1985]. A widespread rule of thumb of taking at least 10 mesh points per wavelength is only a rule of thumb and by no means does it guarantee any number of correct digits.

A simple example of this sort is the logarithmic-singular IE for the 2-D *E*-polarized wave scattering from a perfectly electrically conducting (PEC) flat or curved strip. It is well known that here the condition number of the conventional MOM matrix grows with the number of equations [see *Fikioris,* 2001], thus making the matrix impossible to solve for accuracy better than several digits and a strip greater than 10–20 wavelengths according to *Klien and Mittra* [1973]. Nearly the same can be said of the MOM discretizations of second-kind IEs having strongly singular kernels. A good demonstration of what may sometimes happen to such algorithms was given by *Hower et al.* [1993]. By the simple example of 2-D plane-wave scattering from a tubular dielectric circular cylinder, it was shown that the MOM and finite difference time domain (FDTD) solutions could be 1000% or more in error in a vicinity of sharp resonance. The "pain points" of the conventional MOM approach have been excellently reviewed by *Dudley* [1985]; since then, essentially, nothing has changed. The final statement of *Dudley* [1985] is worth reciting: "It is misleading to refer to the result as *solution* when, in fact, it is *numerical approximation* with no firm mathematical estimate of nearness to solution." Although it is possible to eliminate ill conditioning by using specialized discretization schemes based on the Sobolev-space inner products, this appears to be a purely mathematical exercise, impractical in computations.

Meanwhile, there exists a general approach to overcome all of the mentioned difficulties. It consists in obtaining the second-kind IEs of the Fredholm type, with smoother kernels, from the first-kind equations. Discretization of these new equations, either by collocation or by a Galerkin-type projection on a set of basis functions, generates matrix equations, whose condition numbers remain small when the number of mesh points or "impedance-matrix" size is progressively increased. The approach mentioned is collectively called the method of analytical regularization (MAR) and can be found in *Nosich* [1999] and *Fikioris* [2001]. The term has apparently been introduced by *Muskhelishvili* [1953]; sometimes semi-inversion is used as a synonym. It is based on the identification and analytical inversion of the whole singular part of the original IE or its most singular component. It must be admitted that the whole idea of MAR can be traced back to the pioneering work of the founders of singular IEs theory, Hilbert, Poincare, and Noether, well before the first appearance of a computer.

For the sake of completeness, it should be also mentioned that convergent numerical solutions to electromagnetics IEs with smooth and singular kernels can be obtained using the Nystrom-type algorithms developed by *Tsalamengas* [2010a, 2010b, 2015], *Balaban et al.* [2012], *Bulygin et al.* [2012], and others. Such algorithms do not use partial inversion and, instead, rely on the theorems of approximation of integrals with quadratures. Their numerical performance is generally at the same level as those based on MAR although they do not allow analytical solutions in specific circumstances (see section 5) of nearly canonical shape or small optical contrast of a scatterer.

2. Electromagnetic Characterization of Materials in the Optical Wavelength Range

The optical range of wavelengths occupies the part of electromagnetic spectrum between 300 nm and 900 nm and presents specific features when it comes to the full-wave modeling of time-harmonic electromagnetic-wave scattering, absorption, and emission. These features are considerably different from what is common at microwaves and relate to the characterization of material properties of media and components. Explicitly, (1) there are no perfect electric conductors (PEC) in optics because even good metals like gold and silver have considerable bulk losses; high-quality dielectric materials can be assumed lossless; (2) for metals, both real and imaginary parts of their dielectric permittivities depend on the wavelength, i.e., they are functions rather than constants; high-quality dielectrics can have almost constant permittivities; (3) Metals behave like plasma (i.e., free electron gas in metal is responsible for its material properties); therefore, real parts of their dielectric functions show negative values as certified by the measurements done, for instance, by *Johnson and Christy* [1972]; and (4) for semiconductors under pumping, imaginary parts of dielectric permittivities can be negative, which corresponds to the material gain and eventually provides the lasing; the gain is a function of the wavelength.

From the viewpoint of modeling and computations all the above mentioned means that the PEC boundary conditions (ubiquitous at microwaves) should be discarded. Instead, even for good metals either the surface-impedance conditions [*Colton and Kress*, 1983] or dielectric-interface conditions [*Muller*, 1969] must be used. The choice between them depends on the thickness of the metal. Thinner-than-skin depth layers are partially transparent and hence call for the dielectric-interface description (although with one material treated as "negative dielectric"). Thicker layers allow neglecting the transparency and using the surface-impedance conditions, with metal's impedance showing "inductive" behavior.

Other conditions, which are included in the formulations of the electromagnetic-field boundary value problems in optics, remain as usual: the condition of local power finiteness and the radiation condition at infinity for the scattered field. These conditions guarantee that the solution, if it exists, is unique. Note that both the electric field IE for impedance scatterer and the Muller IE for dielectric scatterer are free of spurious eigenvalues.

It should be noted, in advance of further treatment that the "negative-dielectric" or "inductive-impedance" behavior of metals in the optical range is absolutely unusual with respect to the common experience with much lower microwave frequencies. It can be anticipated that this drastic difference can lead to something unusual in the scattering properties. Indeed, it leads to the appearance of optical *localized surface plasmon* natural modes [*Raether*, 1986] on metal particles of very small subwavelength size, i.e., on nanoparticles. If a metal sample is long enough, in at least one dimension, to be considered as infinite, then metal surfaces, nanostrips, and nanowires can guide the electromagnetic waves, i.e., possess the natural complex waves called *surface plasmon* (SP) waves (here, sometimes adjective *delocalized* is added).

3. Regularization as Transformation to a Fredholm Second-Kind IE

To present a formal scheme of MAR, assume that the boundary condition and some suitable integral representation of the unknown field function (e.g., using the potential theory) generate a first-kind singular IE. In operator notation, this can be written as

$$GX = Y, \tag{1}$$

where X and Y stand for the unknown and given function, respectively. A direct analytical inversion of G is normally not possible, while a numerical inversion, as has been mentioned, has no guaranteed convergence. Now split operator G into two parts: $G = G_1 + G_2$ and assume that the first of these has a known inverse, G_1^{-1}. Then, by acting with this operator on the original equation, one obtains a second-kind IE:

$$X + AX = B, \tag{2}$$

where $A = G_1^{-1}G_2$ and $B = G_1^{-1}Y$. However, this simply looking scheme is mathematically justified only if the resulting IE (2) is of the Fredholm type. This means that the operator A must be compact, e.g., has a bounded L_2 norm, $||A||_{L_2} < \infty$, and the right-hand side B must belong to the same space L_2, i.e., $||B||_{L_2} < \infty$. It is easy to see that compactness of A is achieved only if the inverted operator G_1 contains at least the most singular part of G, and hence, the operator G_2 is less singular than G and G_1. Then, all the power of the classical Fredholm theorems, found, for instance, in *Colton and Kress* [1983] and generalized for operators by *Steinberg* [1968] can be fully exploited. This proves both the existence of the exact solution, $X = (I + A)^{-1}B$ (where I stands for the identity operator) and the convergence by the l_2 norm of discretization schemes, without resorting to residual error estimations as commonly done for the first-kind IEs (see, e.g., *Dudley,* 1985).

Indeed, suppose that we have discretized the second-kind equation (2) by projecting it on some set of local or global expansion functions. Besides the obvious observation that such a set should possess the completeness in L_2, a matrix counterpart of (2) can be equivalent to IE only if this counterpart is infinite dimensional, and in this case the latter is a Fredholm second kind in the discrete space l_2 for the unknown expansion coefficients. Considering its "truncated" counterpart, with a matrix $A^{(N)}$ filled in with zeros off the $N \times N$ square (and similarly for the right-hand-part vector $B^{(N)}$), it is easy to show the following estimation for the relative computational error, by the norm in l_2:

$$e(N) \equiv \frac{||X - X^{(N)}||}{||X||} \le \mathrm{cond}(I + A)\left(\frac{||A - A^{(N)}||}{||I + A||} + \frac{||B - B^{(N)}||}{||B||}\right), \tag{3}$$

where $X^{(N)}$ is the solution of finite-dimensional matrix equation, $X^{(N)} + A^{(N)}X^{(N)} = B^{(N)}$, and $\mathrm{cond}\, C = ||C|| \cdot ||C^{-1}||$ is the condition number of matrix C; note that $\mathrm{cond}\,(I + A) < \infty$ thanks to Fredholm nature of (2).

It is clear that (3) is destined to go to zero with $N \to \infty$, as the first factor in the right-hand part above is a bounded constant, while the second is decreasing. Theoretically, in finite-digit arithmetic, this decrement is limited only by the machine precision. However, in practical computations it can be limited sooner by the accuracy of intermediate operations—e.g., the accuracy of numerical integration for filling in A. The rate of decay of $e(N)$ determines *the cost of the algorithm*, and this rate can be different for different ways of selecting the invertible singular part, G_1. Generally speaking, the best is to invert as much as possible of the singular part. Here comes a key question: how to select the operator G_1? There are at least four basic principles for extracting an invertible singular part of the original operator. This can be (i) the *static part*, as used in the scattering by PEC and imperfect thin screens; (ii) a frequency dependent *canonical-shape part*, which corresponds to either a circular cylinder or a flat PEC strip, in 2-D, and to a sphere, in 3-D, each solvable by separation of variables in the cylindrical, degenerate elliptical, and spherical coordinates, respectively; (iii) the *high-frequency part*, which corresponds to the PEC halfplane scattering and can be solved by the Wiener-Hopf method; note that a PEC halfplane is also a sort of canonical-shape scatterer, however its size is infinite in terms of any length parameter, including the wavelength; and (iv) the *small-contrast part* of the problem, as used in the scattering by dielectric objects.

As mentioned in section 2, in optics and photonics all scatterers must be considered using either the surface impedance or the dielectric-interface boundary conditions. In the first case, the choice of (i) or (iii) is natural, while in the second case the choice of (iv) is usually the most obvious; the choice of (ii) can be very promising if the shape is close to the corresponding canonical scatterer independently of other parameters.

The "small-contrast" regularization is based on the judicious combination of electric and magnetic field IEs on the dielectric-scatterer boundary, derived using the Green's formulas in the interior and exterior domains and the dielectric-boundary conditions (i.e., the continuity of the tangential field components across the boundary). This procedure cancels the hyperorder singularities in the IE kernels. The remaining part of the Muller IE operator has L_2 norm, which behaves as $O(\varepsilon - 1)$ for a scatterer with relative dielectric constant ε, placed in the free space (see *Burghignoli et al.* [2003] for a shorthand derivation in 3-D and *Smotrova et al.* [2013] in 2-D). As already mentioned, the Muller IE is free of spurious eigenfrequencies, which infest other, non-Muller, IE types and spoil all numerical algorithms based on them.

4. Preconditioning as Casting to a Fredholm Second-Kind Matrix Equation

Analytical inversion of the IE static or high-frequency part is usually based on quite specialized functional techniques such as Titchmarsh, Wiener-Hopf, and Riemann-Hilbert Problem techniques. However, eventually one always needs a discretized counterpart of IE, that is, a matrix equation, to find a solution numerically. This suggests a general approach to treat all the above mentioned cases, outlined in *Nosich* [1999] and in more detail in *Fikioris* [2001].

If it is possible to find a set of orthogonal eigenfunctions of the separated singular operator G_1, then the Galerkin-projection technique applied to the original singular IE of the first kind, i.e., to (1), with these functions as a basis, immediately results in a regularized discretization scheme (i.e., yields a Fredholm second-kind infinite matrix-operator equation). This is especially evident with canonical-shape inversion, as in this case, the orthogonal eigenfunctions are just trigonometric (entire-order azimuth exponents or trigonometric polynomials) or spherical polynomials (products of the former with the Legendre functions).

Another simple example is the 2-D scattering by a flat PEC strip—here the weighted Chebyshev polynomials of the first- or the second-kind invert logarithmic or hypersingular static part of the full-wave IE operator, as discussed by *Medina et al.* [1989], *Fikioris* [2001], and *Florencio et al.* [2013]. Such a judicious projection, in fact, combines both regularization (semi-inversion) and discretization in one single procedure and avoids intermediate step of a Fredholm second kind-IE. One may easily see that it bridges the gap between MAR and conventional MOM solutions. Indeed, the intuitive idea that a good choice of expansion functions in MOM can facilitate convergence obtains the form of a clear mathematical rule: to have the convergence guaranteed, take the expansion functions as orthogonal eigenfunctions of G_1. The finding of such functions is called diagonalization of a singular integral operator.

Similar techniques were developed by *Losada et al.* [1999] and *Di Murro et al.* [2015] in the scattering by a PEC disk; here the weighted Jacobi polynomials were used as regularizing basis functions in MOM-like projection. From the viewpoint of numerical analysis, this procedure plays the role of a perfect preconditioning of the original hypersingular IE, the conventional MOM-like discretizations of which are ill conditioned. Therefore, to distinguish it from classical MAR of the IE theory, one can call the outlined scheme a method of analytical preconditioning (MAP).

Note also that similar ideas can be applied to the strip-scattering singular IE after its transformation to the Fourier-transform (or "spectral") domain as it was done by *Matsushima and Itakura* [1990] and *Lucido*

[2012]. In view of linear character of such transform, the necessary basis functions become the Fourier-transforms of the Chebyshev polynomials.

This very powerful and mathematically faultless technique can be also used, after modification, in the scattering by thin imperfect strips (resistive, thin-dielectric, and impedance) because here the strongest kernel singularities are still the same as in the PEC-strip case. In fact, this is what one needs in the optical-range scattering by the metallic strips and disks.

One other generalization of such advanced technique was developed by *Lucido et al.* [2010] in the analysis of the scattering by polygonal dielectric cylinders. Here one can view a broken boundary of polygon as a collection of M strip-like elements, introduce local basis functions diagonalizing integral operators at these elements, and then obtain an $M \times M$ block-type infinite-matrix equation of the Fredholm second kind, in the space of sequences l_2^M.

5. Analytical Solutions

As noted by *Nosich* [1999], the analytical semi-inversion or the preconditioning results in the fact that the norm of the compact operator A in (2) becomes proportional to certain small parameter. Depending on the choice of the inverted part (see section 3), this is either electrical dimension of the scatterer (i), or its inverse value (iii), or the normalized deviation of the surface from the canonical shape (ii), or the optical contrast (iv). Therefore, denoting this parameter, say, as δ, one can see that $||A(\delta)||_{L_2} < \text{const}\cdot\delta$. This enables one to exploit one important feature of the Fredholm second-kind equations. Provided that $||A(\delta)||_{L_2} < 1$, which can always be satisfied for a small enough δ, an iterative solution to (2) is given by the Neumann-operator series

$$X = \sum_{s=0}^{\infty} [-A(\delta)]^s B, \tag{4}$$

which converges by the corresponding norm to the exact solution. Hence, one can avoid inverting (2), at least in a certain domain of parameters. Moreover, if the IEs based on the static and high-frequency parts inversion have overlapping domains of the Neumann series convergence, then the need of solving a matrix is completely eliminated—one has only to perform a matrix-vector multiplication. Besides numerical efficiency, this has another attractive consequence. On expanding (4) in terms of the power series of δ, one obtains, analytically, rigorous asymptotic formulas for the low-frequency or high-frequency scattering, or the scattering from a nearly canonical or small-contrast object, $X = C_0 + C_1\delta + C_2\delta^2 + \ldots$. Such asymptotics have been published for zero-thickness PEC screens in 2-D: flat and circularly curved strips, and in 3-D: finite circular pipes, flat and spherical disks, and also for PEC and imperfect strip gratings (see *Nosich* [1999] for the references). What is worth noting is that this can be done for various excitations specified by different right-hand parts B: plane or cylindrical waves, a complex source-point beam, a surface wave in the layered-media scattering, etc.

6. Eigenvalue Problems

These problems are closely tied to the wave scattering problems. For the passive configurations, they can be classified as natural-frequency or natural-wave problems, although other eigenparameters can be also considered. The natural-wave problems appear only in the analysis of geometries, infinite along some axis, and assuming a traveling-wave field solution, i.e., $\sim e^{ihz - ikct}$. Correspondingly, the (complex-valued) eigenvalue, which has to be determined, is either the wave number k or the natural-wave propagation constant h. What is important, in either case, is that a MAR/MAP treatment leads to a homogeneous equation analogous to the scattering problem:

$$X + A(h,k)X = 0 \tag{5}$$

This is a Fredholm operator equation, with the compact operator A normally being a continuous function of the geometrical parameters and a meromorphic function of the material parameters, k, and h. Hence, due to theorems of *Steinberg* [1968], it is guaranteed that the eigenvalues form a discrete set on a complex k plane (in 3-D case) or on the logarithmic Riemann surface of $Ln\, k$ (in 2-D case) or on the more complicated Riemann surface $Ln\,(k+h)(k-h)$ for the natural waves, respectively. There are no finite accumulation points;

eigenvalues can appear or disappear only at those values of the other parameters where continuity or analyticity of A is lost. Moreover, after discretization, the determinant of the infinite matrix, **Det[*I* + *A*(*k*, *h*)],** exists as a function of parameters, and its zeroes are the needed k or h eigenvalues. The latter are piecewise continuous or piecewise analytic functions of geometrical and material parameters: these properties can be lost only at the points where two or more eigenvalues coalesce. From a practical viewpoint, it is important that eigenvalues can be determined numerically: the convergence of discretization schemes is guaranteed, the number of equations needed being dependent on the desired accuracy and the nature of the inverted part. No spurious eigenvalues appear, unlike many approximate numerical methods. Note that nothing of the above can be established for an infinite-matrix equation of the first-kind and non-Fredholm equations of the second kind, which are common in conventional M**O**M analyses.

Additionally, if a corresponding parameter δ is small, then the matrix $A(k, h; \delta)$ is quasi-diagonal, and the eigenvalues in terms of k or h can be obtained in the form of asymptotic series. Such analytical study has been done, for instance, for a PEC axially slotted cylinder by *Veliyev et al.* [1977] and for a PEC spherical cap by *Vinogradov et al.* [2002], assuming a narrow slot or a small circular aperture, respectively. These asymptotics serve as a perfect starting guess when searching for eigenvalues numerically, with a Newton or another iterative algorithm—this has been done, e.g., for the modes on planar and circular-cylindrical strip and slot lines, and on arbitrary-cross-section dielectric fibers. Such treatment can be extended to imperfect thin-screen objects, although this will need considerable human efforts.

Talking about eigenvalue problems, it is necessary to mention that in the optical range there appears a very interesting version of such problem, adapted to the modeling of the phenomenon of lasing. As explained in *Smotrova et al.* [2011], the lasers can be considered as open resonators equipped with active regions (for example, filled in with a semiconductor or dye-doped polymer or Erbium-doped crystalline material under pumping). In this case, the time-harmonic wave scattering loses the guaranteed uniqueness of solution and hence cannot be studied any more. However, another extremely important analysis becomes possible —this is extraction of lasing thresholds (more precisely, threshold values of material gain in the active region) of the natural modes as eigenvalues, together with the emission wavelengths.

7. Convergence and Accuracy

As has been emphasized, MAR/MAP numerical solutions, based on the Fredholm second-kind matrix equations, have a guaranteed l_2 convergence and thus a controlled accuracy of numerical results. Provided that all intermediate computations necessary for filling in the matrix and the right-hand part have been done with superior accuracy, the parameter controlling the final accuracy is just the size of the matrix, i.e., the order of its truncation—see examples in *Nosich* [1999] and *Di Murro et al.* [2015]. Depending on the nature of the inverted part, the number of equations needed for the usual in practice 3–4 digit accuracy is only slightly greater than, respectively, the electrical dimension of the scatterer, or its inverse value, or the deviation of the surface from the canonical shape, in terms of both distance and curvature.

Here the optical range brings a necessity of revision of the concept of “electrical dimension” of scatterer. In the case of a thick dielectric object with relative dielectric permittivity ε, the wavelength in the material, $\lambda_\varepsilon = \lambda_0 \varepsilon^{-1/2} < \lambda_0$, becomes more important parameter than the wavelength in free space, λ_0 (as with PEC scatterers). In the case of metal scatterers, the negative-dielectric nature of such materials leads to existence of the mentioned in section 2 SP waves. The length of such waves λ_{SP} is a function of λ_0 and can be much shorter than λ_0. Therefore, in optics, there is no “nonresonant” range of wavelengths—even nanoscale metal objects can display strong resonances.

As one can see, by using the MAR/MAP, it is possible to overcome many difficulties encountered in conventional M**O**M treatments. Theoretical merits of the MAR/MAP are numerous: exact solution existence is established, convergence is guaranteed, and rigorous asymptotic formulas can be derived. Computationally, the MAR/MAP results in a small matrix size for practical 3–4 digit accuracy, and sometimes no numerical integrations are needed for filling in the matrix. Thus, *the cost of MAR/MAP algorithms is record low* in terms of both CPU memory and time. A frequent feature is that both power conservation and reciprocity are satisfied at the machine-precision level, independently of the number of equations, whatever it is. As the resolvent operator $(I + A)^{-1}$ is bounded, the condition number of (2) is small and stable, not growing with mesh refinement or with the number of basis functions. The latter fact means that conjugate-gradient iterative algorithms are very promising even in spite of a squaring of the condition number, as was already emphasized by *Rokhlin* [1990]. *Nosich* [1999, p. 43] suggested that using the fast iterative methods, applied to the MAR/MAP matrix equations with static-part inversion, it would be possible to perform accurate full-wave analysis of the Arecibo reflector with a moderate desktop computer. Five years later, this was demonstrated by *Smith et al.* [2004]. Still the high-frequency part inversion can do the same thing more economically.

Sometimes, on observing that in electromagnetics, convergence proofs of usual M**O**M schemes remain impossible, it is erroneously stated "accuracy is more important than convergence" [see *Dudley et al.*, 2002]. Here the accuracy remains not quantified and substituted with elusive "nearness" of solution to the true one. However, there exists unambiguous definition of accuracy based on the convergence—this is the distance, in the l_2 norm, between X and $X^{(N)}$. This leads to conclusion that the convergence is primary. If it takes place, then the accuracy is guaranteed within machine precision and in wide range of variation of geometrical and material parameters.

From a practical viewpoint, it is also important that the accuracy of the MAR/MAP solutions is uniform, including resonances, both in near-field and far-field predictions. Indeed, one must be reminded that near sharp resonances (e.g., whispering-gallery modes of dielectric objects), conventional M**O**M, and FDTD solutions suffer heavy inaccuracy as convincingly demonstrated by *Hower et al.* [1993], which cannot be removed, in principle. All this makes MAR/MAP algorithms perfect candidates for computer-aided design software in the numerical optimization of multielement or clustered 2-D and 3-D scatterers, where interaction between separate elements plays important role, and in the quasioptical range, where both ray-like and mode-like phenomena coexist. In fact, quite complicated 2-D models of reflector and lens antennas, radomes, and microcavity lasers have been accurately studied, showing the features not predicted by ray tracing techniques and inaccessible by rough numerical approximations (early references can be found in *Nosich* [1999] and some of the later ones given in this paper). Many of the solutions developed originally for PEC scatterers can be modified to treat the optics and photonics configurations.

8. General Remarks of MAR and MAP

One of reviewers of this paper requested to place the MAR in the context of other "regularization-related approaches such as Calderon preconditioning" of *Bagci et al.* [2009]. Indeed, at the first glance one may think that any preconditioning entails regularization. However, this is not true: the regularized equations, either IE or equivalent infinite-dimension matrix equation, must be the Fredholm second-kind ones, while the works employing Calderon regularisation and/or preconditioning approaches rarely achieve that property, except under restricted circumstances: for example, it seems that smooth closed bodies can be treated successfully whereas open bodies cannot. As a result, in these works the existence of the solution to the resulting infinite matrix equations is not established, and the convergence of the solutions of their truncated counterparts is out of the question. Note that in the mentioned and other relevant works the question of convergence appears only for the iterative solutions, and it is not proved but illustrated numerically. Full analysis of the shortcomings of the Calderon preconditioning is however out of the scope of this paper. Similar comments can be made, of course, about all conventional M**O**M algorithms using the local basis and testing functions. It should be emphasized that it is the convergence in the l_2 sense that is needed to have reliable and efficient computational instrument however is absent in the above mentioned works. Early examples of clear understanding of the importance of the Fredholm second-kind property are rare and belong mainly to *Colton and Kress* [1983] and *Rokhlin* [1990]. More recently, MAR/MAP related to the static-part inversion in the scattering of electromagnetic (and acoustic) waves by zero-thickness PEC (and rigid) screens was systematically presented and discussed by *Vinogradov et al.* [2002].

The other request of the same reviewer was to discuss the limitations of MAR/MAP and the scope of solvable, though as yet unsolved, problems. Here it can be said that the limitations are obvious however not principal and relate mainly to human efforts and preferences. While for writing an in-house FDTD code, knowledge of four arithmetical operations is sufficient, the MAR needs good experience with mathematical physics and special functions. In general, practically every 2-D scattering problem can be considered with this approach: open and closed, single and multiple scatterers, thin and thick, penetrable and impenetrable, and perfect and imperfect. This is true, so far, as the scatterers are lossy or lossless; the active scatterers (made of gain materials) could be considered as well if the solution uniqueness were not undermined however this is a defect of not the MAR but the time-harmonic formulation in general. Still, as mentioned, for active open resonators one can study the lasing eigenvalue problems, which have mathematically faultless formulation.

MAR works especially well if the boundaries and contours (open or closed) are perfectly smooth (infinitely differentiable) and can be characterized analytically. In 2-D, complicated contours can be tackled using the spline approximations (at least cubic) that preserve sufficient degree of smoothness [see *Nosich et al.*, 2007]. Finite ensembles and infinite periodic arrays can be efficiently attacked with MAR as soon as each single element is amenable to this approach. The same relates to scatterers placed into complicated environments, which still allow derivation of their Green's functions analytically—say, a nanolaser configured as a thin noble-metal strip encased by a circular shell made of the gain material.

Still the real-life configurations of electromagnetic scatterers, both at microwaves and in optics, have complicated 3-D shapes. In 3-D, rotational symmetry of the scatterers enables one to split the azimuth orders, reduce the problem to a set of independent IEs along the contour of rotation, and use the schemes typical for 2-D scatterers of all sorts.

If a 3-D body has no rotational symmetry, the difficulty of tackling the boundary can be overcome or bypassed in several ways although well-known Rao-Wilton-Glisson discretizations are not good candidates because they introduce broken boundaries and display low-frequency collapse. It is apparently better to use a triangular meshing combined with 2-D quadrature formulas as suggested by *Burghignoli et al.* [2003]. Then the Muller boundary IE can be applied to study many important effects and configurations, for instance, to find the emission modes of a 10 by 10 wavelength finite-thickness 3-D dielectric slab perforated with 100 round holes and equipped with an active region, as a model of photonic crystal laser. Further developments of this formulation should consider the use of conformal patches for a more accurate simulation of arbitrary curved surfaces.

Problems presently unsolved but amenable to MAR are many; some of them were mentioned by *Nosich* [1999] and are still untouched. The whole direction of MAR based on the inversion of the half-plane (high frequency) scattering operators is still very little studied. Here the only configurations, solved in the 1970s, were a flat PEC strip and a flat PEC disk, and even their circularly and spherically curved counterparts were only marginally touched with this approach. More recently, systematic efforts were done by *Kuryliak and Nazarchuk* [2008] to develop the MAR-based numerical solutions to the scattering by truncated PEC cones.

Still, even the much better developed static-part inversion solutions have not been systematically applied yet to the scattering problems involving negative dielectrics (i.e., metals in optics) and patterned graphene configurations. Instead, the bulk of researchers in optics and photonics resort to running COMSOL, LUMERICAL, and other commercial codes which are based upon algorithms that are non-convergent, in the mathematical sense (see the citation of *Dudley* [1985] in section 1). Fortunately, these codes are still able to deliver results with a few-digit accuracy that is often enough to obtain a quick answer to "what if" questions.

As already mentioned, the Muller IE is the most adequate starting ground for many interesting problems in optics and photonics because metals can be considered as negative dielectrics and pumped semiconductors or dye-doped polymers can be considered as dielectrics with gain. Claus Muller derived and published his IE for a 3-D object in the late 1950s. Applications of them to analysis of 2-D scatterers are published quite regularly although are still infrequent [see *Rokhlin*, 1990; *Smotrova et al.*, 2013, and references therein]. However, as concerns the 3-D objects, the promising MAR algorithm suggested in *Burghignoli et al.* [2003] seems so far to remain applied only to the wave scattering by a sphere. Even the analysis of a finite smooth rotationally symmetric dielectric body using the Muller IE was published only last year by *Bulygin et al.* [2015] and only for the axially symmetric field case. The closely related problem of the electromagnetic-wave propagation along an infinite uniform dielectric cylinder (fiber) of arbitrary smooth cross section was converted to 3-D Muller IE only "very recently" by *Lai and Jiang* [2015], and their work is still not published in a regular journal.

9. Conclusions

We presented the essentials of the method of analytical regularization in computational electromagnetics and discussed the influence of peculiar material properties of metals and dielectrics in the optical range. These properties change the formulation of wave scattering problems, which cannot now involve the PEC boundary conditions, common at lower frequencies. Besides, material parameters become dependent on the wavelength, and both real (for metals) and imaginary (for semiconductors of dyes under pumping) parts of dielectric functions can display negative values. Still all ideas and techniques associated with MAR are valid, and the development of convergent numerical algorithms is possible. Moreover, it is possible to formulate new class of eigenvalue problems tailored to the adequate modeling of self-excitation thresholds of lasers. In the practical implementation of such algorithms, one has to remember that the "electrical size" of the scatterers, in optics, must be modified as even subwavelength (nanoscale) objects can be strongly resonating. All these fascinating effects, which attract great attention of today's electromagnetics researchers, can be and are already studied with MAR-based techniques.

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References

Bagci, H., F. P. Andriulli, K. Cools, F. Olyslager, and E. Michielssen (2009), A Calderon multiplicative preconditioner for the combined field integral equation, *IEEE Trans. Antennas Propag.*, *57*(10), 3387–3392.

Balaban, M. V., E. I. Smotrova, O. V. Shapoval, V. S. Bulygin, and A. I. Nosich (2012), Nystrom-type techniques for solving electromagnetics integral equations with smooth and singular kernels, *Int. J. Numer. Modell. Electron. Networks Devices Fields*, *25*(5), 490–511.

Bulygin, V. S., A. I. Nosich, and Y. V. Gandel (2012), Nystrom-type method in three-dimensional electromagnetic diffraction by a finite PEC rotationally symmetric surface, *IEEE Trans. Antennas Propag.*, *60*(11), 4710–4718.

Bulygin, V. S., Y. V. Gandel, A. Vukovic, T. M. Benson, P. Sewell, and A. I. Nosich (2015), Nystrom method for the Muller boundary integral equations on a dielectric body of revolution: Axially symmetric problem, *IET Microwaves Antennas Propag.*, *9*(11), 1186–1192.

Burghignoli, P., C. Di Nallo, F. Frezza, and A. Galli (2003), A simple Nystrom approach for the analysis of 3D arbitrarily shaped conducting and dielectric bodies, *Int. J. Numer. Modell.*, *16*(2), 179–194, doi:10.1002/jnm.495.

Colton, D., and R. Kress (1983), *Integral Equation Methods in Scattering Theory*, Wiley, New York.

Di Murro, F., M. Lucido, G. Panariello, and F. Schettino (2015), Guaranteed-convergence method of analysis of the scattering by an arbitrarily oriented zero-thickness PEC disk buried in a lossy half-space, *IEEE Trans. Antennas Propag.*, *63*(8), 3610–3620.

Dudley, D. G. (1985), Error minimization and convergence in numerical methods, *Electromagnetics*, *5*(2–3), 89–97.

Dudley, D. G., W. A. Johnson, and L. K. Warne (2002), Some convergence and accuracy issues in method of moments solutions to integral equations, in *IEEE APS-URSI Symposium Digest, San Antonio*, vol. 1, pp. 50–53, IEEE, doi:10.1109/APS.2002.1016248.

Fikioris, G. (2001), A note on the method of analytical regularization, *IEEE Antennas Propag. Mag.*, *43*(2), 34–40.

Florencio, R., R. R. Boix, and J. A. Encinar (2013), Enhanced MOM analysis of the scattering by periodic strip gratings in multilayered substrates, *IEEE Trans. Antennas Propag.*, *61*(10), 5088–5099, doi:10.1109/TAP.2013.2273213.

Hower, G. L., R. G. Olsen, J. D. Earls, and J. B. Schneider (1993), Inaccuracies in numerical calculation of scattering near natural frequencies of penetrable objects, *IEEE Trans. Antennas Propag.*, *41*(7), 982–986.

Johnson, P. B., and R. W. Christy (1972), Optical constants of the noble metals, *Phys. Rev. B*, *6*, 4370–4378.

Klien, C., and R. Mittra (1973), Stability of matrix equations arising in electromagnetics, *IEEE Trans. Antennas Propag.*, *21*(6), 902–905.

Kuryliak, D. B., and Z. T. Nazarchuk (2008), Convolution type operators for wave diffraction by conical surfaces, *Radio Sci.*, *43*, RS4S03, doi:10.1029/2007RS003792.

Lai, J., and S. Jiang (2015), Second kind integral equation formulation for the mode calculation of optical waveguides, Applied Comput. Harmonic Analysis, vol. 40, 2016. doi:10.1016/j.acha.2016.06.009.

Losada, V., R. R. Boix, and M. Horno (1999), Resonant modes of circular microstrip patches in multilayered substrates, *IEEE Trans. Microwave Theory Tech.*, *47*(4), 488–498.

Lucido, M. (2012), A new high-efficient spectral-domain analysis of single and multiple coupled microstrip lines in planarly layered media, *IEEE Trans. Microwave Theory Tech.*, *60*(7), 2025–2034.

Lucido, M., G. Panariello, and F. Schettino (2010), Scattering by polygonal cross-section dielectric cylinders at oblique incidence, *IEEE Trans. Antennas Propag.*, *58*(2), 540–550, doi:10.1109/TAP.2009.2038181.

Matsushima, A., and T. Itakura (1990), Singular integral equation approach to plane wave diffraction by an infinite strip grating at oblique incidence, *J. Electromagn. Waves Appl.*, *4*(6), 505–519.

Medina, F., M. Horno, and H. Baudrand (1989), Generalized spectral analysis of planar lines on layered media including uniaxial and biaxial dielectric substrates, *IEEE Trans. Microwave Theory Tech.*, *37*(3), 504–511.

Muller, C. (1969), *Foundations of the Mathematical Theory of Electromagnetic Waves*, Springer, Berlin.

Muskhelishvili, N. I. (1953), *Singular Integral Equations*, Noordhoff, Groningen.

Nosich, A. I. (1999), The method of analytical regularization in wave-scattering and eigenvalue problems: Foundations and review of solutions, *IEEE Antennas Propag. Mag.*, *41*(3), 25–49.

Nosich, A. I., A. V. Boriskin, and R. Sauleau (2007), Radiation and focusing of waves by hemielliptic dielectric lenses: 2-D analysis and optimization with boundary integral equations, in *Proceedings of the International Conference on Electromagnetics and Communications (ICECOM-07), Dubrovnik*, pp. 1–5, Univ. of Zagreb Press, Zagreb, doi:10.1109/ICECOM.2007.4544481.

Raether, H. (1986), *Surface Plasmons on Smooth and Rough Surfaces and on Gratings*, Springer, Berlin.

Rokhlin, V. (1990), Rapid solution of IEs of scattering theory in 2D, *J. Comput. Phys.*, *86*(2), 414–439.

Smith, P. D., S. S. Vinogradov, and E. D. Vinogradova (2004), Rigorous analysis of extremely large spherical reflector antennas, in *Proceedings of the International Electromagnetic Theory Symposium (EMTS-2004), Pisa*, pp. 730–732. [Available at http://www.ee.bgu.ac.il/~specmeth/EMT04/pdf/session_3/3_06_03.pdf.]

Smotrova, E. I., V. O. Byelobrov, T. M. Benson, J. Ctyroky, R. Sauleau, and A. I. Nosich (2011), Optical theorem helps understand thresholds of lasing in microcavities with active regions, *IEEE J. Quantum Electron.*, *47*(1), 20–30.

Smotrova, E. I., V. Tsvirkun, I. Gozhyk, C. Lafargue, C. Ulysse, M. Lebental, and A. I. Nosich (2013), Spectra, thresholds and modal fields of a kite-shaped microcavity laser, *J. Opt. Soc. Am. B*, *40*(6), 1732–1742, doi:10.1364/JOSAB.30.001732.

Steinberg, S. (1968), Meromorphic families of compact operators, *Arch. Ration. Mech. Anal.*, *31*(5), 372–379, doi:10.1007/BF00251419.

Tsalamengas, J. L. (2010a), Exponentially converging Nystrom methods in scattering from infinite curved smooth strips. Part 1: TM-Case, *IEEE Trans. Antennas Propag.*, *58*(10), 3265–3274.

Tsalamengas, J. L. (2010b), Exponentially converging Nystrom methods in scattering from infinite curved smooth strips. Part 2: TE-case, *IEEE Trans. Antennas Propag.*, *58*(10), 3275–3281.

Tsalamengas, J. L. (2015), Quadrature rules for weakly singular, strongly singular, and hypersingular integrals in boundary integral equation methods, *J. Comput. Phys.*, *303*(12), 498–513, doi:10.1016/j.jcp.2015.09.053.
Veliyev, E. I., A. I. Nosich, and V. P. Shestopalov (1977), Propagation of electromagnetic waves in a cylindrical waveguide with a longitudinal slot, *Radio Eng. Electron. Phys.*, *22*(3), 29–37.
Vinogradov, S. S., P. D. Smith, and E. D. Vinogradova (2002), *Canonical Problems in Scattering and Potential Theory Part 2: Acoustic and Electromagnetic Wave Scattering*, CRC Press, Boca Raton, Fla.