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TREFFTZ METHOD: FITTING BOUNDARY CONDITIONS

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SUMMARY

The paper presents various ways of fitting the boundary conditions in the T-complete functions method. The authors point out the distinct advantages of the orthogonal collocation in comparison to the equidistant collocation and the integral fit. The convergence of the Collatz error measures and the conditioning of the solution matrices are investigated in detail.

1. INTRODUCTION

There are two main approaches for the formulation of boundary methods; one is based on boundary integral equations (boundary element methods, as well as the boundary series method[1–3]) and the other is based on the use of complete systems of solutions (Trefftz method[4–6]). This article is concerned with the latter approach.

Complete systems of shape functions can be constructed in many alternative ways. Several aspects of such questions, such as completeness and convergence of integral least squares fitting of boundary conditions have been extensively studied by one of the authors.[4,5,7–11] Construction of finite elements with this kind of shape function has also been investigated.[12]

To fit the boundary conditions one can use a direct or, alternatively, an indirect approach.[5] To be more specific, consider the Dirichlet problem for the Laplace equation on a region Ω with boundary Γ. In this case the boundary condition is $u = \bar{u}$ on Γ, where u is a prescribed function. Let $\kappa = \partial u/\partial n$ be the unknown complementary boundary values. To solve such a problem by Trefftz method, one has available a T-complete system of functions $\{U_1, U_2, \ldots\}$. Then, in the direct approach one constructs a linear combination $\hat{u} = \sum_{i=1}^{N} a_i U_i$ which approximates the prescribed boundary values $\bar{u}$, whereas in the indirect approach $\hat{u}$ is required to be such that $\partial \hat{u}/\partial n$ approximates the unknown normal derivative κ, on the boundary. The indirect procedure has been used in previous works and has been called boundary fitting using opposite weights.[12] However, it had not been realized that such a procedure is tantamount to approximating the unknown boundary derivatives. To see that this is indeed so, recall the well-known reciprocity relation

$$\int_{\Gamma} u \frac{\partial v}{\partial n} \mathrm{d}x = \int_{\Gamma} v \frac{\partial u}{\partial n} \mathrm{d}x \tag{1}$$

which holds for harmonic functions in Ω. If we impose the condition

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$$\int \left(\frac{\partial \hat{u}}{\partial n} - \frac{\partial u}{\partial n}\right) U_i \, dx = 0, \quad i = \quad , N \tag{2}$$

it will be granted that the projection of $\partial \hat{u}/\partial n$ on the subspace spanned by the functions $\{U_1, \ldots, U_N\}$ is exact; i.e. it is the same as the projection of $\partial u/\partial n$. In view of equation (1), it is clear that

$$\int_\Gamma \left(\frac{\partial \hat{u}}{\partial n} - \frac{\partial u}{\partial n}\right) U_i \, dx = \int_\Gamma (\hat{u} - u) \frac{\partial U_i}{\partial n} dx = \int_\Gamma (\hat{u} - \bar{u}) \frac{\partial U_i}{\partial n} dx \tag{3}$$

Hence, equation (2) becomes

$$\int_\Gamma \hat{u} \frac{\partial U_i}{\partial n} dx = \int_\Gamma \bar{u} \frac{\partial U_i}{\partial n} dx \tag{4}$$

which is fitting the boundary values with opposite weights.

This article studies the behaviour of solutions obtained using alternative ways of fitting the boundary conditions. Section 2 and 3 study the relation between collocation and integral fit; special attention is given to orthogonal collocation which is quite efficient. In the remaining part of the article the results of numerical experiments are presented and some improvements that can be achieved by multi-step fitting are discussed. Finally, questions related to conditioning of solution matrices are also analysed.

2. RELATION BETWEEN COLLOCATION AND THE INTEGRAL FIT

To be specific we shall consider problems associated with the Laplace operator, although similar considerations apply to other elliptic equations. The boundary of the region Ω will be, as before Γ, and Γ_1, Γ_2 will be a decomposition of Γ. If a function u is harmonic in Ω (i.e. it fulfils Laplace's equation in Ω), then is clear that u is the solution of the problem

$$\Delta u = 0, \quad \text{in} \quad \Omega \tag{5a}$$

$$u = f(x), \quad \text{on} \quad \Gamma_1 \tag{5b}$$

$$u' \equiv \frac{\partial u}{\partial n} = g(x), \quad \text{on} \quad \Gamma_2 \tag{5c}$$

if and only if the quadratic functional

$$X(u) = \int_{\Gamma_1} [u - f(x)]^2 \, dx + \int_{\Gamma_2} \left[\frac{\partial u}{\partial n} - g(x)\right]^2 dx \tag{6}$$

vanishes (i.e. it is minimized).

An approximate solution $\hat{u}$ to this problem can be obtained by replacing the integrals in (6) by their numerical approximation. Thus

$$\sum_{\mu=1}^{\mu^*} W_\mu [\hat{u}(x_\mu) - f(x_\mu)]^2 + \sum_{\mu=\mu^*+1}^{\nu^*} W_\mu [\hat{u}'(x_\mu) - g(x_\mu)]^2 = 0 \tag{7}$$

where the W_μ are weighting constants of integration. Equation (7) is equivalent to the collocation equations

$$\hat{u}(x_\mu) = f(x_\mu), \quad \mu = 1, 2, \ldots, \mu^* \text{—for } \Gamma_1 \tag{8a}$$

$$\hat{u}'(x_\mu) = g(x_\mu), \quad \mu = \mu^* + 1, \ldots, \nu^* \text{—for } \Gamma_2 \tag{8b}$$

If the system of shape functions $U_i(x)$ is used, one can write

$$\hat{u}(x) = \sum_{j=1}^{\nu^*} a_j U_j(x) \tag{9}$$

In this case equations (8) become

$$\sum_{j=1}^{\nu^*} a_j U_j(x_\mu) = f(x_\mu), \quad \mu = 1, \ldots, \mu^* \tag{10a}$$

$$\sum_{j=1}^{\nu^*} a_j U_j'(x_\mu) = g(x_\mu), \quad \mu = \mu^* + 1, \ldots, \nu^* \tag{10b}$$

where the prime stands for the normal derivative. Hence, it is seen that the numerical approximation of the integral fitting leads to simple collocation on the control points used for the integration.

Similar conclusions are obtained if the number of control points is greater than the number of Trefftz functions. Indeed, assume that J is the number of Trefftz functions and that $\nu^* > J$. Then equation (7) can not be fulfilled exactly and one has to be satisfied with

$$\sum_{\mu=1}^{\mu^*} W_\mu [\hat{u}(x_\mu) - f(x_\mu)]^2 + \sum_{\mu=\mu^*+}^{\nu^*} W_\mu [\hat{u}'(x_\mu) - g(x_\mu)]^2 = \min \tag{11}$$

This leads to

$$\sum_{\mu=1}^{\mu^*} W_\mu U_k(x_\mu)[\hat{u}(x_\mu) - f(x_\mu)] + \sum_{\mu=\mu^*+1}^{\nu^*} W_\mu U_k'(x_\mu)[\hat{u}'(x_\mu) - g(x_\mu)] = 0; \quad k = \quad , J \tag{12}$$

and, more explicitly,

$$\sum_{j=1}^{J} a_j \left[\sum_{\mu=1}^{\mu^*} W_\mu U_{k\mu} U_{j\mu} + \sum_{\mu=\mu^*+1}^{\nu^*} W_\mu U_{k\mu}' U_{j\mu}' \right] = \sum_{\mu=1}^{\mu^*} W_\mu U_{k\mu} f(x_\mu)$$
$$+ \sum_{\mu=\mu+1}^{\nu^*} W_\mu U_{k\mu}' g(x_\mu); \quad k = 1, \ldots, J \tag{13}$$

where $U_{k\mu} = U_k(x_\mu)$ and $U_{k\mu}' = U_k'(x_\mu)$.

After the introduction of the following rectangular matrices and vectors:

$$\mathbf{B} = \begin{bmatrix} B_{11} & B_{12} & \cdots & B_{1,J} \\ B_{21} & B_{22} & \cdots & B_{2,J} \\ \\ \\ B_{\nu^*,1} & B_{\nu^*,2} & & B_{\nu^*,J} \end{bmatrix} \quad \tilde{\mathbf{B}} = \begin{bmatrix} W_1 B_{11} & W_1 B_{12} & \cdots & W_1 B_{1,J} \\ W_2 B_{21} & W_2 B_{22} & \cdots & W_2 B_{2,J} \\ \\ \\ W_{\nu^*} B_{\nu^*,1} & W_{\nu^*} B_{\nu^*,2} & & W_{\nu^*} B_{\nu^*,J} \end{bmatrix} \tag{14}$$

$$\begin{bmatrix} f(x_1) \\ f(x_2) \\ \cdot \\ \cdot \\ \cdot \\ \cdot \\ f(x_{\mu^*}) \\ g(x_{\mu^*+1}) \\ \cdot \\ \cdot \\ \cdot \\ \cdot \\ g(x_{\nu^*}) \end{bmatrix} \qquad \mathbf{a} = \begin{bmatrix} a_1 \\ a_2 \\ \\ \\ \\ a_J \end{bmatrix}$$

where

$$B_{rs} = U_s(x_r), x_r \in \Gamma_1, \quad \text{for} \quad r \leqslant \mu^*$$

$$B_{rs} = U_s'(x_r), x_r \in \Gamma_2, \quad \text{for} \quad \mu^* > r \leqslant \nu^*$$

equation (13) can be written as

$$\mathbf{B}^{T}\mathbf{B}\mathbf{a} \quad \mathbf{B}^{T}\mathbf{c} \tag{15}$$

We could have considered, instead, the overdetermined collocation problem

$$\sum_{j=1}^{J} a_j U_j(x_\mu) = f(x_\mu), \quad \mu = 1, \ldots, \mu^* \tag{16a}$$

$$\sum_{j=1}^{J} a_j U_j'(x_\mu) = g(x_\mu), \quad \mu = \mu^* + 1, \ldots, \nu^* \tag{16b}$$

with $J > \nu^*$. Since equations (16) do not have, in general, a solution, one has to be satisfied with

$$\sum_{\mu=1}^{\mu^*} W_\mu R_\mu^2 + \sum_{\mu=\mu^*+1}^{\nu^*} W_\mu R_\mu'^2 = \min \tag{17}$$

where

$$\sum_{j=1}^{J} a_j U_j(x_\mu) - f(x_\mu) = R_\mu, \qquad \mu = 1, \ldots, \mu^* \tag{18a}$$

$$\sum_{j=1}^{J} a_j U_j'(x_\mu) - g(x_\mu) = R_\mu', \qquad \mu = \mu^* + 1, \ldots, \nu^* \tag{18b}$$

Condition (17) leads precisely to equations (13) again. Thus, least squares integral fitting is seen to be equivalent to least squares collocation. In what follows we investigate the influence of the distribution of control points x_μ and the weighting constants W_μ.

3. ORTHOGONAL COLLOCATION AND INTEGRAL FIT WITH GAUSSIAN INTEGRATION

Using T-complete systems of functions, the solution of a boundary value problem only requires the construction of an accurate approximation of the given boundary data $f(x)$, $g(x)$ by the specific series of functions $U_i(\Gamma_1)$, $U_i'(\Gamma_2)$ which are the values of the shape functions on the boundary Γ. This series may have a very complex form, as it depends not only on the T-complete system applied, but also on the shape of the contour Γ.

A related problem which can give hints about the efficiency of alternative distributions of collocation points is the approximation of functions by polynomials. As we know, equidistant points are not very convenient in this case, because such a procedure can be divergent (this is called the 'Runge phenomenon'[13]). However, if the control points are located at the zeros of Legendre polynomials of degree ν^* (where ν^* is the number of control points), then the residue

$$w(x) = \hat{u}(x) - u(x) \tag{19}$$

is the orthogonal to all polynomials of degree smaller than ν^* and the process is necessarily convergent. This will be called Gauss–Legendre integral approximation.

As an extension of this procedure, the idea of using orthogonal collocation inside Ω has been broadly used for solving differential equations.[14–16] Various types of equations are solved with the help of splines as shape functions and estimates of the accuracy of the solutions are available.[17,18] In our case the orthogonal collocation is applied on Γ. An estimate for the error inside the region Ω can be made in the following way. For simplicity, consider the case of a Dirichlet problem (i.e. $\Gamma_2 = \phi$). Assume that orthogonal collocation of degree n is used inside each of the equal segments Γ_α of the contour Γ, where

$$\Gamma = \bigcup_{\alpha=1}^{N} \Gamma_\alpha, \quad N = \frac{L}{h} \tag{20}$$

Here L is the length of the contour and h is the length of each of the segments Γ_α. For this case the error $w(x)$ is given by (19), with

$$\hat{u}(x) = \sum_{j=1}^{J} a_j U_j(x) \tag{21}$$

The error function $w(x)$ inside Ω is given in terms of its values on the boundary by

$$w(x) = \int_\Gamma K(x,\xi) w(\xi)\,d\xi = \sum_{\alpha=1}^{N} \int_{\Gamma_\alpha} K(x,\xi) w(\xi)\,d\xi \tag{22}$$

where $K(x,\xi)$ is the appropriate influence function for the Dirichlet problem in Ω. On the boundary Γ, ξ can be expressed in parametric form, in terms of the arc lengths. Then, for each $\alpha = 1,\ldots,N$, there are n zeros $\{s_1^\alpha, s_2^\alpha, \ldots, s_n^\alpha\}$ of the function $w[\xi(s)]$ which correspond to n collocation points $\{\xi(s_1^\alpha),\ldots,\xi(s_n^\alpha)\}$ inside the segment Γ_α.

Apply now equation (22) at any interior points x of Ω. At any fixed interval Γ_α write

$$K[x,\xi(s)]\,w[\xi(s)] = q(s) \prod_{i=1} (s - s_i^\alpha) \tag{23}$$

which is clearly possible. Even more, the function $\prod_{i=1}^{n}(s - s_i^\alpha)$ is orthogonal to any polynomial in s of degree less than n. When $q(s)$ is C^n, by Taylor's theorem one has

$$q(s) = \text{polynomial of degree } (n-1) + O(h^n) \tag{24}$$

Therefore

$$\int_{\Gamma_\alpha} K[x,\xi(s)]\,w[\xi(s)]\,d\xi(s) = \int_{\Gamma_\alpha} O(h^n) \prod_{i=1} (s - s_i^\alpha)\,ds = O(h^{2n+} \tag{25}$$

going back to (22) we obtain

$$w(x) = \sum_{\alpha=1}^{N} O(h^{2n+1}) = O(h^{2n}) \tag{26}$$

because $N = L/h$.

We have shown in Section 2 that the integral fit, using the same number of control points for the numerical integration as shape functions, is equivalent to collocation at the control points. Thus, in this case, the error estimate we have just obtained is also applicable to integral fit when Gauss–Legendre numerical integration is used.

It must be noticed that although the procedure just explained shows that the error is $O(h^{2n})$ for any interior point x, this fact is less significant when the boundary Γ is approached because the function $K(x,\xi)$ is singular on Γ, so the approximation is slowly convergent. Indeed, equation (26) means that for every x, there exists a positive number M such that

$$|w(x)| < M h^{2n} \tag{27}$$

However, M depends on x and may grow indefinitely when the boundary is approached.

In the case of the least squares fit the system of weights W_μ (equation (15)) considerably influences the final result of the fit. For Gauss–Legendre integral fit this system by the formula

$$W_\mu = \frac{t_2 - t_1}{2} A_\mu \tag{28}$$

where t_1, t_2 are the lower and upper limits of the integral and A_μ are Gaussian weights. The automatic association of weights with the ranges of integration (when the segments Γ_α have different lengths) is not always profitable. More reasonable seems often to be the direct choice of the Gaussian weights in orthogonal collocation ($W_\mu = A_\mu$), which corresponds to the sum of average values of the integrals over the segments Γ_α. A comparison of the numerical results when applying various systems of weights W_μ is presented in the following sections.

4. ERROR CRITERIA

Generally, the error norm must be carefully chosen in order to reflect those aspects of the error most relevant from the engineering viewpoint. Taking $w(x)$ as in (19), the integral error norms

$$E_\Omega = \int_\Omega |w(x)|^p \,\mathrm{d}x \tag{29a}$$

or

$$E_\Gamma = \int |w(x)|^p \,\mathrm{d}x \tag{29b}$$

are in a certain sense representative, as they estimate the solution in the global way. However, the integrals smooth out the local concentrations of the error, which can sometimes be unacceptable from the engineering viewpoint. Hence, in the two-step solution additional weighting functions should be introduced, for example

$$\tilde{E}_\Gamma = \int_\Gamma |w_1(x)|^k |w(x)|^p \,\mathrm{d}x \tag{30a}$$

or

$$\tilde{E}_\Omega = \int_\Omega |w_1(x)|^k |w(x)|^p \,\mathrm{d}x \tag{30b}$$

where $w_1(x)$ is the error associated with the first-step solution of the problem and the exponents p, k are positive numbers which control the influence of the particular factors.

As has already been mentioned, for elliptic problems the maximum error occurs on the boundary.[19] Hence, we have introduced the error norms (Figure 1):

$$E_e = \max_{x\in\Gamma} |w(x)|, \quad E_b = \max_{x\in\Gamma} w - \min_{x\in\Gamma} w \tag{31}$$

The first one is called the extreme error of the fit and the second one, the width of the error band. We consider these measures as sufficiently representative for the problems discussed and applied them in our numerical investigation of the ways of fitting the boundary conditions.

5. BEHAVIOUR OF SOLUTIONS: NUMERICAL EXAMPLES

Two T-complete families of shape functions were used: harmonic polynomials

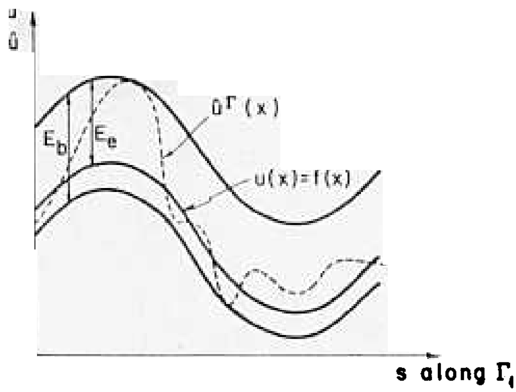

Figure 1. Definition of the Collatz error norms on the boundary Γ

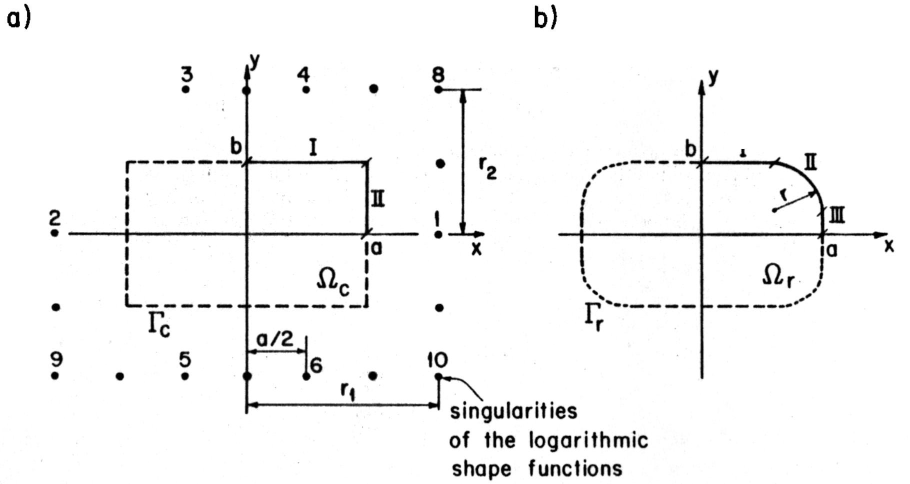

Figure 2. Contours of the areas Ω used in the numerical examples: I, II, III—segments of fitting the boundary conditions

$$U_0^h = 1, \quad U_{2n}^h = \mathrm{Re}(z^n), \quad U_{2n+1}^h = \mathrm{Im}(z^n), \quad n = 1, 2, . \tag{32}$$

and singular logarithmic functions

$$U_0 = 1, \quad U_n = \log r_n, \quad n = 1, 2, \ldots \tag{33}$$

Here $r_n^2 = (x - x_n)^2 + (y - y_n)^2$ and the singular point (x_n, y_n) lies outside the region Ω.

These functions identically satisfy the Laplace equation inside Ω. We investigated their behaviour when fitting Dirichlet boundary conditions:

$$f(x, y) = (x^2 + y^2)/2, \quad \text{on } \Gamma \tag{34}$$

on two different contours—the rectangle Ω_c and the rectangle with rounded corners Ω_r(Figure 2). Because of the symmetry we applied

$$U_n^h = \mathrm{Re}(z^n), \qquad n = 0, 2, 4 \ldots \tag{35}$$

in the case of the harmonic polynomials, and

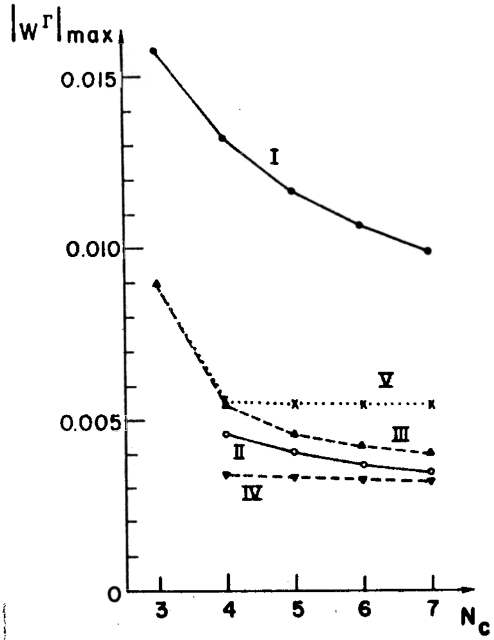

Figure 3. Error $|w^\Gamma|_{max}$ on the boundary of the square, $a = b = 1{\cdot}0$; $N_s(=6)$ is the number of the shape functions applied, N_c is the number of control points on each side of the rectangle: I—equidistant collocation inside the segments; II—equidistant collocation including the corner; III—orthogonal collocation; IV—orthogonal collocation with the additional control point in the corner; V—integral fit with the Gaussian integration

$$
\begin{aligned}
U_1 &= \\
U_2 &= \sum_{i=1}^{2} \log r_i \\
U_3 &= \sum_{i=3}^{6} \log r_i \\
U_4 &= \sum_{i=7}^{10} \log r_i
\end{aligned} \qquad 36)
$$

for the singular logarithmic functions. To investigate the convergence of the solutions and the conditioning of the matrices we also applied 10 additional singular functions (Figure 2(a)) in the latter case. Because of the symmetry they formed three independent shape functions.

In Figures 3 and 4 we can see the results of the calculations for the harmonic polynomials and the rectangles of different shapes. As the number of shape functions applied was $N_s = 6$ (U_n^h for $n = 0, 2, \ldots, 10$), the point $N_c = 3$ (the number of control points on each side of the rectangle) means the direct fit of the boundary conditions and $N_c > 3$ means the least squares solution. In the case of the control point located in the corner, the solution for $N_c = 3$ could not be calculated, as this point was the same for both sides of the rectangle and the solution was singular.

All the calculations showed the evident superiority of the least squares fit over the direct fit of the boundary conditions. In most cases the error decreases rapidly after the application of 1

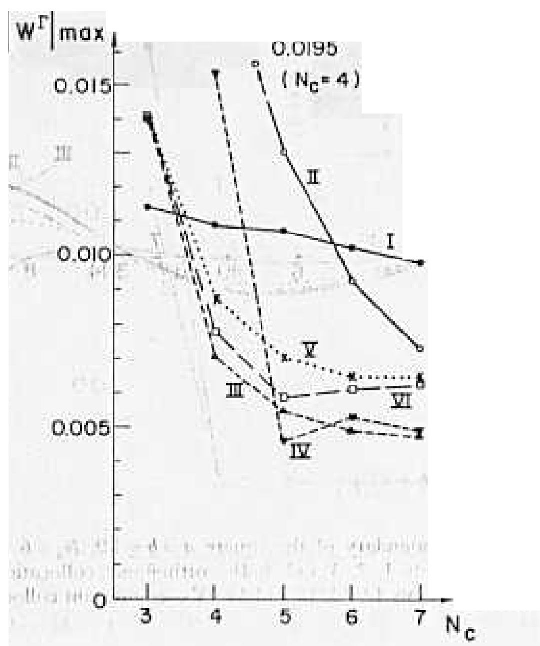

Figure 4. Error $|w^\Gamma|_{max}$ on the boundary Γ_c, $a = 2{\cdot}0$, $b = 0{\cdot}5$, $N_s = 6$; I—V as in Figure 3; VI—orthogonal collocation with the Gaussian weights

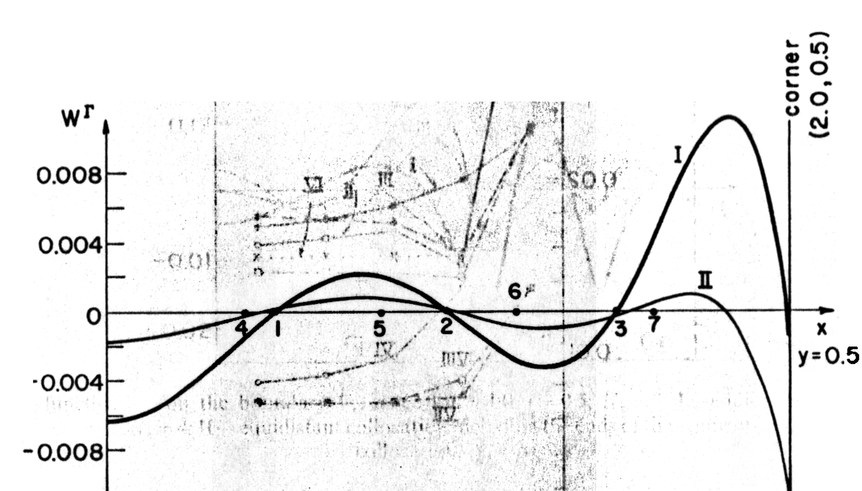

Figure 5. Error function w^Γ on the boundary Γ_c, $a = 2{\cdot}0$, $b = 0{\cdot}5$, $N_s = 6$. The segment $0 \leqslant x \leqslant 2{\cdot}0$; $y = 0{\cdot}5$: I—equidistant collocation at the points 1, 2 and 3; II—equidistant collocation at the points 4, 5, 6 and 7 (least squares)

or 2 additional control points and the error function changes its form considerably (see Figure 5). However, a further increase of the number of the control points does not seem to be profitable, as the results (especially when applying the orthogonal type of collocation) become more stable.

In the case of the square, the corner was the point of the most significant errors. Hence it appeared profitable to place and additional control point at it. This was difficult for the typical integral fit with Gaussian integration. However, when we changed to orthogonal collocation,

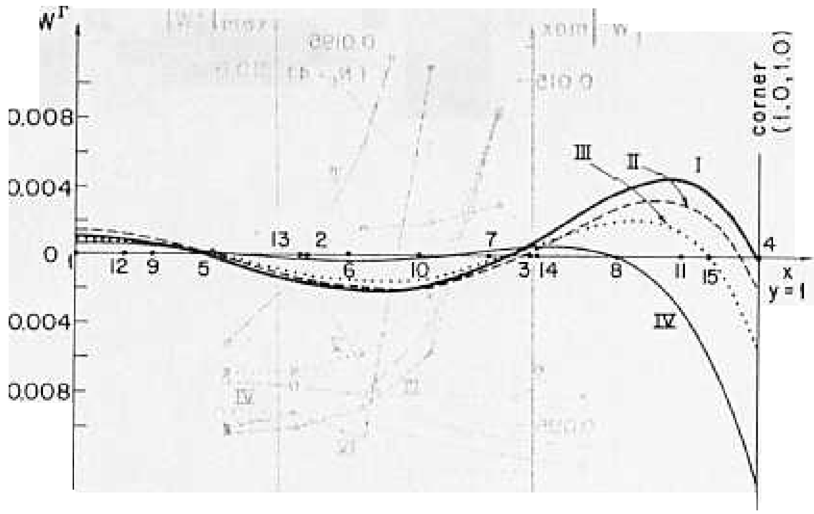

Figure 6. Error function w^{Γ} on the boundary of the square $a=b=1{\cdot}0$; $N_s=6$. The segment $0 \leqslant x \leqslant 1{\cdot}0$; $y=1{\cdot}0$: I—equidistant collocation in the points 1, 2, 3 and 4; II—orthogonal collocation in the points 9, 10, 11 and 4: III—orthogonal collocation in the points 12, 13, 14 and 15; IV—equidistant collocation in the points 5, 6, 7, and 8

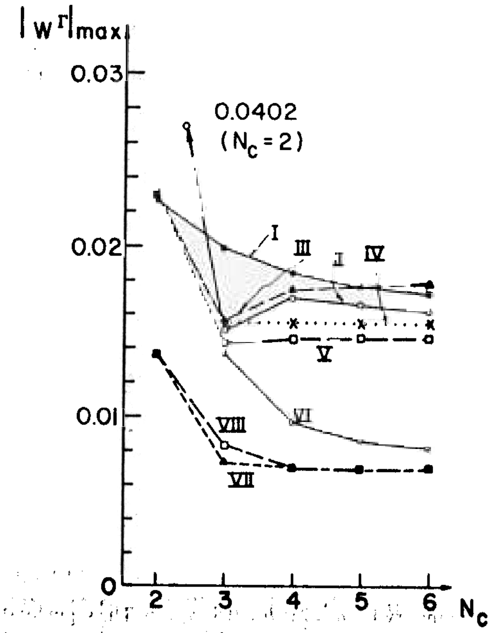

Figure 7. Error $|w^{\Gamma}|_{max}$ on the boundary Γ_r (Figure 2(b)), $a=2{\cdot}0$, $b=1{\cdot}0$, $r=0{\cdot}5$. N_c is the number of the control points on each of the three segments of the boundary: I—equidistant collocation inside the segments; $N_s=4$; II—equidistant collocation including the ends of the segments, $N_s=4$; III—orthogonal collocation, $N_s=4$; IV—integral fit with the Gaussian integration, $N_s=4$; V—orthogonal collocation with the Gaussian weights, $N_s=4$; VI—equidistant collocation including the ends of the segments, $N_s=6$; VII—orthogonal collocation, $N_s=6$; VIII—orthogonal collocation with the Gaussian weights, $N_s=6$

this additional point did not disturb the procedure, and its introduction was very easy. In Figure 6 we can see the influence of the choice of control points on the error function $w(x)$ in this case.

For the smooth contour (Figure 2(b)) we could observe the superiority of the orthogonal collocation with the Gaussian weights, which is clearly visible in Figures 7 and 8. The typical

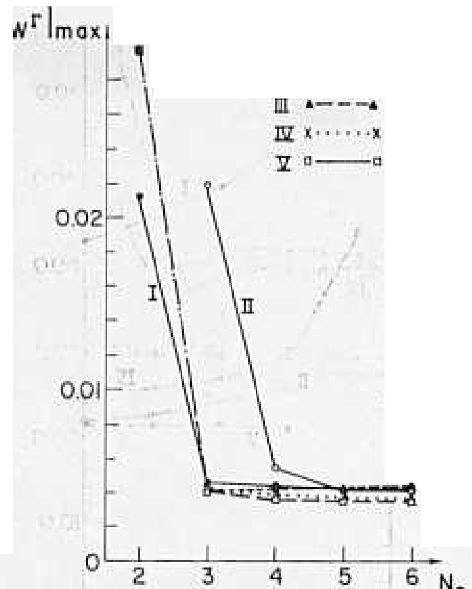

Figure 8. Error $|w^\Gamma|_{max}$ on the boundary Γ_r, $a=2{\cdot}0$, $b=0{\cdot}5$; $r=0{\cdot}25$; $N_s=6$: I—V as in Figure 7 (but for $N_s=6$)

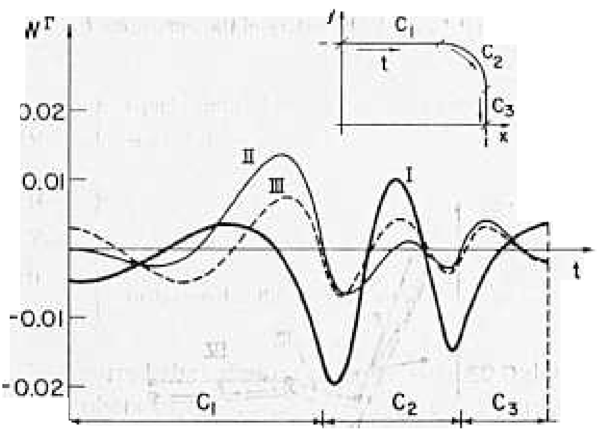

Figure 9. Error function w^Γ on the boundary Γ_r, $a=2{\cdot}0$, $b=1{\cdot}0$, $r=0{\cdot}5$; $N_c=3$: I—equidistant collocation in the points inside the segment, $N_s=4$; II—equidistant collocation including the ends of the segments, $N_s=6$; III—orthogonal collocation, $N_s=6$

distributions of the error functions in this case are presented in Figure 9. The width of the error band on the boundary Γ ($E_b = w^\Gamma_{max} - w^\Gamma_{min}$) behaved, for both shapes of the area Ω, very similarly to E_e, though the differences between the particular procedures were a little smaller. We can see this in Figures 10 and 11, which can be compared to Figures 3 and 7, respectively.

Changing the shape functions to logarithmic type (36) did not introduce basic changes in the behaviour of the solution when applying the different procedures for fitting the boundary conditions. Figures 12 and 13 show the most characteristic results in this case. The rapid decrease of the error after the application of the first additional control point (in comparison to the direct fit) and the stability of the solution with further increase of N_c are evident.

The authors also calculated for all the cases the integral fit with opposite weights, which is often convenient[12] and does not disturb the symmetry of the main matrices. However, the results were similar to those of the least squares integral fit (Figure 14).

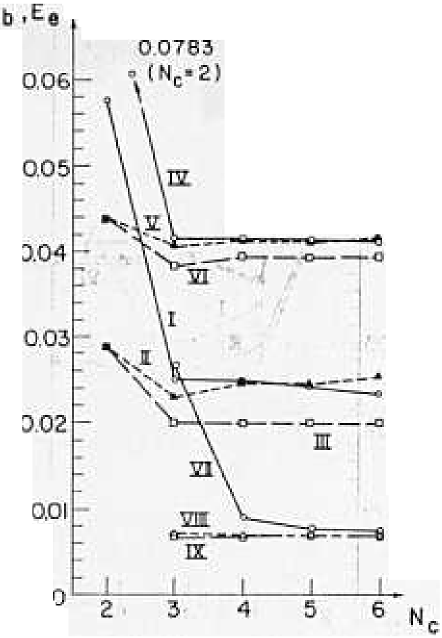

Figure 13. E_e and E_b on the boundary Γ_r, $a = 2{\cdot}0, b = 1{\cdot}0, r = 0{\cdot}5$. Logarithmic shape functions, $r_1 = 3{\cdot}0, r_2 = 2{\cdot}0$: I–VI as in Figure 12; VII—equidistant collocation including the ends of the segments ($N_s = 7$); VIII—orthogonal collocation ($N_s = 7$); IX—orthogonal collocation with the Gaussian weights ($N_s = 7$)

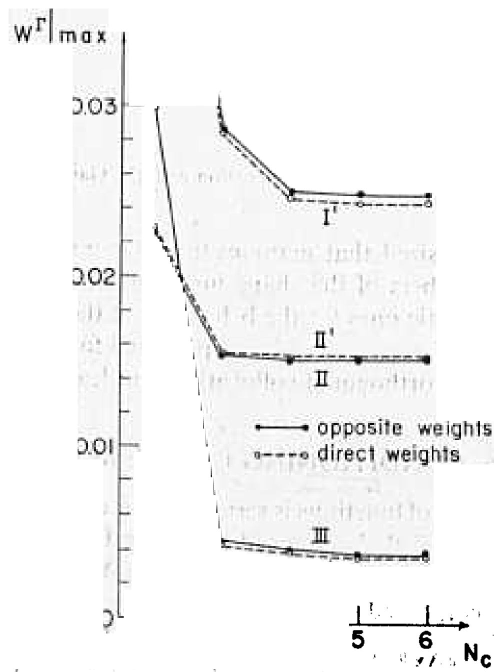

Figure 14. Comparison of the integral fit with the direct and opposite weights. Harmonic polynomials: I—contour Γ_c, $a = 2{\cdot}0$, $b = 1{\cdot}0$, $N_s = 4$; II—contour Γ_r, $a = 2{\cdot}0$, $b = 1{\cdot}0$, $r = 0{\cdot}5$, $N_s = 4$; III—contour Γ_r, $a = 2{\cdot}0$, $b = 0{\cdot}5$, $r = 0{\cdot}25$, $N_s = 6$

where $\Delta \mathbf{A}$ and $\Delta \mathbf{b}$ are the computational errors (e.g. rounding error) of the matrix $\mathbf{A}$ and the vector $\mathbf{b}$, respectively. For a symmetric matrix, we define

$$\|\mathbf{A}\| = \max_{1 \leqslant j \leqslant n} \sum_{i=1}^{n} |a_{ij}| = \max_{1 \leqslant i \leqslant n} \sum_{j=1}^{n} |a_{ij}| \tag{38}$$

and the condition number γ is given by[20,21]

$$\gamma(\mathbf{A}) = \|\mathbf{A}\| \, \|\mathbf{A}^{-1}\| \tag{39}$$

The purpose of our numerical experiments was to determine the influence of the different characteristics involved in γ and $\|\overline{\Delta \mathbf{x}}\|$. For harmonic polynomials such characteristics were the number of shape functions, the number of control points and the shape of the region Ω. An additional characteristic, for singular logarithmic functions, was the distance of the singularities to the boundary Γ. The increase of the number of control points (least squares solutions) caused, as a rule, a certain decrease of the error estimate, but the condition number remained relatively unchanged when the different procedures for fitting the boundary conditions were applied.

Table I shows the results that were obtained for harmonic polynomials. The most conspicuous increase of γ and $\|\overline{\Delta \mathbf{x}}\|$ can be observed with the changes of the contour shape (increase of the ratio a/b) and the number of the shape functions N_s. For the singular logarithmic functions the problem of the conditioning of the matrices is more complicated since the distance of the singularities from the region Ω plays an additional important role. In Figure 15 we can see the results of the calculations for the area Γ_r. It becomes obvious that the optimization of the distances r_1 and r_2 must include not only the error values (as was proposed by Mathon and Johnston[22]) but also the conditioning number γ.

Since increasing the number of shape functions that are used in a given boundary value problem produces an increase in $\|\Delta \mathbf{x}\|$ and γ, in general it is not possible to enlarge the system of shape functions that is used, beyond certain limits. Thus, when such limits are reached all that can be done to improve the solution is to use multi-step fitting (section 7), or to divide the region Ω into elements. However, it must be noticed that using $\|\overline{\Delta \mathbf{x}}\|$ and γ to determine such limits may be too conservative, since $\|\overline{\Delta \mathbf{x}}\|$ is only a bound of the actual error $\|\Delta \mathbf{x}\|$. Table II displays some of the results for the condition number γ, which may be of interest in actual engineering calculations.

We introduced into the matrix $\mathbf{A}$ additional disturbances of the order 10^{-8} situated incidentally inside the matrix [in the example this was introduced by the instruction IF((I + J). EQ. 4. OR. (I + J). EQ. 6) A(I, J) = A(I, J) + 1.E − 8]. The reaction for these disturbances is compared with the estimators of the result error (with the assumed data error of the same order $\delta_a = 10^{-8}$). We can see the considerable difference between this estimation and the real error of the roots. Additionally it is visible that even the great error of the roots can result in relatively small changes of the field functions. All these facts must be taken into account while limiting the solution factors.

Additionally, it should be noted that the order of the final solution error did not increase during the test when changing the places of the matrix disturbances. Hence the test described above can be considered as the image of the real sensitivity of the solution on the matrix errors and the authors suggest it as a helpful tool in the determination of the limiting values of the solution factors a/b, N_s, r_1 and r_2.

7. MULTI-STEP FITTING

An important advantage of the boundary method is the fact that the error of the approximate

Table Conditioning measures of the matrices in the numerical examples (shape functions-harmonic polynomials); the assumed error of the matrix elements, $\delta_a = 10^{-8}$; the accuracy of calculations is 11 digits

Data										
Γ*	a	b	r	N_s	N_c	fit	$\|A\|$	$\|A^{-1}\|$	γ	$\|\Delta x\|$
Γ_c	2	1		4	2†	equidistant collocation	$3{\cdot}140 \times 10^3$	1·426	$4{\cdot}478 \times 10^3$	$3{\cdot}818 \times 10^{-6}$
						orthogonal collocation	$9{\cdot}562 \times 10^3$	0·782	$7{\cdot}480 \times 10^3$	$2{\cdot}661 \times 10^{-6}$
						integral fit	$5{\cdot}838 \times 10^3$	0·777	$4{\cdot}534 \times 10^3$	$2{\cdot}295 \times 10^{-6}$
					6	equidistant collocation	$2{\cdot}122 \times 10^4$	0·338	$7{\cdot}177 \times 10^3$	$1{\cdot}098 \times 10^{-6}$
						orthogonal collocation	$4{\cdot}373 \times 10^4$	0·258	$1{\cdot}127 \times 10^4$	$9{\cdot}288 \times 10^{-7}$
						integral fit	$6{\cdot}850 \times 10^3$	0·902	$6{\cdot}180 \times 10^3$	$2{\cdot}823 \times 10^{-6}$
Γ_c	3	1		4	2†	equidistant collocation	$4{\cdot}803 \times 10^5$	2·072	$9{\cdot}954 \times 10^5$	$1{\cdot}432 \times 10^{-5}$
						orthogonal collocation	$5{\cdot}614 \times 10^5$	0·990	$5{\cdot}558 \times 10^5$	$1{\cdot}024 \times 10^{-5}$
					6	equidistant collocation	$1{\cdot}584 \times 10^6$	0·465	$7{\cdot}384 \times 10^5$	$4{\cdot}034 \times 10^{-6}$
						orthogonal collocation	$1{\cdot}838 \times 10^6$	0·337	$6{\cdot}194 \times 10^5$	$4{\cdot}484 \times 10^{-6}$
Γ_c	3	1		6	3†	equidistant collocation	$5{\cdot}965 \times 10^9$	2·975	$1{\cdot}775 \times 10^{10}$	$9{\cdot}510 \times 10^{-3}$
						orthogonal collocation	$1{\cdot}262 \times 10^{10}$	0·719	$9{\cdot}075 \times 10^9$	$2{\cdot}359 \times 10^{-3}$
					6	equidistant collocation	$1{\cdot}600 \times 10^{10}$	0·673	$1{\cdot}076 \times 10^{10}$	$2{\cdot}267 \times 10^{-3}$
						orthogonal collocation	$3{\cdot}082 \times 10^{10}$	0·392	$1{\cdot}014 \times 10^{10}$	$1{\cdot}037 \times 10^{-3}$
Γ_r	2	1	0·5	4	4	equidistant collocation	$2{\cdot}049 \times 10^4$	0·326	$6{\cdot}681 \times 10^3$	$1{\cdot}767 \times 10^{-6}$
						orthogonal collocation	$2{\cdot}030 \times 10^4$	0·329	$6{\cdot}671 \times 10^3$	$1{\cdot}798 \times 10^{-6}$
				6		equidistant collocation	$6{\cdot}828 \times 10^6$	0·317	$2{\cdot}166 \times 10^6$	$5{\cdot}376 \times 10^{-5}$
						orthogonal collocation	$7{\cdot}129 \times 10^6$	0·315	$2{\cdot}248 \times 10^6$	$5{\cdot}024 \times 10^{-5}$
Γ_r	2	0·5	0·25	6	4	equidistant collocation	$4{\cdot}468 \times 10^6$	10·10	$4{\cdot}514 \times 10^7$	$3{\cdot}120 \times 10^{-4}$
						orthogonal collocation	$4{\cdot}351 \times 10^6$	9·095	$3{\cdot}963 \times 10^7$	$2{\cdot}693 \times 10^{-4}$

* See Figure 2

† For the unification of the programs the formula (15) was applied also in the case of the direct fit

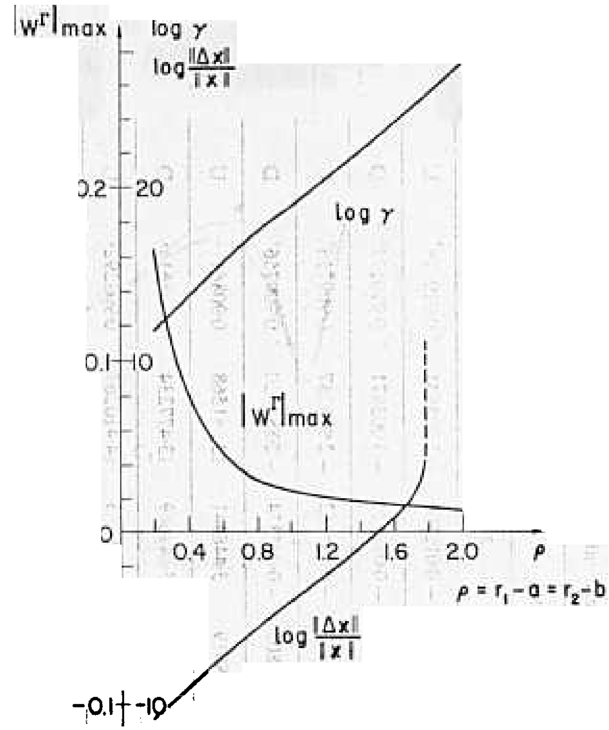

Figure 15. Influence of the distance of the singularities on the results of the example. Logarithmic functions: area Γ_r—$a = 2{\cdot}0$, $b = 1{\cdot}0$, $r = 0{\cdot}5$, $N_s = 4$, $N_c = 4$ on each segment; orthogonal collocation

solution is introduced only through the boundary. For elliptic equations the maximum error occurs just on the boundary.[19] Also, in previous discussions this has been related to the error in the interior of the region Ω.

In solutions with T-complete systems of functions, the boundary error is directly observed as the difference between the prescribed and calculated boundary functions. Observe that the same is not possible when using boundary integral equations. This allows using multi-step fitting of boundary conditions, i.e. applying procedures for successive correction of boundary errors.

Secondary collocation at the points of extreme boundary error in the first-step solution is one of the obvious methods for fit improvement. In Figure 16 we can see the result of the application of three additional control points with weights proportional to the values of the error in the first-step solution. Repeating this procedure we could obtain the optimal fit for a given number of shape functions. This can be especially important when increasing the number of the shape functions is difficult because of conditioning reasons (see section 6).

Treating the boundary error w_1^Γ from the first-step solution (which is known exactly) as a new boundary condition is another possibility for improving the result. Since the exact solution is

$$u(x) = \hat{u}(x) - w_1(x) \tag{40}$$

it is required to find an accurate approximation of $w_1(x)$. The function $\hat{w}_1(x)$ should however, be, calculated in a different way to the first-step solution. For example, one can use different T-complete systems of functions or a different division of Γ into segments. In Figure 17 we can

Table 11. Influence of the disturbances of order 10[illegible] introduced into the matrix **A**. Logarithmic shape functions, $N_s = 4$, contour 1 ($a = 2{\cdot}0$, $b = 1{\cdot}0$, $r = 0{\cdot}5$), $N_c = 4$ in each segment

Fit	r_1, r_2 (Figure 2)	$\Vert\mathbf{A}\Vert$ (for undisturbed data)	$\Vert\mathbf{A}^{-1}\Vert$ (for undisturbed data)	γ (for undisturbed data)	$\Vert\overline{\Delta\mathbf{x}}\Vert$ (for undisturbed data)	Roots of the equation $\mathbf{Ax} = \mathbf{b}$: 1	2	3	4	$u(0,0)$	
equidistant collocation	$r_1 = 3{\cdot}0$	$2{\cdot}702 \times 10^{3}$	$5{\cdot}828 \times 10^{4}$	$1{\cdot}575 \times 10^{8}$	0·5900	32·601693	−0·174134	−0·013509	−3·005841	0·910178†	U
	$r_2 = 2{\cdot}0$					32·602116	−0·174145	−0·013521	−3·005871	0·910178†	D
orthogonal collocation	$r_1 = 3{\cdot}0$	$2{\cdot}702 \times 10^{3}$	$5{\cdot}633 \times 10^{4}$	$1{\cdot}530 \times 10^{8}$	0·5690	32·285155	−0·166791	−0·005362	−2·983287	0·909756†	U
	$r_2 = 2{\cdot}0$					32·285621	−0·166803	−0·005374	−2·883320	0·909756†	D
equidistant collocation	$r_1 = 4{\cdot}0$	$4{\cdot}439 \times 10^{3}$	$1{\cdot}673 \times 10^{8}$	$7{\cdot}425 \times 10^{11}$	$2{\cdot}790 \times 10^{3}$*	−247·5385	6·308819	5·448441	12·681568	0·908618‡	U
	$r_2 = 3{\cdot}0$					−260·7607	6·523186	5·642669	13·477234	0·908614‡	D
orthogonal collocation	$r_1 = 4{\cdot}0$	$4{\cdot}439 \times 10^{3}$	$1{\cdot}669 \times 10^{8}$	$7{\cdot}409 \times 10^{11}$	$3{\cdot}121 \times 10^{3}$*	−276·2433	6·772079	5·869465	14·410267	0·908292‡	U
	$r_2 = 3{\cdot}0$					−288·8782	6·976907	6·055041	15·170618	0·908309‡	D

U—undisturbed results; D—disturbed results

* Formal application of the formula (37), invalid for these values of γ (see Figure 15)

† Extreme difference between disturbed and undisturbed $\hat{u}$ was of the order 10^{-6}

‡ Extreme difference between disturbed and undisturbed $\hat{u}$ was of the order 10^{-4}

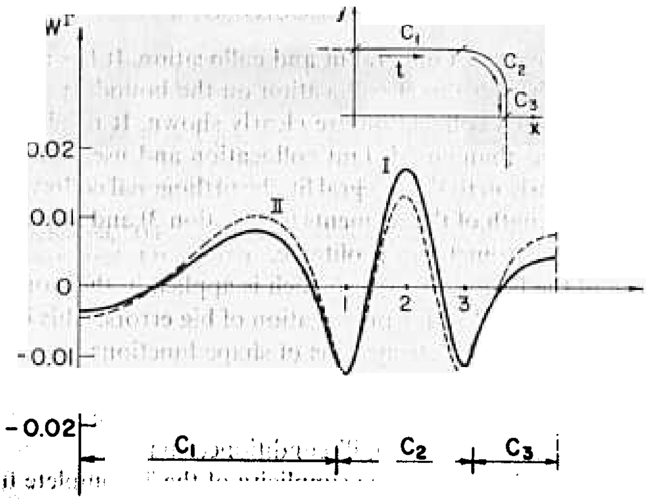

Figure 16. Two-step fitting of the boundary conditions on Γ_r, harmonic polynomials; orthogonal collocation, $N_s = 4$, $N_c = 4$, $a = 2{\cdot}0$, $b = 1{\cdot}0$, $r = 0{\cdot}5$: I—first-step solution; II—improved solution with the three additional control points

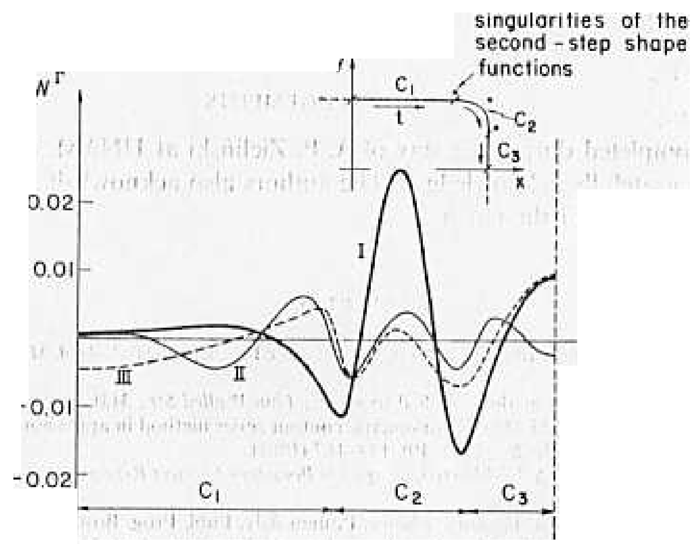

Figure 17. Improvement of fitting the boundary conditions on Γ_r. Logarithmic shape functions. Orthogonal collocation; $a = 2{\cdot}0$, $b = 1{\cdot}0$, $r = 0{\cdot}5$, $r_1 = 3{\cdot}0$, $r_2 = 2{\cdot}0$: I—one-step solution, $N_s = 4$, $N_c = 4$, $\gamma = 1{\cdot}53 \times 10^8$; II—one-step solution, $N_s = 7$, $N_c = 4$; $\gamma = 4{\cdot}70 \times 10^{11}$; III—two-step solution, $N_{s1} = 4$, $N_{c1} = 4$, $N_{s2} = 3$, $N_{c2} = 6$, $\gamma_1 = 1{\cdot}53 \times 10^8$, $\gamma_2 = 4{\cdot}89 \times 10^2$

see the two-step procedure when applying the singular logarithmic shape functions. The diminishing of the error can also be done in the one-step solution with the greater number of shape functions (curve II) but in this case the condition number of the solution matrix would increase.

The multi-step fitting can also be useful in typical engineering calculation which can be considerably improved by application of additional control points in the regions where the greatest values of the investigated field functions occur.

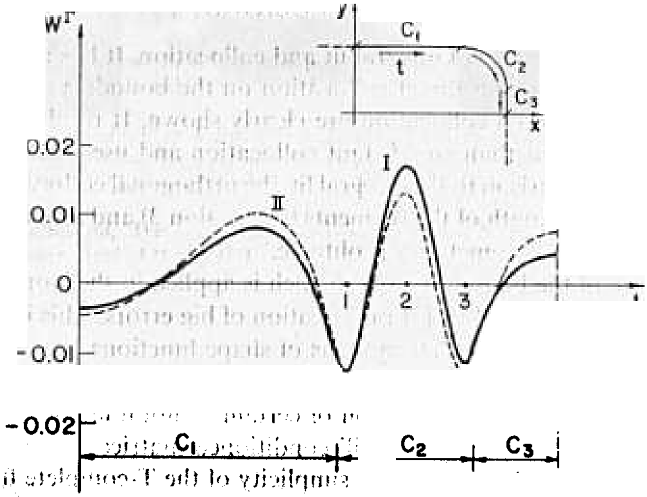

Figure 16. Two-step fitting of the boundary conditions on Γ_r, harmonic polynomials; orthogonal collocation, $N_s = 4$, $N_c = 4$, $a = 2{\cdot}0$, $b = 1{\cdot}0$, $r = 0{\cdot}5$: I—first-step solution; II—improved solution with the three additional control points

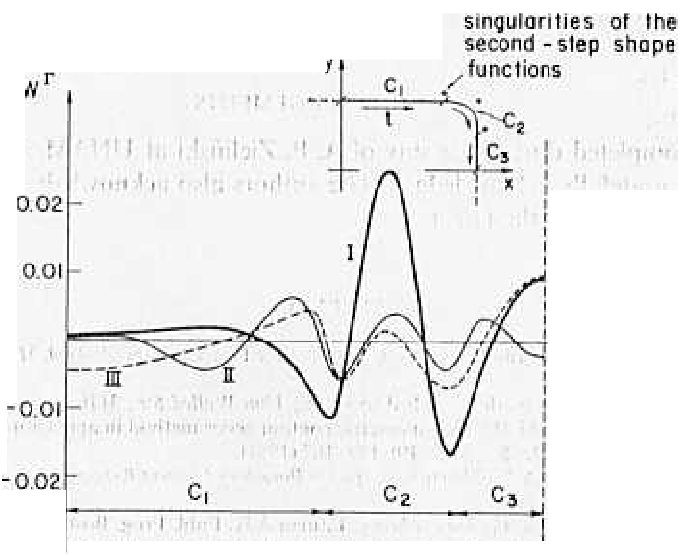

Figure 17. Improvement of fitting the boundary conditions on Γ_r. Logarithmic shape functions. Orthogonal collocation; $a = 2{\cdot}0$, $b = 1{\cdot}0$, $r = 0{\cdot}5$, $r_1 = 3{\cdot}0$, $r_2 = 2{\cdot}0$: I—one-step solution, $N_s = 4$, $N_c = 4$, $\gamma = 1{\cdot}53 \times 10^8$; II—one-step solution, $N_s = 7$, $N_c = 4$; $\gamma = 4{\cdot}70 \times 10^{11}$; III—two-step solution, $N_{s1} = 4$, $N_{c1} = 4$, $N_{s2} = 3$, $N_{c2} = 6$, $\gamma_1 = 1{\cdot}53 \times 10^8$, $\gamma_2 = 4{\cdot}89 \times 10^2$

see the two-step procedure when applying the singular logarithmic shape functions. The diminishing of the error can also be done in the one-step solution with the greater number of shape functions (curve II) but in this case the condition number of the solution matrix would increase.

The multi-step fitting can also be useful in typical engineering calculation which can be considerably improved by application of additional control points in the regions where the greatest values of the investigated field functions occur.

8. CONCLUSIONS

This paper has proved the identity of integral fit and collocation. It has also showed the distinct superiority of least squares fit over direct collocation on the boundary.

The advantages of orthogonal collocation are clearly shown. It results, as a rule, in a better fit of the boundary conditions than equidistant collocation and uses the unique control points inside the segments. In comparison to the integral fit, the orthogonal collocation has no additional weights connected with the length of the segments (see section 3) and also allows for easy adding of the control points, which is sometimes profitable.

The Collatz measure of the boundary error (which is applied in the work) seems to be a good estimate of the fit, as it does not allow for propagation of big errors. This is especially important when forming elements with T-complete systems of shape functions.[12]

The conditioning of the solution matrices has been investigated in detail. The paper points out the danger of the unconscious application of certain solution factors beyond the accessible limits and supplies some guide for avoiding ill-conditioned matrices.

On the positive side the reader can see the simplicity of the T-complete function method, the easy estimation of the solution error and the possibility of reducing it by multi-step fitting the boundary conditions. The main solution gives here directly the coefficients of the shape functions, which allows avoidance of the 'postprocessing' which is a characteristic disadvantage of other boundary methods. However, the conditioning of the solution matrices remains as the main limitation of the method discussed.

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