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USING EXTRAPOLATION IN THE ITERATIVE SOLUTION OF SCATTERING PROBLEMS WITH A VARYING PARAMETER

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ABSTRACT

We consider the determination of electromagnetic fields for a (large) number of values of a physical parameter. We apply an iterative procedure based on the minimization of an integrated squared error, and start this procedure from an initial estimate that is a linear combination of the last few "final" results. When the coefficients in this extrapolation are determined by minimizing the integrated squared error for the actual value of the parameter, the built-in orthogonality in this type of scheme ensures that only a few iteration steps are required to obtain the solution. The algorithm has been available for some time [1], and has already been demonstrated in a number of applications. In the present paper, we illustrate its potential by applying it to two classical implementations of the CGFFT method to three-dimensional geometries i.e., a flat, rectangular conducting plate and an inhomogeneous dielectric cube, both in free space. In both cases, the space discretization preserves the convolution symmetry of the continuous form of the relevant integral equation.

METHOD OF SOLUTION

In the computational modeling of electromagnetic fields for practical applications, typically a large system of linear equations must be solved. This system originates from spatially discretizing Maxwell's differential equations (in "finite" or "local" techniques) or equivalent integral equations (in "global" techniques). In formal notation, such a system can be written as

$$L(p)\,u(p) = f(p), \tag{1}$$

where $L(p)$ is a linear operator that originates from discretizing its counterpart in the continuous equation, $u(p)$ is a discretized field and $f(p)$ corresponds to an impressed source or an incident field. We are interested in the situation where this problem must be solved for a large number of sampled values of the parameter p, e.g., $p = p_0 + m\Delta p$, with $m = 0, 1, \ldots, M$.

Iterative procedure

In this subsection, we consider the iterative procedure that is used to solve the system of equations (1). We summarize the classical description of Van den Berg [2], but restrict ourselves to the case where (1) is a discretized equation. We do account for the case where (1) is an overdetermined system. First, we introduce an inner product. Let g and h be two vectors in data space, i.e., the space in which the vectors Lu and f are defined. Then, we define the inner product as

$$< g \mid h >= \sum_j g_j^* h_j, \tag{2}$$

where g_j and h_j denote the components of g and h, and where the asterisk denotes complex conjugation. Further, we define a norm according to $||g||^2 =< g \mid g >$. The basic idea behind the iterative procedure is to construct a sequence of vectors $\{u^{(n)} \mid n = 0, 1, 2, \ldots\}$ such that the norm of the residual in (1), i.e.,

$$\mathrm{ERR}^{(n)} =< r^{(n)} \mid r^{(n)} >^{\frac{1}{2}}, \quad \text{with } r^{(n)} = Lu^{(n)} - f, \tag{3}$$

decreases with increasing n. At each step of the iterative procedure, we write

$$u^{(n)} = u^{(n-1)} + u_{cor}^{(n)}, \tag{4}$$

where $u_{cor}^{(n)}$ is a suitably constructed correction vector. We start the procedure with an initial guess $u^{(0)}$ with corresponding residual $r^{(0)}$, and a suitably chosen variational vector $\varphi^{(1)}$. Let $u_{cor}^{(1)} = \alpha^{(1)}\varphi^{(1)}$. We now determine the scalar $\alpha^{(1)}$ such

that $< r^{(1)} \mid r^{(1)} >$ is minimized. This leads to

$$\alpha^{(1)} = \frac{- < L\varphi^{(1)} \mid r^{(0)} >}{||L\varphi^{(1)}||^2}. \tag{5}$$

In subsequent steps, we let $u_{cor}^{(n)} = \alpha^{(n)} \hat{u}_{cor}^{(n)}$ with $\hat{u}_{cor}^{(n)} = \varphi^{(n)} + \beta^{(n)} \hat{u}_{cor}^{(n-1)}$, for $n = 2, 3, \ldots$. Here, $\varphi^{(n)}$ is again a suitably chosen variational vector. It now follows that $< r^{(n)} \mid r^{(n)} >$ is minimized when

$$\alpha^{(n)} = \frac{- < L\varphi^{(n)} \mid r^{(n-1)} >}{||L\hat{u}_{cor}^{(n)}||^2} \quad \text{and} \quad \beta^{(n)} = \frac{< L\hat{u}_{cor}^{(n-1)} \mid L\varphi^{(n)} >}{||L\hat{u}_{cor}^{(n-1)}||^2}. \tag{6}$$

With equations (4)–(6) the iterative scheme based on error minimization has been defined. A geometrical interpretation is that, in each iteration step, the component of the residual $r^{(n-1)}$ in the subspace spanned by the basis vectors $L\varphi^{(n)}$ and $Lu_{cor}^{(n-1)}$ is removed by the correction $\alpha^{(n)} \hat{u}_{cor}^{(n)}$. However, for a general choice of the expansion vectors $\{\varphi^{(n)}\}$, the successive basis vectors $\{Lu_{cor}^{(n)}\}$ are not orthogonal. Therefore, the iterative procedure formulated above cannot be interpreted as a full projection scheme.

Choice of expansion vectors

In principle, the iterative procedure outlined above works for any choice of the expansion vectors $\{\varphi^{(n)}\}$. The error is reduced as long as the coefficient $\alpha^{(n)}$ differs from zero, i.e., when

$$< L\varphi^{(n)} \mid r^{(n-1)} > \neq 0. \tag{7}$$

The condition (7) is known as the *improvement condition*. In the *conjugate-gradient method*, the expansion vectors are generated from the residuals:

$$\varphi^{(n)}(p_m) = L^{\dagger}(p_m)\, r^{(n-1)}(p_m), \tag{8}$$

where $L^{\dagger}$ is the adjoint operator corresponding to L. This choice offers the advantage that (7) is inherently satisfied. For this specific choice of expansion vectors, it can be shown that

$$< Lu_{cor}^{(n)} \mid L\varphi^{(j)} > = 0 \quad \text{and} \quad < r^{(n)} \mid L\varphi^{(k)} > = 0, \tag{9}$$

for $j = 0, 1, \ldots, n-1$, and $k = 0, 1, \ldots, n$, respectively. Now, any correction vector $u_{cor}^{(n)}$ is inherently a linear combination of the expansion vectors $\{\varphi^{(n)}\}$. Therefore, we may interpret the conjugate-gradient method as a successive projection of the residual $r^{(0)}$ on the orthogonalized basis vectors $\{L\varphi^{(n)}\}$. In the remainder of this paper, we will restrict ourselves to this choice of expansion vectors. Further, we will attempt to organize the space discretization such that the convolution structure of the continous equation is preserved. In that case, the matrix-vector products in (3) and (8) can be evaluated by FFT operations, which considerably improves the speed of the so-called CGFFT algorithm.

Initial estimate

In many applications of the conjugate-gradient method, a simple initial estimate is used. Typically, the scheme is started from $u^{(0)} = 0$. Depending on the nature of the problem at hand, we can also start from an incident field or from the Kirchhoff approximation to an unknown surface current. Our choice of the initial estimate is inspired by the fact that $u(p)$ depends in a well-behaved manner on the parameter p. Therefore, it should be possible to extrapolate, by choosing

$$u^{(0)}(p_m) = \sum_{k=1}^{K} \gamma_k\, u(p_{m-k}). \tag{10}$$

The interpretation of the conjugate-gradient scheme given above suggested that the $\{\gamma_k \mid k = 1, \ldots, K\}$ should be found by minimizing the squared error

$$< L(p_m)u^{(0)}(p_m) - f(p_m) \mid L(p_m)u^{(0)}(p_m) - f(p_m) > . \tag{11}$$

Because of the built-in orthogonality of the conjugate-gradient method, we are then certain that this procedure must start its search for components of $f(p_m)$ outside the space spanned by the "previous" functions $\{Lu(p_{m-k}) \mid k = 1, \ldots, K\}$. The coefficients γ_k that minimize the squared error (11) can be found from the system of linear equations

$$\sum_{k'=1}^{K} < L(p_m)u(p_{m-k}) \mid L(p_m)u(p_{m-k'}) > \gamma_{k'} = < L(p_m)u(p_{m-k}) \mid f(p_m) >, \tag{12}$$

with $k = 1, \ldots, K$. Typically, we choose $K = 2$ (linear extrapolation) or $K = 3$ (quadratic extrapolation). For larger values of K, the basis vectors $L(p_m)u(p_{m-n})$ with $n = 1, \ldots, K$ become almost linearly dependent, and therefore the coefficients $\{\gamma_k\}$ can no longer be resolved from (12).

SCATTERING BY A FLAT PLATE

To illustrate our approach, we have extended existing implementations of the CGFFT procedure for two three-dimensional objects that have become standards in the literature. In both cases, no special precautions were taken to enhance the discretization, which is first-order accurate as a function of the mesh size. The first example is a flat, rectangular plate in free space located at $0 < x < a$, $0 < y < b$ and $z = 0$ [3]. For this problem, we solve the well-known electric-field integral equation

$$\left[\nabla_T \nabla_T \cdot + \frac{s^2}{c_0^2}\right] \int_0^a dx' \int_0^b dy' \, \frac{\exp(-sR/c_0)}{4\pi R} \, \boldsymbol{J}_S(\boldsymbol{r}'_T, s) = -s\varepsilon_0 \, \boldsymbol{E}^i_T(\boldsymbol{r}_T, s), \tag{13}$$

where s is a complex frequency, $R = |\boldsymbol{r}_T - \boldsymbol{r}'_T|$, and where the subscript $_T$ stands for a transverse component. The unknown surface current $\boldsymbol{J}_S(\boldsymbol{r}_T, s)$ is approximated by rooftop functions, and we use a weak formulation of (13), weighted by the same rooftop functions. In the resulting discretized form, the convolution symmetry is preserved, so that the matrix-vector products in the conjugate-gradient procedure can be evaluated with the aid of two-dimensional FFT operations.

In particular, we have computed the monostatic radar cross section of a $\lambda \times \lambda$ plate for the special case $s = -i\omega$. A plane wave is incident on the plate at an angle θ with respect to the z-axis and an angle $\phi = 90^\circ$ with respect to the x-axis. The incident plane wave is x-polarized. The discretized plate has a mesh of 31×31 points. Figure 1 shows the number of iterations for increasing θ. The red line represents starting from a zero initial estimate, and the blue line is for two previous results in the initial estimate, i.e. $K = 2$.

The second result for the plate concerns marching on in length. The idea was inspired by the shape sensitivity analysis in [4]. Here, we start from a $\lambda \times \lambda$ plate and we increase the length of the plate in 100 steps to a $2\lambda \times \lambda$ plate. We used a fixed space discretization of 62×31 mesh points. The number of iterations required to reach a relative error of 10^{-3} versus the length of the plate is shown in Figure 2.

SCATTERING BY AN INHOMOGENEOUS DIELECTRIC CUBE

The second example is an inhomogeneous dielectric cube, again in free space. We formulate the scattering problem as a domain integral equation over the object domain $\mathcal{D}$ as

$$\boldsymbol{E}^i(\boldsymbol{r}, s) = \frac{\boldsymbol{D}(\boldsymbol{r}, s)}{\varepsilon(\boldsymbol{r}, s)} + \left(\frac{s^2}{c_0} - \nabla\nabla\cdot\right) \boldsymbol{A}(\boldsymbol{r}, s), \tag{14}$$

where s is a complex frequency and where the vector potential $\boldsymbol{A}(\boldsymbol{r}, s)$ is given by

$$\boldsymbol{A}(\boldsymbol{r}, s) = \frac{1}{\varepsilon_0} \iiint_{\mathcal{D}} \frac{\exp(-sR/c_0)}{4\pi R} \, \frac{\varepsilon(\boldsymbol{r}, s) - \varepsilon_0}{\varepsilon(\boldsymbol{r}, s)} \, \boldsymbol{D}(\boldsymbol{r}, s) \, dV', \tag{15}$$

where $R = |\boldsymbol{r} - \boldsymbol{r}'|$. We take the contrast function in (15) constant in each rectangular subdomain in the space discretization. Like the current in the plate problem, the dielectric displacement $\boldsymbol{D}(\boldsymbol{r}, s)$ is approximated by an expansion that is piecewise linear in the longitudinal direction and constant in the transverse directions. The Green's function is replaced by a weak form, and the result is weighted by testing functions that are identical to the expansion functions. Again, the space discretization preserves the convolution symmetry of the continuous form of the integral equation given in (14) and (15). More details can be found in [5].

As an illustration, we have modeled a cube of muscle tissue centered inside a cube of fat tissue. The incident field is x-polarized with propagation vector parallel to the z-axis and a strength of 1 V/m. The dispersive tissues are modeled using a Debye model, and the dimensions of the inner and outer cubes are 0.14 m and 0.30 m, respectively. The discretized object has $30 \times 30 \times 30$ mesh points. The field is computed in the middle of the muscle cube for real-valued frequencies $s = -i\omega = -2\pi i f$ with f between 100 and 600 MHz and then converted to a time domain signal. The number of iterations needed is shown in Figure 3, where the red line is for a zero initial estimate, and the blue line for minimization using two previous results. Again, using $K = 2$ in the extrapolation procedure led to the most rapid convergence. The time signal, shown in Figure 4, is computed by an FFT using the waveform $\exp\left[-\frac{(t-\tau)^2}{2T^2}\right] \sin(\omega_0 t)$, where $\tau = 14$ ns, $T = 2.75$ ns and $\omega_0/2\pi = 450$ MHz.

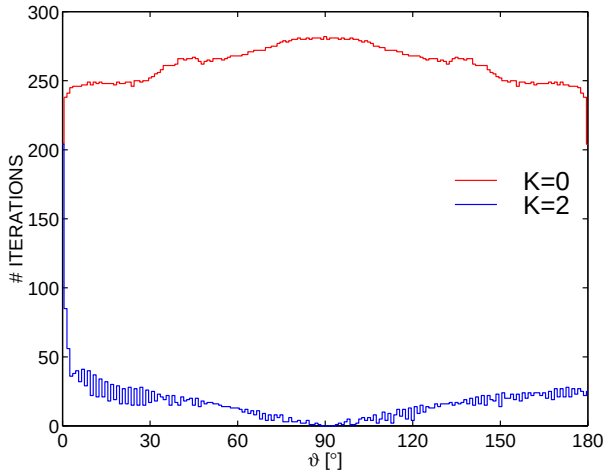

Fig.1. Number of iterations required to reach a relative error of 10^{-3} versus angle of incidence for the marching-on-in-angle version of the CGFFT method for a flat plate using zero (red line) and two previous results (blue line) as an initial estimate.

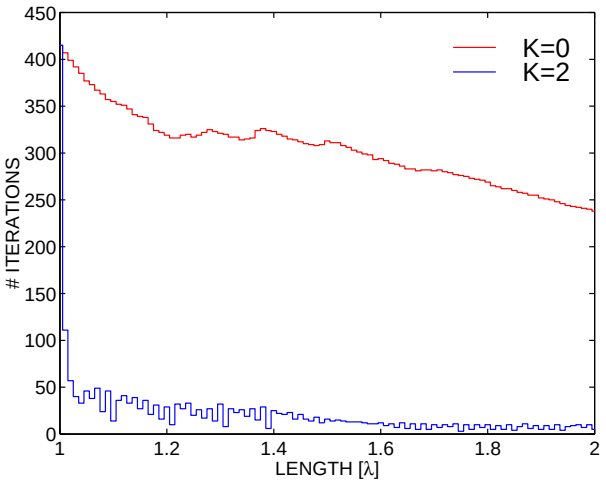

Fig.2 Number of iterations required to reach a relative error of 10^{-3} versus length of the plate for the marching-on-in-length version of the CGFFT method for a flat plate using zero (red line) and two previous results (blue line) as an initial estimate.

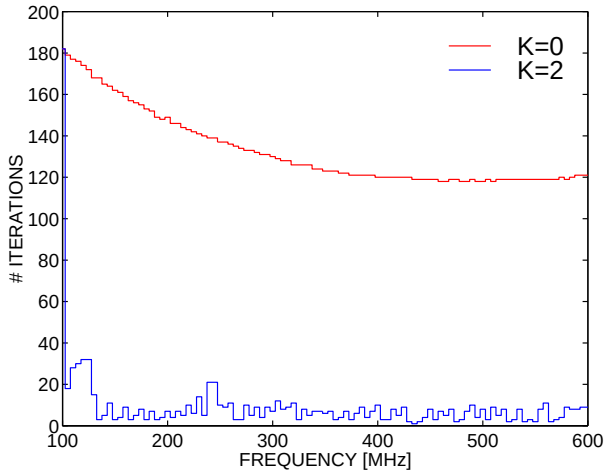

Fig. 3. Number of iterations required to reach a relative error of 10^{-3} versus frequency for the marching-on-in-frequency version of the CGFFT method for an inhomogeneous dielectric cube using zero (red line) and two previous results (blue line) as an initial estimate.

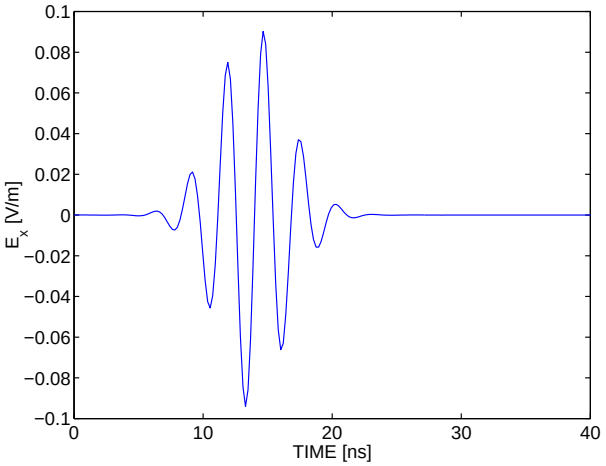

Fig. 4. Time domain signal at the center of the muscle cube for an incident x-polarized wave with amplitude 1 V/m.

REFERENCES

[1] A.G. Tijhuis and Z.Q. Peng, "Marching-on-in-fequency method for solving integral equations in transient electromagnetic scattering," *IEE Proc. H*, vol. 138, pp. 347–355, August 1991.

[2] P.M. van den Berg, "Iterative schemes based on the minimization of the error in field problems," *Electromagnetics*, vol. 5, pp. 237–262, April 1985.

[3] A.P.M. Zwamborn and P.M. van den Berg, "The weak form of the conjugate gradient method for plate problems", *IEEE Trans. Antennas Propagat.*, Vol. 39, pp. 224-228, February 1991.

[4] J. Ureel and D. De Zutter, "Shape sensitivities of capacitances of planar conducting surfaces using the method of moments," *IEEE Trans. Microwave Theory Tech.*, vol. 44, pp. 198–207, February 1996.

[5] A.P.M. Zwamborn, and P.M. van den Berg, "The three-dimensional weak form of the conjugate gradient FFT method for solving scattering problems", *IEEE Trans. Microwave Theory Tech.*, 40, 1757–1766, September 1992.