BOUNDARY CONDITIONS IN THE FINITE-DIFFERENCE METHOD

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RESUMO

Apresenta-se o procedimento usual para tratar as condições de contorno, ao usar o método das diferenças finitas. Tal procedimento resulta em erros que podem ser muito grandes, e não assegura a convergência para os valores exatos quando o intervalo tende a zero.

Desenvolve-se em seguida um procedimento sem tais inconvenientes, baseado na série de Taylor. Mostra-se como aplicá-lo a condições de contorno lineares e não-lineares.

ABSTRACT

The usual procedure to treat boundary conditions, when the finite-difference method is used, is shown here. Such procedure results in errors that may be very large and does not assure convergence to the exact value when the interval tends to zero.

A procedure without such inconveniences is then developed, based on Taylor series. It is shown how to apply it to linear and non-linear boundary conditions.

INTRODUCTION

The finite-difference method is widely used to get numerical solutions of differential equations. In this method the derivatives are substituted by central differences. The differential equation is substituted by a system of algebraic equations giving the values of the unknown function at pivotal points.

When the central difference is applied at a point of the boundary or near the boundary, a difficulty arises; it is necessary to use points outside the domain; it is admitted therefore that the differential equation remains valid outside the domain. Boundary conditions are used to get relations among points outside and inside the domain.

The external points can be eliminated from the equations using those relations.

In this paper it is made a critical analysis of this procedure, and another one is proposed to treat boundary conditions.

The dissimilarities between the procedures are shown in problems with one dimension, with linear and non-linear boundary conditions.

THE USUAL PROCEDURE

Consider that point 1 is an extremity of a beam, Fig. 1. Points $\underline{a}$ and $\underline{b}$ are outside the domain and points 2, 3, 4 are inside the beam. The usual approximations for derivatives at point 1 give the following results, where $\underline{u}$ is the vertical displacement:

$$u_a = u_2 - 2h\, u_1' \tag{1}$$

$$u_a = 2\, u_1 - u_2 + h^2\, u_1'' \tag{2}$$

$$u_b = 2\, u_a - 2u_2 + u_3 - 2h^3\, u_1''' \tag{3}$$

If point 1 is a fixed end, the following result will represent the fourth derivative at point 2 in finite differences, incorporating boundary conditions at 1:

$$h^4 u_2'''' = 7\ u_2 - 4\ u_3 + u_4 = \frac{h^4\ q}{EJ} \tag{4}$$

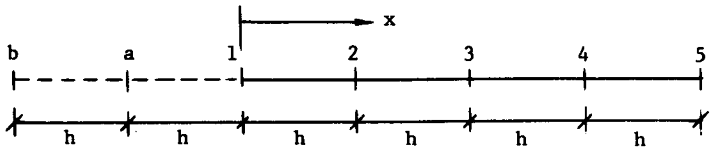


Fig. 1

In this equation q is the load acting on the beam and EJ is the bending rigidity.

If point 1 is simply-supported, the fourth derivative at point 2 is:

$$h^4\ u_2'''' = 5\ u_2 - 4\ u_3 + u_4 = \frac{q\ h^4}{EJ} \tag{5}$$

Consider now that point 1 is a free end. Then the fourth derivative at points 1 and 2 are:

$$h^4\ u_1'''' = u_1 - 2\ u_2 + u_3 = \frac{q\ h^4}{EJ} \tag{6}$$

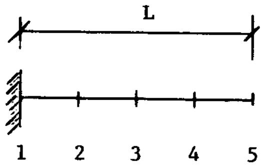
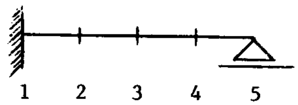
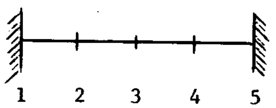
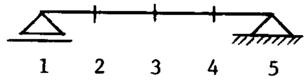
$$h^4\ u_2'''' = -\ 2u_1 + 5\ u_2 - 4\ u_3 + u_4 = \frac{q\ h^4}{EJ} \tag{7}$$

With these equations it is easy to find the displacements of a beam of constant EJ subjected to a uniformly distributed load. As the solution is given by a fourth degree polynomial, five points are needed to get the answer without errors.

In Table 1 are the results obtained with finite-differences and using the fourth degree polynomial. As it can be seen the results are not exact, as they should be. The use of a small number of points cannot be claimed as responsible for the inaccuracies. As the fourth derivative of the polynomial is obtained without error, then the only explanation for this fact is the poor treatment given to boundary conditions.

TABLE 1 - Values of α for uniformly distributed load

$$u = \alpha \frac{q L^4}{EJ}$$

		Finite-difference	Exact	Error %
	u_2	5/256	27/8 x 256	48
	u_3	16/256	17/8 x 48	41
	u_4	30/256	171/8 x 256	40
	u_5	45/256	32/256	41
	u_2	20/5632	15/6144	45
	u_3	37/5632	32/6144	26
	u_4	30/5632	27/6144	21
	u_2	5/2048	3/2048	67
	u_3	1/256	1/384	50
	u_4	5/2048	3/2048	67
	u_2	5/512	19/2048	5,2
	u_3	7/512	5/384	5
	u_4	5/512	19/2048	5,2

A CRITICAL ANALYSIS OF THE USUAL PROCEDURE

The first objection to the usual procedure is that external points cannot give any help in order to obtain discrete values inside the domain. Indeed, if a problem has a correct formulation, the differential equation and boundary conditions permit the determination of the unknown function. It is not necessary to extend the domain artificially.

Therefore in the numerical solution this is not necessary.

This restriction can be considered at a first view only a formal one. However it is really important. The use of external points gives a wrong idea of how the boundary conditions should be treated. Furthermore it introduces errors if an analysis taking into account the first term neglected is not made. As a matter of fact the approximations involved have different errors and the resulting expression can come with a precision smaller than what it should be.

As it can be seem from Table 1, the value of the error is highly dependent on the boundary conditions. The fixed-fixed beam presents an error greater than 50%. The simply-supported beam has an error of 5%. The beam with one end fixed and the other simply supported has an interesting behavior: near the fixed end the error is twice the error near the other end.

These facts show clearly that the approximations used are not reliable.

To understand how the error was introduced, consider eq. (1) with the first term in the error series:

$$u_1' = \frac{u_2 - u_a}{2h} - \frac{h^2}{6} u_1''' + \dots \qquad (8)$$

As the first derivative is zero, the point outside the domain is found by

$$u_a = u_2 - \frac{1}{3} h^3 u_1''' + \dots \qquad (9)$$

If this value is substituted in the usual approximation for the fourth derivative

$$u_2'''' = \frac{1}{h^4} (u_a - 4 u_1 + 6 u_2 - 4 u_3 + u_4) = (\frac{q}{EJ})_2 \qquad (10)$$

one gets considering $u_1 = 0$:

$$u_2'''' = \frac{1}{h^4}(7 u_2 - 4 u_3 + u_4) - \frac{1}{3h} u_1''' + \dots = (\frac{q}{EJ})_2 \qquad (11)$$

This is eq. (4) with an additional term. When h tends to zero, the expression in parenthesis tends to the fourth derivative. The second term, however with h in the denominator grows without limit. Due to this, the answer will not converge to the exact one. The error terms that were omitted have h in the numerator, therefore they go to zero with h.

THE PROPOSED PROCEDURE

Instead of using points outside the domain as shown, an unsafe procedure, the formulation of the problem must be changed. In a beam with a fixed support for example it is, Fig. 1: determine the best approximation for the fourth derivative at point 2 in terms of u_1, u_2, u_3, u_4 and the first derivative at point 1.

Expanding in Taylor series u_1, u_2, u_3, u_4, u_1' about x_2, it is possible to write:

$$\begin{Bmatrix} u_1 \\ u_2 \\ u_3 \\ u_4 \\ u_1' \end{Bmatrix} = \begin{bmatrix} 1 & -h & h^2/2 & -h^3/6 & h^4/24 \\ 1 & 0 & 0 & 0 & 0 \\ 1 & h & h^2/2 & h^3/6 & h^4/24 \\ 1 & 2h & 4h^2/2 & 8h^3/6 & 16h^4/24 \\ 0 & 1 & -h & h^2/2 & -h^3/6 \end{bmatrix} \cdot \begin{Bmatrix} u_2 \\ u_2' \\ u_2'' \\ u_2''' \\ u_2'''' \end{Bmatrix} \tag{12}$$

Multiply the first equation by A, the second by B, the third and fourth by C and D and the last by hE; now add all these equations.

$$\begin{aligned} Au_1 + Bu_2 + Cu_3 + Du_4 + E\,h\,u_1' &= (A + B + C + D)\,u_2 + \\ &+ h\,u_2'\,(-A + C + 2D + E) + \frac{h^2}{2}\,u_2''\,(A + C + 4D - 2E) + \\ &+ \frac{h^3}{6}\,u_2'''\,(-A + C + 8D + 3E) + \frac{h^4}{24}\,u_2''''\,(A + C + 16D - 4E) + \\ &+ \dots \end{aligned} \tag{13}$$

If the left hand side of this equation must be the best approximation of u_2'''', then the coefficients of u_2, u_2', u_2''' must be zero and the coefficient of u_2'''' must be one. Therefore:

$$\begin{bmatrix} 1 & 1 & 1 & 1 & 0 \\ -1 & 0 & 1 & 2 & 1 \\ 1 & 0 & 1 & 4 & -2 \\ -1 & 0 & 1 & 8 & 3 \\ 1 & 0 & 1 & 16 & -4 \end{bmatrix} \begin{Bmatrix} A \\ B \\ C \\ D \\ E \end{Bmatrix} = \frac{24}{h^4} \begin{Bmatrix} 0 \\ 0 \\ 0 \\ 0 \\ 1 \end{Bmatrix} \tag{14}$$

Solving the system:

$$A = \frac{-22}{3h^4} \quad B = \frac{12}{h^4} \quad C = -\frac{6}{h^4} \quad D = \frac{4}{3h^4} \quad E = -\frac{4}{h^4} \tag{15}$$

The best approximation for the fourth derivative then is:

$$u_2'''' = \frac{1}{h^4}\left[-4h\,u_1' - \frac{22}{3}u_1 + 12\,u_2 - 6\,u_3 + \frac{4}{3}u_4\right] \tag{16}$$

In the particular case of a fixed end $u_1 = u_1' = 0$ and the fourth derivative incorporating these conditions is

$$u_2'''' = \frac{1}{h^4}\left(12\,u_2 - 6\,u_3 + \frac{4}{3}u_4\right) \tag{17}$$

With the same procedure, for the simply-supported beam, the result is:

$$u_2'''' = \frac{1}{11h^4}\left(-24u_1 + 12h^2\,u_1'' + 60u_2 - 48u_3 + 12u_4\right) \tag{18}$$

But as $u_1 = u_1'' = 0$, eq. (18) simplifies:

$$u_2'''' = \frac{1}{11h^4}\left(60\,u_2 - 48\,u_3 + 12\,u_4\right) \tag{19}$$

For a free end $u_1'' = u_1''' = 0$ and one gets:

$$u_1'''' = \frac{1}{7h^4} (12\ u_1 - 24\ u_2 + 12\ u_3) \tag{20}$$

The fourth derivative at point 2 comes from eq. (18) with $u_1'' = 0$:

$$u_2'''' = \frac{1}{11h^4} (-24\ u_1 + 60\ u_2 - 48\ u_3 + 12\ u_4) \tag{21}$$

Comparing these equations with those found previously, eqs. (4) to (7) it is easy to verify that only for a simply-supported end they are nearly equal; for a fixed end or a free end they differ too much. Those conclusions agree with the values shown in Table 1.

If eqs. (17) to (21) are used, it is easy to verify that the displacements got are exact. With a proper treatment of boundary conditions and not by the use of a more refined formulas, the error disappears.

It is quite common to see researchers complaining of the poor results they get with a small number of points, Ref. [1]. But those bad results are due to a poor boundary treatment. They improve with an increase in nodal points; really in the fixed beam shown, with three nodal points, two equations depend on the condition $u_1' = 0$. Using 100 nodal points two equations again will depend on that condition. The results improve but they will never approach the exact ones.

The procedure proposed is general and reliable; it can be used in ordinary and partial differential equations, with any type of conditions.

It requires the solution of a system of algebraic equations though.

It is possible, however, to avoid this work. In eq. (9) the exponent of $\underline{h}$ is the order of the derivative added to the order of the error; this exponent is $\underline{p}$. The order of the differential equation is $\underline{n}$. If $p > n + 1$, the first term of the error series is of the form h^m ( ), where $\underline{m}$ is a positive number, in eq. (11). If $p < n + 1$, $\underline{m}$ will be non positive and convergence fails.

This means that to solve a fourth order differential equation with a condition on the first derivative, it is needed a formula with an error of h^4. In Ref. [2] it is found the following approximation

$$u_1' = \frac{1}{12h}\,(-3u_a - 10u_1 + 18u_2 - 6u_3 + u_4) - \frac{1}{20}\,h^4\,u_1''''' \qquad (22)$$

Then the for the fixed end of the beam

$$u_a = \frac{-\,10u_1 + 18u_2 - 6u_3 + u_4}{3} - \frac{h^5}{5}\,u_1''''' \qquad (23)$$

Substituting this value in eq. (10), eq. (17) is obtained.

Non-linear conditions can be operated by the general procedure. Consider the problem of free convection from a heated vertical plate. In Ref. [3] it is shown a system of two equations with two unknowns, $f(x)$ and $g(x)$ with adequate conditions. Eliminating the function $g(x)$, the governing equation of the problem is

$$-f''''' + (f'')^2 - 2f'f''' - 3(1+\sigma)f\,f'''' + 3\sigma\,(f\,f'f'' - 3f^2f''' = $$

$$= 0 \qquad (24)$$

and the conditions are:

$$x = 0 \qquad f = 0 \qquad f' = 0 \qquad f''' = -1 \qquad (25)$$

$$x = \infty \qquad f' = 0 \qquad f''' + 3\,f\,f'' = 0 \qquad (26)$$

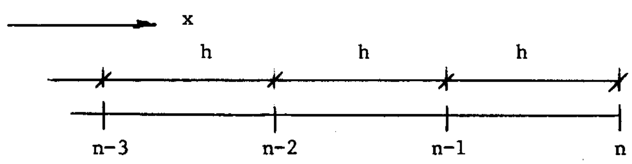


Fig. 2

In eq. (24) σ is the Prandtl number.

The terminal point is n. Taylor series expansions are:

$$\begin{bmatrix} 1 & 0 & 0 & 0 & 0 & 0 \\ 1 & -h & h^2/2 & -h^3/6 & h^4/24 & -h^5/120 \\ 1 & -2h & 4h^2/2 & -8h^3/6 & 16h^4/24 & -32h^5/120 \\ 1 & -3h & 9h^2/2 & -27h^3/6 & 81h^4/24 & -243h^5/120 \end{bmatrix} \begin{Bmatrix} f_n \\ f'_n \\ f''_n \\ f'''_n \\ f''''_n \\ f'''''_n \end{Bmatrix} = \begin{Bmatrix} f_n \\ f_{n-1} \\ f_{n-2} \\ f_{n-3} \end{Bmatrix} \qquad (27)$$

Multiply the first equation by A, and others by B, C and D, and add. Then,

$$A\, f_n + Bf_{n-1} + Cf_{n-2} + Df_{n-3} = (A+B+C+D)f_n - h\, f'_n\, (B + 2C + 3D)$$

$$+ \frac{h^2}{2}\, f''_n\, (B + 4C + 9D) - \frac{h^3}{6}\, f'''_n\, (B + 8C + 27D) +$$

$$+ \frac{h^4}{24}\, f''''_n\, (B + 16C + 81D) - \frac{h^5}{120}\, f'''''_n\, (B + 32C + 243D) + \ldots \qquad (28)$$

Next include boundary conditions in eq. (28). The third derivative is substituted by $-\ 3f_n\, f''_n$.

$$A\, f_n + Bf_{n-1} + Cf_{n-2} + Df_{n-3} = (A + B + C + D)f_n +$$

$$+ \frac{h^2}{2}\, f''_n \left[B + 4C + 9D + h\, f_n\, (B + 8C + 27D)\right] + \frac{h^4}{24}\, f''''_n\, (B + 16C + 81D)$$

$$- \frac{h^5}{120}\, f'''''_n\, (B + 32C + 243D) \qquad (29)$$

The equations to get the unknowns for the fifth derivative of f at n are, with $\alpha = h\, f_n$:

$$\begin{bmatrix} 1 & 1 & 1 & 1 \\ 0 & 1+\alpha & 4(1+2\alpha) & 9(1+3\alpha) \\ 0 & 1 & 16 & 81 \\ 0 & -1 & -32 & -243 \end{bmatrix} \begin{Bmatrix} A \\ B \\ C \\ D \end{Bmatrix} = \frac{120}{h^5} \begin{Bmatrix} 0 \\ 0 \\ 0 \\ 1 \end{Bmatrix} \qquad (30)$$

Solving the system, the above equation is get

$$f_n'''''=\frac{1}{h^5(11+6\alpha)}\left[\frac{(600+850\alpha)}{3}f_n-60\ (5+6\alpha)f_{n-1}+\right.$$

$$\left.+\ 30\ (4+3\alpha)\ f_{n-2}-\frac{20}{3}(3+2\alpha)\ f_{n-3}\right] \qquad (31)$$

CONCLUSIONS

The usual procedure to consider external points for the finite difference method recommended by several authors, Refs. [4], [5], [6], must be avoided. In some cases the error is small, but it is possible to have large errors. It is important to realize that when the interval goes to zero there is no guarantee that the error will go to zero.

The only way to be sure to get the best approximation with the desired number of terms is the use of Taylor series or equivalent algorithm, as exposed above.

REFERENCES

[1] Szilard, R., "Theory and Analysis of Plates", Prentice Hall, 1974.

[2] Southwell, "Relaxation Methods in Theoretical Physics", Oxford Clarendon, 1952.

[3] Yih, C.S., "Fluid Mechanics", McGraw-Hill, 1969.

[4] Crandall, S., "Engineering Analysis", McGraw-Hill, 1956.

[5] Wang, P.C., "Numerical and Matrix Methods in Structural Mechanics", John Wiley, 1966.

[6] Collatz, L., "The Numerical Treatment of Differential Equations", Springer-Verlag, 1966.