A Numerical Solution to Electromagnetic Scattering by Three-Dimensional Nonlinear Objects in Free Space Using a Statistical Cooling Procedure

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A Numerical Solution to Electromagnetic Scattering by Three-Dimensional Nonlinear Objects in Free Space Using a Statistical Cooling Procedure

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Résumé. — Cet article analyse la diffraction par des objets non-linéaires illuminés par des champs électromagnétiques incidents et périodiques. Nous décrivons une formulation intégrale de la diffraction tridimensionnelle (vectorielle) par des objets diélectriques limités et nous dérivons une solution formelle en série. Puis nous obtenons une solution numérique par discrétisation du modèle continu et par l'utilisation d'une procédure de refroidissement statistique (ou recuit simulé) pour résoudre la fonction d'énergie résultante. L'article présente quelques résultats numériques obtenus pour des objets non-linéaires simples.

Abstract. — This paper deals with the scattering by nonlinear objects illuminated by time-periodic incident electromagnetic fields. An integral formulation of the three-dimensional full-vector scattering by bounded dielectric objects is described and a formal series solution is obtained. A numerical solution is then achieved by discretizing the continuous model and by using a statistical-cooling procedure (i.e., simulated annealing) to solve the resulting energy function. Numerical results on simple nonlinear objects are reported.

1. Introduction

This paper deals with the electromagnetic scattering by nonlinear dielectric objects of limited dimensions. In the last few years, the topic of nonlinear wave propagation has been extensively investigated, especially for infinite and semi-infinite nonlinear media. Many interesting phenomena (e.g., shock-wave generation and propagation, solitary waves, and soliton formation and decay) have been studied (see, for example [1-4]) and several applications have been described in the literature. In this paper, we aim to develop a numerical approach to the full-vector three-dimensional scattering by bounded nonlinear bodies of arbitrary shapes, illuminated by time-periodic incident electromagnetic fields. We consider nonmagnetic isotropic dielectric objects, whose dielectric permittivities depend on the total internal electric fields in such a way that the objects keep their scalar nature (isotropic nonlinear material). We start with an integral-equation formulation, the theoretical basis of which was first introduced in reference [5] and subsequently discussed from a numerical point of view in references [6, 7] with reference to scattering in free space and in a rectangular waveguide excited in the TE_{10} mode. In particular, the present paper is focused on the problem previously addressed in reference [6], where the nonlinear electromagnetic problem was described in detail. A formal solution to the direct scattering problem is derived as a series solution in which the nonlinear effects are taken into account by considering an equivalent current distribution (based on the equivalent principle) that depends on the harmonic mixing. The simplifying hypotheses are: neglecting the frequency dependence of the dielectric permittivity and limiting the analysis to weak nonlinearities. As a result, it is possible to obtain a formal series solution in which the coefficients are the solutions of a set of integral equations written in terms of Green's dyadic function for free space. The static vector component is also taken into account by using an integral equation for the polarization vector, which depends on the generated electric field vector component at zero frequency. By truncating the series at a suitable term and by discretizing the continuous problem using the method of moments [8], we obtain a nonlinear system of algebraic equations to be solved for the complex harmonic amplitudes of the electric field vector. The solution of this system is a critical point, and the approach presented in reference [6] did not address the resulting numerical problem in an adequate way. In other words, in order to obtain preliminary numerical results, the solution of the above nonlinear system was otained by using Wolfe's method [9], which is a deterministic iterative method that can be regarded as the result of a generalization of the secant method. As shown in reference [6], the application of Wolfe's method to such a complex problem (i.e., the solution of a nonlinear full-vector three-dimensional scattering problem) results in a high computational load and does not ensure that a solution corresponding to a global minimum will be reached.

In the present paper, the numerical problem is handled from a different point of view. In particular, the problem solution is reduced to the minimization of a multivalue multivariable function. In order to find a global minimum for the resulting (usually, multimodal) *energy* function, we use an efficient implementation of a statistical-cooling procedure [10, 11]. The iterative procedure employs the Metropolis algorithm and is governed by a suitable scheduling of a control parameter (often called *system temperature*).

In the following sections, the mathematical problem formulation is outlined and the implementation of the statistical-cooling procedure is described. Moreover, the results of several numerical simulations are reported and utilized to discuss the validity of the proposed approach.

2. Method Description

In this section, we outline the mathematical formulation for the proposed approach. Let us assume a time-periodic incident electric field vector, $\mathbf{E}_{\mathrm{I}}(\mathbf{x}, t)$ ($\mathbf{x}$: position vector), illuminating a bounded nonlinear object. The object is assumed to be lossless, isotropic and inhomogeneous; its inhomogeneity is due both to the nonlinear nature of the dielectric permittivity and to the inhomogeneities of the linear part of the dielectric permittivity. General relationships between induction vectors and field vectors can be derived by using Volterra series expressions [12]. However, in many practical cases, some heuristic assumptions are made (e.g., Kerr-like nonlinearities) that seem acceptable for a wide range of applications. In this paper, we assume that the nonlinear dielectric permittivity can be expressed as:

$$\varepsilon_{\mathrm{NL}}(\mathbf{x}, t) = \varepsilon_0[\varepsilon_{\mathrm{Lr}}(\mathbf{x}) + \Re\{\mathbf{E}(\mathbf{x}, t)\}] \tag{1}$$

where $\mathbf{x}$ is the position vector, t denotes the time, $\varepsilon_{\mathrm{Lr}}(\mathbf{x})$ is the linear part of $\varepsilon_{\mathrm{NL}}(\mathbf{x},t)$, and $\Re\{\mathbf{E}(\mathbf{x},t)\}$ is an operator that is assumed to fulfil the constraint of not modifying the scalar nature of the dielectric permittivity and to be a time-periodic function. Then, we consider the harmonic vector components of the total electric field, $\mathbf{e}_k(\mathbf{x})\exp(j2\pi k f_0 t)$, $k = 1,\ldots A$, where f_0 is the fundamental frequency of the time-periodic incident electric field and A is the maximum order of the harmonic terms (a series truncation is used). For any harmonic vector component, an inhomogeneous wave equation can be derived as described in reference [6]:

$$\nabla \times \nabla \times \mathbf{e}_k(\mathbf{x}) - k_k^2 \mathbf{e}_k(\mathbf{x}) = \mathbf{y}_k(\mathbf{x}) \tag{2}$$

where $k_k = 2\pi k f_0(\varepsilon_0\mu_0)^{1/2}$ and $\mathbf{y}_k(\mathbf{x})$ is an equivalent excitation term that can be written as the sum of a linear and a nonlinear term

$$\mathbf{y}_k(\mathbf{x}) = k_k^2(\varepsilon_{\mathrm{Lr}}(\mathbf{x}) - 1)[\mathbf{e}_k(\mathbf{x}) + \mathbf{e}_k^{\mathrm{i}}(\mathbf{x})] + k_k^2 \mathbf{t}_k(\mathbf{x}) \tag{3}$$

where $\mathbf{e}_k^{\mathrm{i}}(\mathbf{x})$ is the k-th harmonic vector component of $\mathbf{E}_{\mathrm{i}}(\mathbf{x})$ and $\mathbf{t}_{\mathrm{k}}(\mathbf{x})$ is given by:

$$\mathbf{t}_k(\mathbf{x}) = \sum_p \sum_q \delta_{pq}^k g_p(\mathbf{x}) \mathbf{e}_q(\mathbf{x}) \tag{4}$$

where $\delta_{pq}^k = 1$, if $p + q = k$, $\delta_{pq}^k = 0$, otherwise; $g_p(\mathbf{x})$ is the p-th harmonic component of $\Re\{\mathbf{E}(\mathbf{x},t)\}$ [6]. Once $\Re\{\mathbf{E}(\mathbf{x},t)\}$ has been specified, the vectors $\mathbf{t}_{\mathrm{k}}(\mathbf{x})$ can be rendered explicit. By using the well-known integral solution of equation (2) in terms of the Green tensor for free space [15,16], we obtain a set of A coupled integral equations ($k = 1,\ldots A$):

$$\mathbf{e}_k(\mathbf{x}) = \mathbf{e}_k^{\mathrm{i}}(\mathbf{x}) - \int_D k_k^2(\varepsilon_{\mathrm{Lr}}(\mathbf{x}') - 1)\mathbf{y}_k(\mathbf{x}') \cdot \Gamma_k(\mathbf{x},\mathbf{x}')\mathrm{d}\mathbf{x}' \tag{5}$$

where $\mathbf{y}_k(\mathbf{x})$ (relation (3)) contains the unknown terms $\mathbf{e}_k(\mathbf{x}')$ and $\mathbf{t}_k(\mathbf{x}')$, D is the domain of the nonlinear object, and $\Gamma_k(\mathbf{x},\mathbf{x}')$ is Green's dyadic function (at a frequency $f_k = kf_0$). Moreover, the static component ($k = 0$) can be taken into account by considering the polarization vector $\mathbf{p}_0(\mathbf{x})$ given by:

$$\mathbf{p}_0(\mathbf{x}) = \varepsilon_0(\varepsilon_{\mathrm{Lr}}(\mathbf{x}) - 1)[\mathbf{e}_0(\mathbf{x}) + \mathbf{y}_0(\mathbf{x})] \tag{6}$$

from which we obtain:

$$\mathbf{e}_0(\mathbf{x}) = (4\pi\varepsilon_0)^{-1} \int_S \gamma(\mathbf{x},\mathbf{x}')\mathbf{p}_0(\mathbf{x}') \cdot \mathbf{n}\mathrm{d}\mathbf{x}' - \int_D \gamma(\mathbf{x},\mathbf{x}')\nabla \cdot \mathbf{p}_0(\mathbf{x}')\mathrm{d}\mathbf{x}' \tag{7}$$

where $\gamma(\mathbf{x},\mathbf{x}') = (\mathbf{x} - \mathbf{x}')/|\mathbf{x} - \mathbf{x}'|^3$, S is the surface including D, and $\mathbf{n}$ is the outward normal unit vector. Relations (5) and (7) indicate explicit functional relationships among the harmonic components of the electric field vector. By discretizing the continuous model, we obtain an algebraic system of nonlinear equations that can be expressed as:

$$\Im_i(F) - \Re_i = 0 \quad i = 1,\ldots 3(A + 1) \times N \tag{8}$$

where N is the number of subdomains used and the unknown array F has $3 \times (A + 1) \times N$ elements corresponding to the Cartesian components (cp, $p = 0,\ldots 2$) of the $(A + 1)$ harmonic vector components (including the static one) of the total electric fields inside the N subdomains ($n = 1,\ldots N$):

$$\begin{aligned} F \;=\; & [e_{0,c0}^1, e_{0,c1}^1, e_{0,c2}^1, \ldots, e_{0,c0}^N, e_{0,c1}^N, e_{0,c2}^N, \ldots, e_{k,c0}^n, e_{k,c1}^n, e_{k,c2}^n, \ldots, \\ & e_{A,c0}^n, e_{A,c1}^n, e_{A,c2}^n, \ldots, e_{0,c0}^N, e_{0,c1}^N, e_{0,c2}^N]^t \end{aligned} \tag{9}$$

where t indicates the transposition operation. The problem solution can now be reduced to the minimization of an *energy* function, $\aleph(F)$, defined as follows:

$$\sum_i (\Im_i(F) - \Re_i)^2 \tag{10}$$

In order to find a global minimum for $\aleph(F)$ (usually, multimodal), we apply a statistical-cooling procedure [10,11]. This procedure employs the Metropolis algorithm and requires that a suitable scheduling of a control parameter (often called *system temperature*) be defined. The iterative scheme of the procedure requires that F be initialized as follows:

$$F \leftarrow F_0 \tag{11}$$

where F_0 is randomly generated. In this paper, we use two sequences (for the real and imaginary parts) with uniform distributions and zero mean values. The sequences are such that the amplitude of any field component does not exceed twice the maximum amplitude of the incident electric field inside the dielectric object. At each step, a sequence of random arrays F_{hj} is generated (h being the step index and $j = 1, ...3(A+1) \times N$) and assigned to F. The range for the choice of the values F_{hj} is *dynamically* changed according to the degree of *thermodynamic* equilibrium (related to the probability that a local minimum may be reached). This procedure can be expressed as:

$$F_{hj} \leftarrow F_{(h-1)j} + V_{hj}\eta_{hj} \tag{12}$$

where V_{hj} is the half-amplitude of the range (at step h) for the choice of the values of F, and η_{hj} is an *array* whose single non-zero value (the j-th) is a random variable uniformly distributed between -1 and 1. The generated configuration is accepted or not according to the Metropolis criterion [10], which states that:

- if a given configuration produces a change $\Delta\aleph(F)$ (in the *energy* function)

$\Rightarrow$ accept that configuration if:

$$\Delta\aleph(F) < 0 \tag{13}$$

$\Rightarrow$ accept it with a probability $u = \exp(-\Delta\aleph(F)/T)$, if:

$$\Delta\aleph(F) > 0 \tag{14}$$

Therefore, reject it with a probability $v = 1 - u$. The control parameter T is then modified according to a logarithmic *scheduling*, similar to that proposed in reference [17] and given by:

$$T_{h+1} = T_0[\ln(1+h)]^{-1}\xi \tag{15}$$

where h is the step index, T_0 is the initial value of T, and ξ denotes a value that allows a fine tuning of the temperature value. It allows the algorithm to escape local minima in an efficient way.

3. Numerical Simulations and Discussion

In this section, we report the results of some numerical simulations. We consider the three-dimensional dielectric scattering object shown in Figure 1 (λ_0 being the free-space wavelength of the fundamental frequency). The object is assumed to be homogeneous in the linear part of its nonlinear dielectric permittivity, $\varepsilon_{\mathrm{Lr}}(\mathbf{x}) = 4.0$, and its nonlinear part shows a Kerr-like dependence on the total electric field:

$$\Re\{\mathbf{E}(\mathbf{x},t)\} = \beta|\mathbf{E}(\mathbf{x},t)|^2 \tag{16}$$

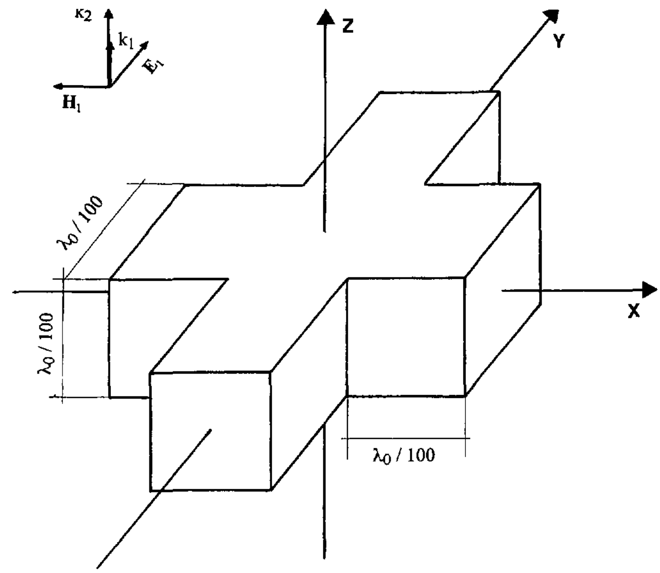


Fig. 1. — Problem configuration.

The scatterer is illuminated by an incident electric field resulting from the sum of two uniform plane waves at the frequencies f_0 and $2f_0$, polarized with the electric field in the $\mathbf{z}$ direction and propagating in the $\mathbf{y}$ direction. For the electric field, we consider a series expansion truncated at the 4-th harmonic term.

In Figure 2, the amplitudes of the harmonic vector components $|e^k_{c1}(\mathbf{x})|$ are plotted *versus* different values of the nonlinear index β inside the object at the positions (see Fig. 1) (a) $\mathbf{x}_1 = (0,0,0)$, (b) $\mathbf{x}_2 = (\lambda_0/100, 0, 0)$, (c) $\mathbf{x}_3 = (0, \lambda_0/100, 0)$, (d) $\mathbf{x}_4 = (-\lambda_0/100, 0, 0)$ and (e) $\mathbf{x}_5 = (0, -\lambda_0/100, 0)$. Note that, as the the nonlinear index β increases, a significant generation of harmonic components occurs at frequencies different from those of the incident fields. Moreover, the amplitudes of the total electric electric field, for $\beta = 0.0$, coincide with those obtained by the authors (as a consistency check) by using the moment method [8] for direct scattering by linear dielectrics.

For illustrative purposes, Figures 3 and 4 present the trends of the characteristic parameters of this minimization method. Figure 3 gives the decrease in the energy function $\aleph(F)$, as compared with that of the control parameter T, at different cooling iterations.

In Figure 4, the number of generated configurations accepted for the statistical cooling procedure is plotted *versus* the number of temperature iterations: (a) configuration adjournments for which the energy function increases; (b) adjournments for which the energy function decreases; in this case, the trend is approximately the same as that of positive adjourments, for the statistical equilibrium is reached at only one temperature iteration, i.e., equal numbers of positive and negative resets of unknown accepted configurations; (c) configuration adjournments for which the energy function value is minimum as compared with other values calculated at the previous temperature iterations. The time-dependent relative dielectric permittivity was also computed. Figure 5 gives the obtained results for the same points inside the object as in Figure 2. Table I gives the CPU times for some significant values of the nonlinear index β. An IBM RISC 6000 computer was used.

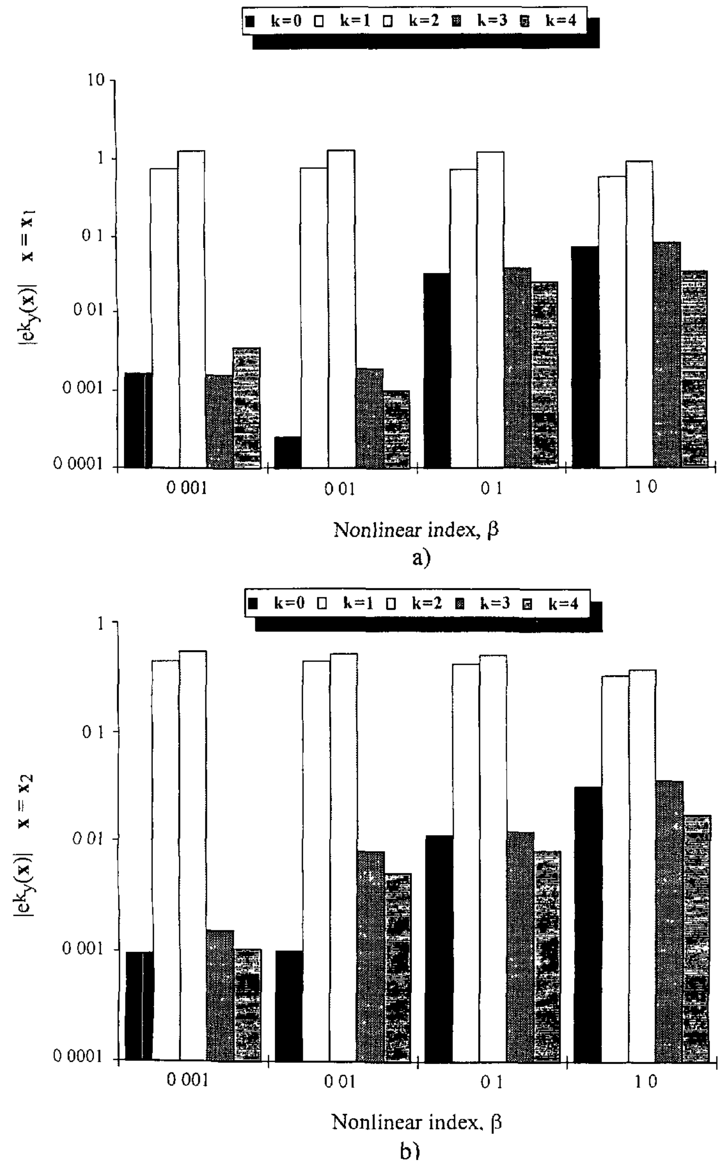
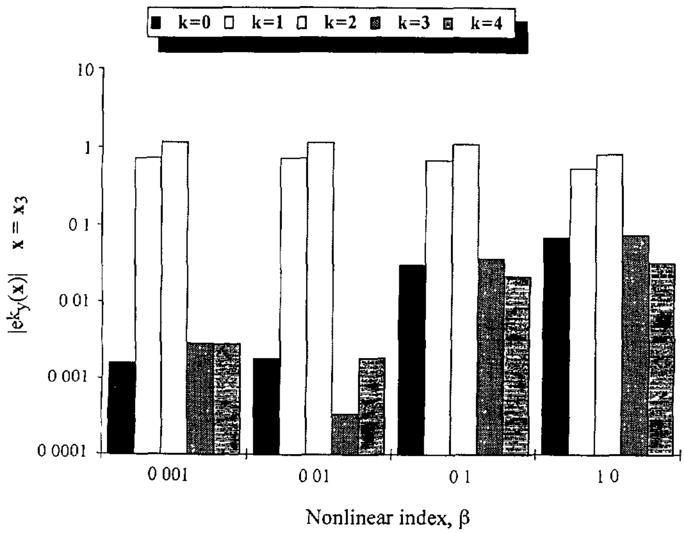
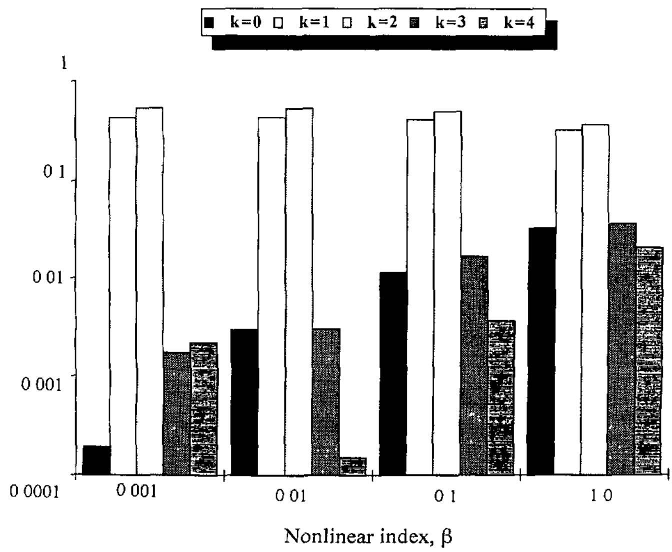


Fig. 2. — Amplitudes of the harmonic components of the electric field *versus* the nonlinear parameter β, for $\varepsilon_b = 4.0$, inside the dielectric object (Fig. 1) at the positions a) $\mathbf{x}_1 = (0, 0, 0)$, b) $\mathbf{x}_2 = (\lambda_0/100, 0, 0)$, c) $\mathbf{x}_3 = (0, \lambda_0/100, 0)$, d) $\mathbf{x}_4 = (-\lambda_0/100, 0, 0)$ and e) $\mathbf{x}_5 = (0, -\lambda_0/100, 0)$.

Finally, it is worth noting that the consideration made in reference [17] about the possibility of extending the formulation of the functional dependence $\mathbf{D}(\mathbf{E})$ to the functional dependence of $\mathbf{B}(\mathbf{H})$ holds true even for the present approach. According to the duality principle, an analogous formulation, in particular, a similar series solution can be derived for the distributions of the magnetic field vectors scattered by bounded magnetic objects. For such objects, a relationship (analogous to Eq. (1)) can be defined that relates $\mathbf{H}(\mathbf{x}, t)$ to $\mu_{\mathrm{NL}}(\mathbf{x}, t)$, under



c)



d)

Fig. 2. — *(Continued)*

the same assumptions as valid for the dependence of the dielectric permittivity on the total internal electric field vector. In the present case, as each harmonic vector component of $\mathbf{H}(\mathbf{x}, t)$ would satisfy a vector equation analogous to equation (2), where the excitation term would be an equivalent magnetic source, the duality theorem [15] only requires that, in the formulation developed in Section 2, $\mathbf{E}(\mathbf{x}, t)$ $\varepsilon_{\mathrm{NL}}(\mathbf{x}, t)$, ε_0, and μ_0 be replaced with $\mathbf{H}(\mathbf{x}, t)$, $\mu_{\mathrm{NL}}(\mathbf{x}, t)$, μ_0, and ε_0, respectively.

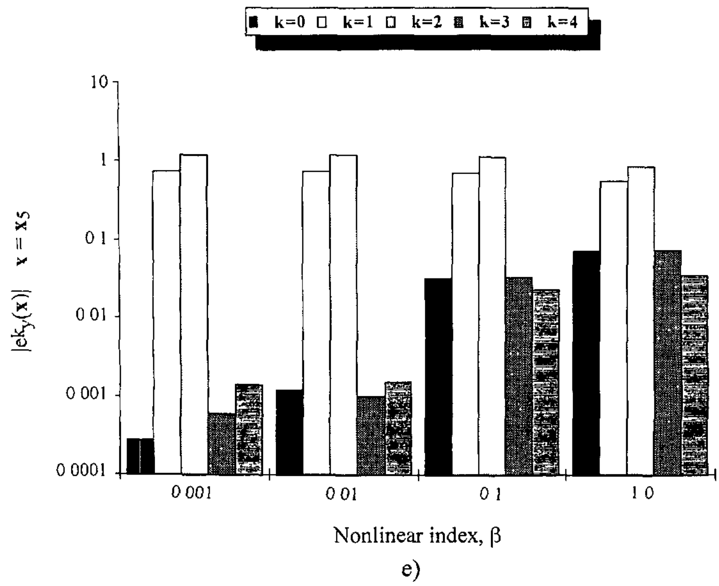


Fig. 2. — *(Continued)*

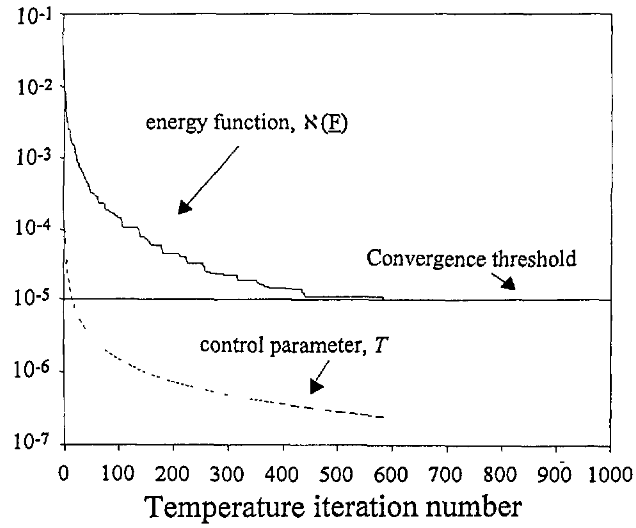


Fig. 3. — Behaviour of the norm of the residual error *versus* number of temperature iterations.

4. Conclusion

A numerical approach to the computation of the full-vector electromagnetic scattering by three-dimensional nonlinear bounded dielectric objects in free space has been proposed. The approach starts with an integral-equation formulation previously derived and suitable for weak nondispersive nonlinear isotropic media whose dielectric permittivities can be expressed as functions of the internal electric fields through an operator that produces a time-periodic

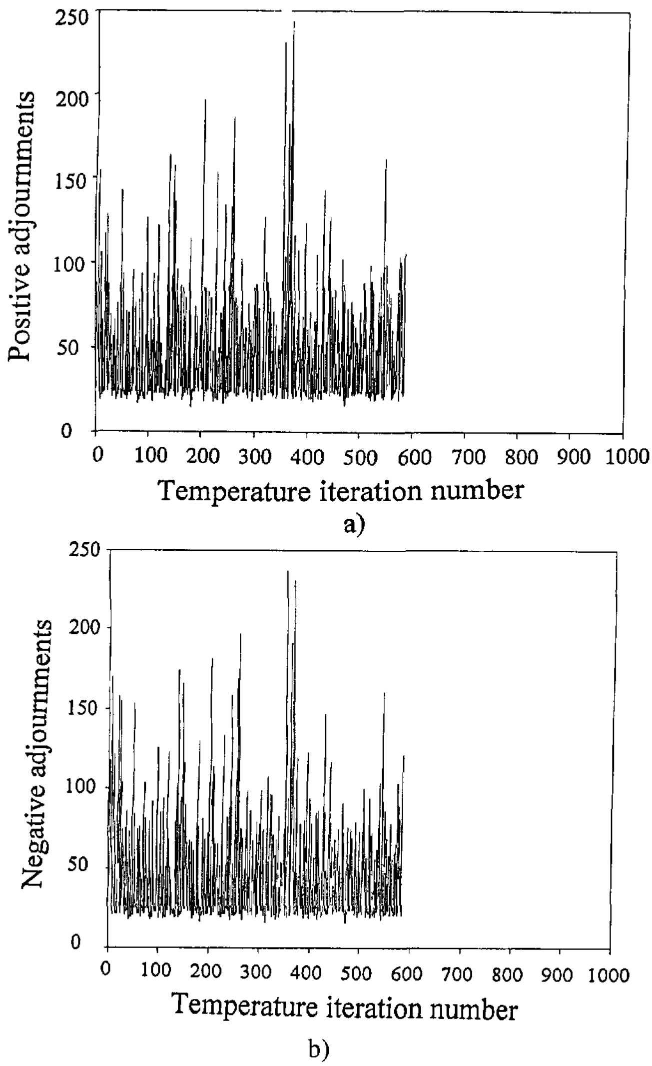
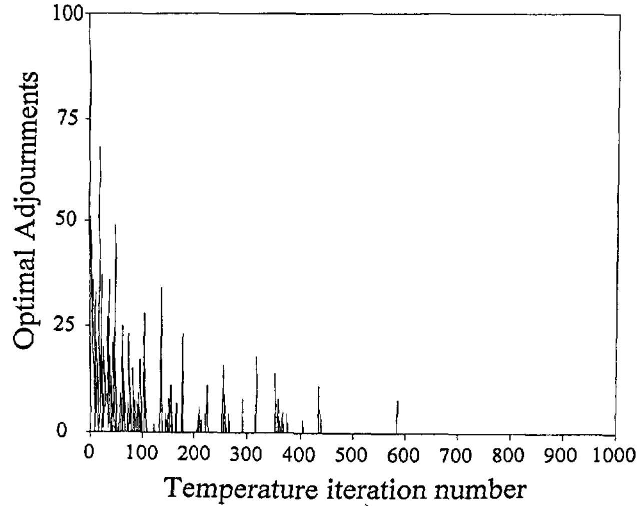


Fig. 4. — Number of adjournments required by the statistical-cooling procedure *versus* number of temperature iterations: a) *positive* adjournments, b) *negative* adjournments, c) *optimal* adjournments.

Table I. — *CPU times (ms) required for the solutions of the electromagnetic problems related to the geometrical configuration shown in Figure 1, for different values of the nonlinear index β.*

β = 0.001	**β = 0.01**	**β = 0.1**	**β = 1.0**
9.0	3.0	66.0	1094.0



c)

Fig. 4. — *(Continued)*

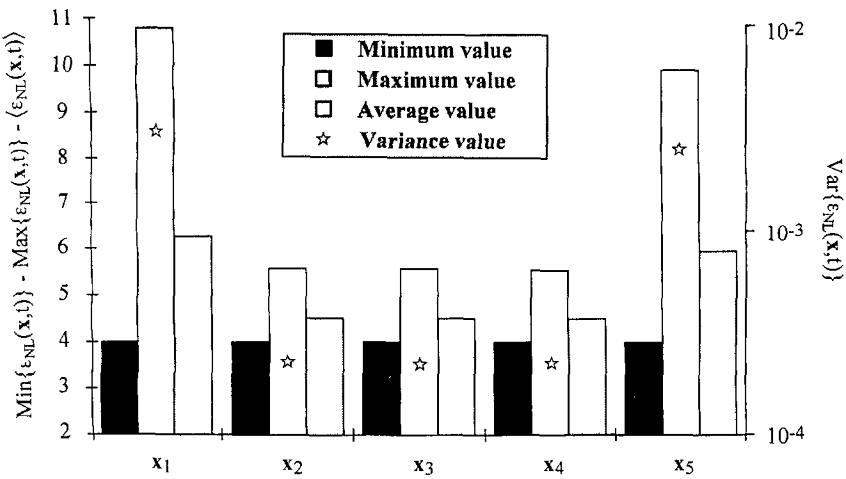


Fig. 5. — Minimum values, maximum values, mean, variance values of the equivalent dielectric permittivity $\varepsilon_{\mathrm{NL}}(\mathbf{x},t)$ inside the dielectric object (Fig. 1) at the positions $\mathbf{x}_1 = (0,0,0)$, $\mathbf{x}_2 = (\lambda_0/100,0,0)$, $\mathbf{x}_3 = (0,\lambda_0/100,0)$, $\mathbf{x}_4 = (-\lambda_0/100,0,0)$ and $\mathbf{x}_0 = (0,-\lambda_0/100,0)$, during a period of the fundamental frequency ($t_0 = 1/f_0$) for a nonlinear entity denoted by $\beta = 1.0$.

function when the incident illumination is periodic in time. The numerical problem has then been dealt with by developing a numerical solution based on a statistical-cooling procedure. The reported results seem to confirm the possibility of solving the above complex nonlinear problem effectively by a numerical approach, in particular, by computing the distributions of the fields scattered at the fundamental frequency and the harmonic components of the fields inside nonlinear objects of arbitrary shapes, to which analytical methods cannot be applied.

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