Modified least squares method with application to diffraction and eigenvalue problems

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Abstract: The paper offers a new approach to boundary value problems. It is a variant of the least squares boundary residual method (LSBRM), combined with the fast Fourier transform (FFT) of basis functions and boundary conditions. This variant makes possible a considerable saving of computation time in comparison with the original LSBRM. The procedure was successfully demonstrated on diffraction and eigenvalue problems.

1 Introduction

The least squares residual method for electromagnetic problems in the microwave domain, e.g. scattering and eigenvalue problems [1, 2] shows considerable advantages over the other possible methods. It was also successfully used in dielectric waveguides [3], and acoustic wave propagation along periodic grating [4]. Its applicability was demonstrated in electrostatic and eddy currents, and also for nonharmonic field problems [5, 6]. The method makes possible a very effective analysis of waveguides with complex cross-sections [7]. The high accuracy of the method and the simplicity of programming make this method very attractive in a large number of boundary value problems.

The only difficulty may be the choice of appropriate basis functions; although this choice is almost always dictated by the nature of the problem. In many cases it is possible to choose the basis functions so that the boundary conditions are fulfilled at least at some parts of the boundary. However, the numerical integration of the products of the basis functions should be carried out along the rest of the boundary. This is the most time consuming part of the whole numerical procedure. Several attempts to decrease the computation time have been made. One of them is based on the transformation of basis functions into rectangular pulse functions satisfying the boundary conditions over only one part of the interface [8]. We shall present a variant of LSBRM combined with the fast Fourier transform of basis functions and boundary conditions. resulting in a substantial saving of computation time.

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2 Theory

Let us consider a two dimensional equation of the Helmholtz type:

$$\frac{\partial^2 U}{\partial x^2} + \frac{\partial^2 U}{\partial y^2} + k^2 U = 0 \tag{1}$$

with the boundary condition along the line $L = L_1 + L_2$ defined by the function $l(x)$. The boundary condition on L_1 is of the Dirichlet type, and that on L_2 is of the Neumann type:

$$g(x) = \begin{cases} U[x, l(x)] & \text{on } L_1 \\ \dfrac{\partial U[x, l(x)]}{\partial n} & \text{on } L_2 \end{cases} \tag{2}$$

The solution will be sought as a sum of the basis functions $\phi_m(x, y)$ of eqn. 1:

$$U(x, y) = \sum_{m=1}^{M} \alpha_m \phi_m(x, y) \tag{3}$$

If we define the functions $f_m(x, y)$ as

$$f_m(x) = \begin{cases} \phi_m[x, l(x)] & \text{on } L_1 \\ \dfrac{\partial \phi_m[x, l(x)]}{\partial n} & \text{on } L_2 \end{cases} \tag{4}$$

and if they meet conditions to be developed in Fourier series, then we can express them in a form

$$f_m(x) = \sum_{n=-N/2}^{N/2-1} \tilde{F}_m(n) e^{jn(2\pi/a)x} \tag{5}$$

where a denotes the length of periodicity on the x-axis. If the functions $f_m[x, l(x)]$ are bandlimited, we can get the coefficients $\tilde{F}_m(n)$ from samples of the functions $f_m[x, l(x)]$ at $x = a(i/N)$, using the FFT algorithm (see Reference 9 for example). So we can write

$$\tilde{F}_m(n) = \text{FFT}\{f_m(n)\} \tag{6}$$

where $f_m(n) = f_m[x, l(x)]\,|_{x=(a/N)n}$ denotes the nth sample of the mth basis function on the boundary.

Deviation of the bounary condition is given by

$$e(x) = \sum_{m=1}^{M} \alpha_m f_m[x, l(x)] - g(x) \tag{7}$$

The FFT of the boundary condition function is denoted by $\tilde{F}_g(n)$:

$$\tilde{F}_g(n) = \text{FFT}[g(n)] \tag{8}$$

and after interchanging the order of summation, the error at any point can be written as

$$e(x) = \sum_{n=-N/2}^{N/2-1} \left[\sum_{m=1}^{M} \alpha_m \tilde{F}_m(n) - \tilde{F}_g(n) \right] e^{jn(2\pi/a)x} \quad (9)$$

The mean of the absolute square value of the error is equal to the sum of the mean square values of all the harmonics:

$$\overline{|e(x)|^2} = \sum_{n=-N/2}^{N/2-1} \left[\sum_{m=1}^{M} \alpha_m \tilde{F}_m(n) - \tilde{F}_g(n) \right] \times \left[\sum_{m=1}^{M} \alpha_m^* \tilde{F}_m^*(n) - \tilde{F}_g^*(n) \right] \quad (10)$$

We shall find the developing coefficients from the condition that the right-hand side of eqn. 10 should be a minimum. This means that the first derivative of the real part of α_m is zero, which gives

$$\sum_{n=-N/2}^{N/2-1} \sum_{l=1}^{M} \mathrm{Re}\,\{\alpha_l \tilde{F}_l(n) \tilde{F}_m^*(n)\} = \sum_{n=-N/2}^{N/2-1} \mathrm{Re}\,\{\tilde{F}_g(n) \tilde{F}_m^*(n)\} \quad (11)$$

By analogy, the derivative of the imaginary part of α_m is

$$\sum_{n=-N/2}^{N/2-1} \sum_{l=1}^{M} \mathrm{Im}\,\{\alpha_l \tilde{F}_l(n) \tilde{F}_m^*(n)\} = \sum_{n=-N/2}^{N/2-1} \mathrm{Im}\,\{\tilde{F}_g(n) \tilde{F}_m^*(n)\} \quad (12)$$

Eqns. 11 and 12 can be condensed to

$$\sum_{l=1}^{M} \alpha_l A_{ml} = B_m \quad m = 1, 2, \ldots, M \quad (13)$$

A_{ml} and B_m denote

$$A_{ml} = \sum_{n=-N/2}^{N/2-1} \tilde{F}_l(n) \tilde{F}_m^*(n) \quad B_m = \sum_{n=-N/2}^{N/2-1} \tilde{F}_g(n) \tilde{F}_m^*(n) \quad (14)$$

Therefore the unknown developing coefficients are given by the following system of linear equations:

$$\begin{Vmatrix} A_{11} & \cdots & A_{1M} \\ \vdots & & \vdots \\ A_{M1} & \cdots & A_{MM} \end{Vmatrix} \begin{Vmatrix} \alpha_1 \\ \vdots \\ \alpha_M \end{Vmatrix} = \begin{Vmatrix} B_1 \\ \vdots \\ B_M \end{Vmatrix} \quad (15)$$

Note that the relationship $A_{ml} = A_{lm}^*$ holds for the coefficients A_{ml}, which saves time in filling up the matrix in eqn. 15. In the case of the boundary condition $g(x) = 0$, the same approach can be applied, taking $\alpha_1 = -1$, i.e. $g(x) = f_1[x, l(x)]$, and then finding the other coefficients.

3 Application in diffraction problems

The applicability of the method will be demonstrated on electromagnetic wave diffraction, from periodic gratings which have perfect conductivity. The grating of sinusoidal profile (Fig. 1*a*) has often been used as a test problem for many methods (for extensive references see [10, 11].

As usual, we shall assume an incident plane wave of normal polarisation:

$$\boldsymbol{E}_i = \boldsymbol{E}_0 e^{-jk(\gamma x - \delta z)} \quad (16)$$

where $\gamma = \sin\theta$, $\delta = \cos\theta$, $k = 2\pi/\lambda$ and $\boldsymbol{E}_0 = 1$.

The reflected field will be represented as a sum of propagating and attenuated waves:

$$\bar{E}_r = \sum_{m=-M_1}^{M_1} \bar{E}_m e^{-jk(\gamma_m x + \delta_m z)} \quad (17)$$

with

$$\gamma_m = \sin\theta + m\lambda/d \quad \delta_m = \sqrt{(1 - \gamma_m^2)}$$

We shall determine the unknown coefficients $\bar{E}_m$ by the procedure described previously, which satisfies the boundary condition on the grating wall:

$$\bar{E}_r = -\bar{E}_i \quad (18)$$

Thus, here we have

$$f_m[x, l(x)] = e^{-jk(\gamma_m x + \delta_m h \sin(2\pi/d)x)}$$
$$g(x) = -e^{-jk(\gamma x - \delta h \sin(2\pi/d)x)} \quad (19)$$

After finding the field amplitudes $\bar{E}_m$, we plotted the reflection coefficients

$$R_m = |\bar{E}_m|^2 \frac{\delta_m}{\delta} \quad (20)$$

against the incidental angle (Figs. 2*a* and *b*), for two sets of grating parameters.

In the same way we solved the diffraction problem on triangular cross-section grating (Fig. 1*b*), which is of greater practical interest. The reflection coefficients are shown on Fig. 3.

A simple and reliable test is the energy balance equation:

$$\sum_m |\bar{E}_m|^2 \frac{\delta_m}{\delta} = 1 \quad (21)$$

where summation is over those m for which δ_m is real. From Table 1 it can be seen that the requirement of eqn. 21 is adequately satisfied.

The error is less than 1% for a triangular grating, and even less than 0.06% for a sinusoidal grating. This was achieved with $M_1 = 15$, i.e. with 31 modes in eqn. 17, and with 64 samples along the grating wall, i.e. within the interval (0, *d*).

For the sinusoidal grating, the same parameters have been taken as in Reference [10], and the results are in complete agreement.

The fulfilment of the boundary condition, eqn. 18, can be used as another accuracy check. Although it is not presented here, this check has been performed and it has proved the high accuracy of this numerical procedure.

Generally, better accuracy, with less calculation, can be achieved with the suggested modification than with the original LSBRM. If N is the number of integral steps, then in LSBRM for M modes (i.e. for M developing coefficients) the total $M \times M \times N$ multiplications and summations are performed. In our modification, with N basis function samples and m developing coefficients, the number of calculations is $M \times N \times \log_2 N$. Then, taking N_1 as the number of harmonics which mainly contribute to the field value (i.e. their amplitudes are greater than a certain small value), additional $M \times M \times N1$ operations are performed. Altogether, the ratio of the number of calculation is

$$R_t = \frac{N_1}{N} + \frac{\log_2 N}{M} \quad (22)$$

The above ratio does not include the number of calculations required for solving eqns. 15. Since this number is of the order $M^3/3$, the total ratio is

$$R_t = \frac{(M/3N) + (N_1/N) + (\log_2 N/M)}{(M/3N) + 1} \quad (23)$$

It should be noted that, in all realistic problems, the number of modes M is considerably smaller than the number of samples (integral steps) N in the original LSBRM.

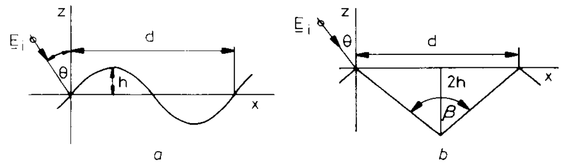

Fig. 1 *Gratings*
a Sinusoidal
b Triangular

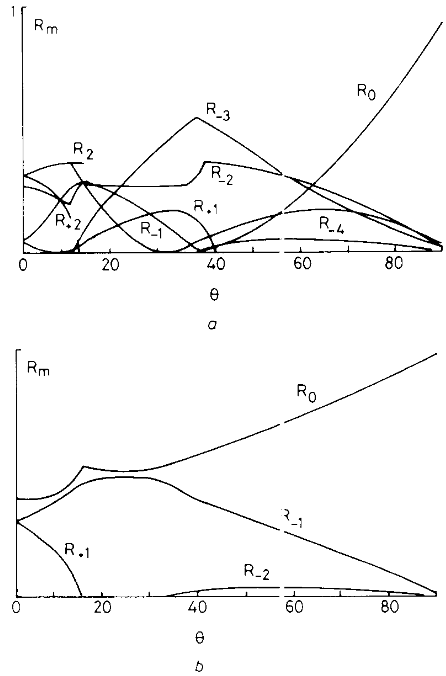

Fig. 2 *Reflection coefficients for sinusoidal grating*
(*a*) $h/\lambda = 0.375$; $d/\lambda = 2.5$
(*b*) $h/\lambda = 0.1333$; $d/\lambda = 1.3$

Table 1: Energy balance

Diffraction from triangular grating		Diffraction from sinusoidal grating	
$d/\lambda = 2.5$ $h/\lambda = 0.375$		$M_1 = 15$	
Angle, degrees	Energy summation	Angle, degrees	Energy summation
0	0.9907514	0	0.9995761
10	0.9923179	10	0.9994044
20	0.9910881	20	0.9997635
30	0.9908311	30	0.9993797
40	0.9969598	40	0.9998330
50	0.9950774	50	0.9996443
60	0.9950853	60	0.9995366
70	0.9988487	70	0.9993890
80	0.9991010	80	0.9999954
89	1.000253	89	0.9999812

Even if we assume that $M = N$, and that M is a large number, the ratio given by eqn. 23 shows that the reduction in computation time is still considerable.

The summation limit N_1 is defined by the basis function of faster convergence, and for our basis function it is usually up to ten times smaller than N. As can be seen from Fig. 4, the significant values given by eqn. 14 are located around the carrier numbers. The latter depend on the basis functions indices, m and l, and not on the grating shape.

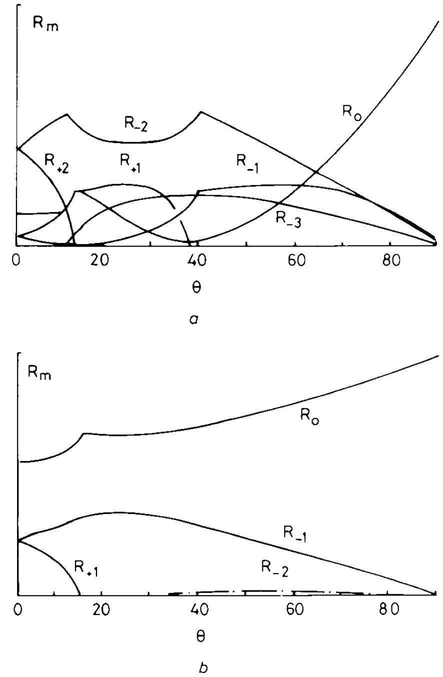

Fig. 3 *Reflection coefficients for triangular grating*
(*a*) $h/\lambda = 0.375$; $d/\lambda = 2.5$
(*b*) $h/\lambda = 0.1333$; $d/\lambda = 1.3$

Table 2: Normalised eigenvalue $k/(\pi/a)$ of H_{10} mode and normalised bandwidth of the round-ridged waveguide for different cross-sectional parameters

h/d	0.9	0.8	0.7	0.6	0.5	0.4
H_{10}	0.969	0.929	0.883	0.831	0.774	0.721
$H_{20} - H_{10}$	1.037	1.086	1.141	1.206	1.269	1.336

$b/a = 0.3$; $a/d = 2$

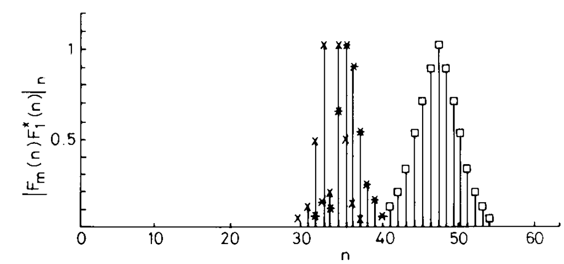

Fig. 4 *Normalised value of* $|\tilde{F}_m(n)\tilde{F}_l^*(n)|$ *against n for different harmonics*
○○○ $m = 1$; $l = 1$
∗∗∗ $m = 1$; $l = 15$
× × × $m = 15$; $l = 15$

So, for $N = 64$, $M = 31$ and $N_1 = 13$, eqn. 22 gives the ratio of performed calculations as 0.4. This means that our modified version of the LSBRM is approximately 2.5 times faster than the original method. The reduction in computation time comes from replacing the N-point numerical integration by the summation of N_1 terms. For the basis functions treated in this paper, the convergence regarding N_1 is fast. It has been demonstrated [13], that, in some cases of practical interest, only one of the most significant terms ($N_1 = 1$), may produce sufficiently accurate results. However, for the most general form of basis functions, the convergence regarding N_1 is to be considered in each case separately.

4 Eigenvalue problems

As a demonstration of the applicability of the suggested method in eigenvalue problems, we shall consider two complex cross-section waveguides (Fig. 5) carrying with

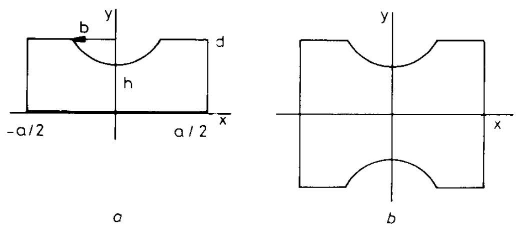

Fig. 5 *Cross-section of round-ridged waveguide*

H wave. The differential equation for the longitudinal magnetic field component $U = H_z$, is the same as eqn. 1, and the boundary condition on the waveguide walls is:

$$\partial H_z/\partial n = 0 \tag{24}$$

so system eqns. 15 become

$$\begin{Vmatrix} A_{11} & \cdots & A_{1M} \\ \vdots & & \vdots \\ A_{M1} & \cdots & A_{MM} \end{Vmatrix} \begin{Vmatrix} \alpha_1 \\ \vdots \\ \alpha_M \end{Vmatrix} = 0 \tag{25}$$

Assuming H_z for the H_{10} and H_{20} modes to be:

$$H_{z10} = \sum_{m=1}^{M} \alpha_m \sin \frac{(2m-1)}{a} \pi x \cos k_y y$$

$$\div \exp\left[\frac{2m-1}{a} \pi d\right]$$

$$H_{z20} = \sum_{m=1}^{M} \alpha_m \cos \frac{2m\pi}{a} x \cos k_y y$$

$$\div \exp\left[\frac{2m\pi d}{a}\right] \quad k_x^2 + k_y^2 = k^2 \tag{26}$$

then the boundary condition (eqn. 24) on the walls, $x = \pm a/2$ and $y = 0$, is exactly satisfied.

The nontriviality condition for the eqns. 25 requires that

$$\det \|A_{mn}\| = 0 \tag{27}$$

where $A_{mn} = A_{mn}(k)$. For different values of the relative eigenvalue, $k_r = k/(\pi/a)$, we calculate det (A_{mn}). The unknown eigenvalues are those for which the determinant is a minimum.

Better results were obtained by using eqn. 25 to give the coefficients α_m with $\alpha_1 = 1$, and e^2 from eqn. 10. By altering the value of κ_r, we can find the minimum of e^2 and thus the required eigenvalue.

In analogous manner we found the bandwidth of a round-ridged waveguide (Fig. 5). The results (Table 3) are almost identical to those obtained by the original method [7].

Another example we studied was a variant of π ridged-waveguide. The sharp ridge edge caused reduced accuracy when the same co-ordinate system (Fig. 6*a*) was

Table 3: Normalised eigenvalue $k/(\pi/a)$ of H_{10} mode of the waveguide for different cross-sectional parameters

h/d	0.1	0.2	0.3	0.4	0.5	0.6	0.7	0.8	0.9
$k/(\pi/a)$	0.45	0.58	0.62	0.71	0.79	0.85	0.91	0.94	0.99
by Ref. 12	0.49	0.58	0.64	0.71	0.79	0.84	0.90	0.94	0.99

$a/d = 2$

used. Therefore the analysis was carried out in the system shown in (Fig. 6*b*). This co-ordinate system was also appropriate for our intended demonstration of the inclusion of mixed boundary conditions in the suggested variant.

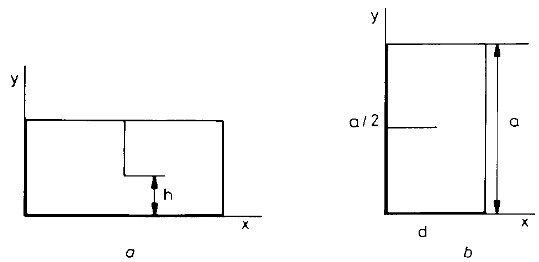

Fig. 6 *Cross-section of π-waveguide*

When

$$\phi_m(x, y) = \cos \frac{m\pi x}{d} \cos \sqrt{\left[k^2 - \left(\frac{m\pi}{d}\right)^2\right]} y \tag{28}$$

the boundary conditions (eqn. 24) are exactly fulfilled on the walls $x = 0$, $x = d$ and $y = 0$. The boundary condition (eqn. 24) is approximately fulfilled along the ridge, while the field continuity conditions met along the rest of the line $y = a/2$. So, we have

$$f_{1m}(x) = \begin{cases} \dfrac{\partial \phi_m}{\partial y} & 0 < x < d - h \\ \dfrac{\partial \phi_m}{\partial x} & d - h < x < d \end{cases} \tag{29}$$

$$f_m(x) = \begin{cases} 0 & 0 < x < d - h \\ \phi_m & d - h < x < d \end{cases}$$

The square error is now

$$e^2(x) = \left[\sum_{m=0}^{M-1} \alpha_m f_m(x)\right]^2 + g\left[\sum_{m=0}^{M-1} \alpha_m f_{1m}(x)\right]^2 \tag{30}$$

The minimisation procedure of e^2, described in chapter 2 gives:

$$A_{ml} = \sum_{n=-N/2}^{N/2-1} [\tilde{F}_l(n)\tilde{F}_m^*(n) + g\tilde{F}_{1l}(n)\tilde{F}_{1m}^*(n)] \tag{31}$$

Otherwise, calculation of eigenvalues is identical to the round-ridged waveguide. The results are shown in Table 3, where we give the eigenvalues from Reference [12] for comparison. Again, we use $N = 64$ samples of basis functions, the number of modes $M = 11$, and the weighting factor $g = 1$.

This shows the results to be very close for all ridge depths of practical interest.

5 Conclusion

The modification of the LSBRM was achieved using FFT, instead of the usual integration procedure of the original method. This variant was applied to the wave diffraction produced by sinusoidal and triangular gratings, and also to eigenvalue problems of two types of ridged waveguide. In all these cases, the accuracy was very high, and computation was very fast. The shorter computation time in the modified method is due to the fact that, in FFT, we take only those harmonics that contribute significantly to the basis function value. This number can be much smaller than the number of integration steps in the original LSBRM.

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