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UNIFIED APPROACH TO DISCRETE METHODS.

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ABSTRACT

Applying the method of weighted residuals and then interpreting the resulting equations by means of Green's formulas for discontinuous functions a direct method of analysis is constructed. The manner in which finite elements, boundary methods and finite differences can be incorporated in this scheme is explained. This brief article constitutes a summary of the theory which soon will appear in full.

INTRODUCTION

Three of the most powerful techniques for the numerical treatment of partial differential equations are finite elements, finite differences and boundary element methods. The foundations of each one of these methodologies, as originally formulated, appeared to be unrelated.

More recently, however, it has been recognized that it is desirable, and it has been suspected possible, to develop foundations common for all of them. Indeed, for some specific cases developments of the sort have been done. Zienkiewicz, for example [1983; Zienkiewicz, et. al., 1977, 1979; Zielinski and Zienkiewicz, 1984] has given examples of procedures which permit coupling finite elements with boundary methods. Brebbia [1983] on the other hand, stresses the unifying power of the principle of virtual work.

Regarding finite differences, although it is well known that some specific algorithms, such as central differences, can be derived applying the finite element formulation, the general theory is based on Taylor series developments [Lapidus and Pinder, 1982].

Here a summary of a unifying theory recently developed by the author is presented [Herrera, 1984a]. The approach is quite general, since it is applicable to any linear operator. The procedure consists in applying the method of weighted residuals [Finlayson, 1972] and then interpreting the resulting equations by means of general Green's formulas for discontinuous functions, which have just been obtained by the author [Herrera, 1984a] for general non-symmetric operators. They constitute generalizations of previous result which have already been published in book form [Herrera, 1984b].

The use of Green's formulas permits formulating variational principles for arbitrary non-symmetric operators, thus allowing a very systematic formulation of the numerical approach. Even more, by their use the constraint imposed by the weighted residuals on the differential operator is transformed into a restriction which is imposed explicitly on the possible solutions, deriving in this manner the information which is sought about the actual solution.

Explicit knowledge of the information that is being derived by each one of the weighting functions is quite valuable, not only as a powerful tool of analysis which can be used to evaluate the error, but also as a guide which yields insight and orientation to develop more efficient approximate methods.

The unified formulation is presented in Section 3 and then it is specialized for finite elements, boundary methods and finite differences in Sections 4, 5 and 6, respectively. The finite difference schemes presented in Section 6, yield exact values of the solution at the nodes. Such kind of results were first obtained by Rose [1964, 1975] for Sturm-Liouville operators.

BOUNDARY VALUE PROBLEMS

Let $P:D\to D^*$ and $B:D\to D^*$ be functional valued operators [Herrera, 1980, 1984b] such that B is a boundary operator for P. Generally, boundary value problems can be formulated as follows. Given functionals $f \in D^*$ and $g \in D^*$, such that f is in the range of P, while g is in the range of B, the boundary value problem consists in finding $u \in D$ such that

$$Pu = f \quad \text{while} \quad Bu = g \tag{1}$$

The theory shows that equations (1) hold, if and only if [Herrera, 1980]

$$(P-B)u = f - g \tag{2}$$

Typical example is Dirichlet problem, which can be obtained by letting

$$\langle Pu,v\rangle = \int_{\Omega} v\Delta u dx \quad ; \langle Bu,v\rangle = -\int_{\partial\Omega} u\frac{\partial v}{\partial n}dx \qquad (3a)$$

and

$$\langle f,v\rangle = \int_{\Omega} vf_{\Omega}dx \quad \text{and} \quad \langle g,v\rangle = -\int_{\partial\Omega} g_{\partial}\frac{\partial v}{\partial n}dx \qquad (3b)$$

where Ω is a region, $\partial\Omega$ its boundary, f_{Ω} is defined in Ω while g_{∂} are the prescribed boundary values on $\partial\Omega$.

Let Q^* be formal adjoint of P and

$$P - B = Q^* - C^* \qquad (4)$$

be a Green's formula. Here, the star refers to the transposed bilinear functional. Then $u \in D$ is solution of the boundary value problem, if and only if

$$(Q^* - C^*)u = f - g \qquad (5)$$

The boundary values associated with any function $u \in D$ are characterized by Bu and C^*u. Thus, Bu are the prescribed boundary values while C^*u are the complementary boundary values which can be evaluated only after the solution has been obtained. When P and B are given by (3a), one can take $Q = P$ and $C = B$ in (4) to obtain a Green's formula. Hence

$$\langle Q^*u,v\rangle = \int_{\Omega} u\Delta v dx \quad \text{and} \quad \langle C^*u,v\rangle = -\int_{\partial\Omega} v\frac{\partial u}{\partial n}dx \qquad (6)$$

Thus the prescribed boundary values Bu are associated with the values of the function u on $\partial\Omega$ and the complementary boundary values C^*u with the normal derivative on $\partial\Omega$. For Elasticity, when the displacements are prescribed on the boundary $\partial\Omega$, the complementary boundary values are the tractions.

Observe also that Pu is prescribed in the boundary value problem, while P^*u, in view of (6), is associated with the sought values of the function in the region Ω.

UNIFIED FORMULATION

The unified formulation is based on the application of weighted residuals and subsequent use of Green's formulas for problems in which the admissible functions may be discontinuous.

Let π be a partition of Ω into a finite collection of E subdomains Ω_e, e=1,...,E, [Babuska, et. al., 1977, 1978]. If the space of admissible functions D is made of functions which are smooth in every one of the subdomains Ω_e separately, then one can still define $P:D\to D^*$, $B:D\to D^*$, $Q^*:D\to D^*$ and $C^*:D\to D^*$, by means of (3a) and (6), if the integrals are interpreted as sums of the contributions coming from every one of the subdomains (i.e. $\int_\Omega = \sum_{e=1}^{E} \int_{\Omega e}$ and similarly for $\int_{\partial\Omega}$).
However, equation (4) has to be modified to be

$$P - B - J = Q^* - C^* - K^* \qquad (7)$$

Where the "jump" operator $J:D\to D^*$ is given by [Herrera, 1980]

$$\langle Ju,v\rangle = \int_\Gamma \{[u] \frac{\partial \dot{v}}{\partial n} - \dot{v}[\frac{\partial u}{\partial n}]\}dx \qquad (8a)$$

while the "average" operator $K^*:D\to D^*$ is given by

$$\langle K^*u,v\rangle = \int_\Gamma \{[v]\frac{\partial \dot{u}}{\partial n} - \dot{u}[\frac{\partial v}{\partial n}]\}dx \qquad (8b)$$

Clearly $K^* = J^*$, for this case. Here, Γ is the union of all interelement boundaries, while

$$[u] = u_f - u_e \quad ; \quad [\frac{\partial u}{\partial n}] = \frac{\partial u_f}{\partial n} - \frac{\partial u_e}{\partial n} \qquad (9a)$$

$$\dot{u} = \frac{1}{2}(u_f + u_e) \quad ; \quad \frac{\partial \dot{u}}{\partial n} = \frac{1}{2}(\frac{\partial u_f}{\partial n} + \frac{\partial u_e}{\partial n}) \qquad (9b)$$

at every point $\underset{\sim}{x} \in \partial\Omega_e \cap \partial\Omega_f$. In equations (9), the unit normal vector is taken pointing outwards from Ω_e.

Green's formulas (7) for arbitrary formally symmetric operators in discontinuous fields were published by the author [Herrera, 1980] and have just appeared in book form [Herrera, 1984b]. The extension to non-symmetric operators will son appear [Herrera, 1984a]. For arbitrary linear boundary value problems with prescribed jumps, including initial value problems, since the region Ω may be space-time, the problem is formulated by means of the functional equation

$$(P - B - J)u = f - g - j \qquad (10)$$

In general, f, g and j are defined in terms of the data for the differential operator, the boundary values and the prescribed jumps in Ω, on $\partial\Omega$ and on interelement boundaries Γ, respectively. In this manner Pu, Bu and Cu are prescribed, while Q^*u, C^*u and K^*u supply pieces of information about the sought solution. Indeed, knowing Q^*u is tantamount to know u

Taking into account (12), it is clear that equations (13a) are also satisfied by the exact solution u (recall $j = 0$); i.e. an exact is necessarily an approximate solution. Therefore, by substraction one gets

$$<Q^*(u' - u),\varphi_\alpha> - <C^*(u' - u),\varphi_\alpha> - <K^*(u' - u),\varphi_\alpha> = 0 ;$$

$$\alpha = 1,\dots,N \qquad (14)$$

The system of N equations (14), shows that all what is required of an approximate solution is that certain linear combinations of the weighted averages (defined by $<Q^*u',\varphi_\alpha>$) of the values in the interior of the finite elements Ω_e ($e=1,\dots,E$), with those of the complementary boundary values (defined by $<C^*u',\varphi_\alpha>$) and with those of the averages on the interelement boundaries (defined by $<K^*u',\varphi_\alpha>$), be precisely equal to those associated with the exact solution. Thus, if these weighted averages are computed after an approximate solution has been obtained, the values associated with the exact solution are derived. Thus, this is information about the exact solution; indeed, the only information about the exact solution that one can derive from an approximate solution. Observe, the solution of system (13) is non-unique but the information about the exact solution supplied by an approximate solution u', is the same independently of the specific approximate solution u' considered.

Keeping Dirichlet problem as illustrative example, equation (13a) is equivalent to (14). The latter states that

$$\int_\Omega u'\Delta\varphi_\alpha dx + \int_{\partial\Omega}\varphi_\alpha \frac{\partial u'}{\partial n}dx + \int_\Gamma\{\dot{u}'\left[\frac{\partial\varphi_\alpha}{\partial n}\right] - [\varphi_\alpha]\frac{\partial\dot{u}'}{\partial n}\}dx; \qquad (15a)$$

be equal to

$$\int_\Omega u\Delta\varphi_\alpha dx + \int_{\partial\Omega}\varphi_\alpha \frac{\partial u}{\partial n}dx + \int_\Gamma\{u\left[\frac{\partial\varphi_\alpha}{\partial n}\right] - [\varphi_\alpha]\frac{\partial u}{\partial n}\}dx \qquad (15b)$$

In view of the fact that either one of the equivalent systems (13), possesses infinitely many solutions, in the finite element method one usually assumes that u' is given by

$$u' = \sum_{\alpha=1}^{N} a_\alpha \Phi_\alpha, \qquad (16)$$

where $\{\Phi_1,\dots,\Phi_N\} \subset D$ is an additional family of functions, the base functions. Since the information (about the exact solution u) supplied by the approxiin the interior of the subdomain (finite elements) Ω_e; C^*u is associated to the complementary boundary values on $\partial\Omega$, while K^*u represents the average values across the interelement boundaries. For example, in finite element formulations the sought solution is usually smooth, so that $j = 0$. When equations (9) apply, this implies that the average $\hat{u}$ across interelement boundaries coincides with the function. Therefore, knowing K^*u is tantamount to know the function u and $\partial u/\partial n$ there.

Equation (10) is equivalent to

$$(Q^* - C^* - K^*)u = f - g - j \tag{11}$$

by virtue of (7). The advantage of (11) over (10) is that the latter involves the sought information Q^*u, C^*u and K^*u, explicitly. This will be discussed more thoroughly in the next section.

FINITE ELEMENTS

Equation (11) is a functional equation, since f, g, $j \in D^*$; i.e. f, g and j are linear functionals defined on the space D of admissible functions. Thus, we can write

$$<(Q^* - C^* - K^*)u,v> = <f - g - j,v> \; \forall \; v \in D \tag{12}$$

instead of equation (11). In what follows it will be assumed that the sought solution is smooth, so that $j = 0$.

Equation (12) is satisfied, if and only if, the function $u \in D$ is an exact solution. Generally, the dimension of D is infinity and approximate methods are formulated replacing D by a finite family $\{\varphi_1,\ldots,\varphi_N\} \subset D$ of linearly independent functions; these are called test or weighting functions. Thus, we say that $u' \in D$ is an approximate solution when

$$(P - B - J)u',\varphi_\alpha> = <f - g, \varphi_\alpha> \tag{13a}$$

or equivalently

$$<Q^*u',\varphi_\alpha> - <C^*u',\varphi_\alpha> - <K^*u',\varphi_\alpha> = <f,\varphi_\alpha> - <g,\varphi_\alpha> ;$$
$$\alpha = 1,\ldots,N \tag{13b}$$

Observe, the system of N equations (13a), imposes restrictions on (i.e. it supplies information on) the values of the function in the interior of the finite elements Ω_e (through Q^*u') the complementary boundary values on $\partial\Omega$ (C^*u') and the average value of u on the interelement boundaries $\Gamma(K^*u)$.

mate solution is independent of the particular base system $\{\Phi_1,\ldots,\Phi_N\}$ used to represent u', it is clear that the base functions $\{\Phi_1,\ldots,\Phi_N\}$ only define the nature of the interpolation used to extend the actual information available.

Equations (14) can be used to carry out an analysis of the errors which is independent of the interpolating functions used. This can then be complemented by the analysis of the error introduced by the interpolating functions $\{\Phi_1,\ldots,\Phi_N\}$.

For Laplace operators, by integration by parts it is seen that the functional $<(P-B-J)u',v> = <(Q^*-C^*-K^*)u,v>$ can also be written as

$$(P-B-J)u',v> = -\int_\Omega \nabla u'\nabla v\,dx - \int_\Gamma \{[u']\frac{\partial \dot{v}}{\partial n} + [v]\frac{\partial \dot{u}'}{\partial n}\}dx + \int_{\partial\Omega}\{v\frac{\partial u'}{\partial n} + u'\frac{\partial v}{\partial n}\}dx \qquad (17)$$

When conforming elements are used, the functions are continuous across interelement boundaries so that $[u] = [v] = 0$ on Γ.

When in addition, $u' = v = 0$ on the boundary, the functional of equation (17) reduces to the well known functional $\int_\Omega \nabla u\,\nabla v\,dx$. When less restrictive conditions apply, the functional (12) has to be used.

BOUNDARY ELEMENT METHODS

Observe that

$$<Q^*u',\varphi_\alpha> = <Q\varphi_\alpha,u'> \qquad (18)$$

Therefore, if

$$Q\varphi_\alpha = 0 \quad , \quad \text{for } \alpha = 1,\ldots,N \qquad (19)$$

then the term containing Q^*u' in (13b) drops out, reducing to

$$<C^*u',\varphi_\alpha> + <K^*u',\varphi_\alpha> = <g - f,\varphi_\alpha>, \ \alpha = 1,\ldots,N \qquad (20)$$

This is a system of equations involving the complementary boundary values C^*u' and the averages across interelement boundaries K^*. Thus, a boundary method. Using (14) it is seen that this system is equivalent to

$$<C^*(u' - u),\varphi_\alpha> + <K^*(u' - u),\varphi_\alpha> = 0; \ \alpha=1,\ldots,N \qquad (21)$$

The author has shown [Herrera, 1984b], that when the system of weighting functions φ_α is T-complete, the system (21) implies that $C^*u' = C^*u$ and $K^*u' = K^*u$. Hence, the exact complementary boundary values and the exact values on interconnecting boundaries Γ, are obtained in that case by solving (20). For problems in several dimensions T-complete systems are not finite and the system (20) yields approximate values only. However, there is an important case for which T-complete systems are finite; these are one-dimensional problems. Thus, for ordinary differential equations one gets exact values and these will be discussed in the next Section.

Application of formula (20) allows formulating two classes of boundary methods. If the test functions φ_α are required to be smooth in Ω (i.e. $J\varphi_\alpha = 0$), boundary methods in a restricted sense are obtained. In this case

$$\langle K^*u',\varphi_\alpha\rangle = \langle K\varphi_\alpha,u'\rangle = 0 \qquad (22)$$

because the theory shows that $K\varphi_\alpha = 0$ if and only if $J\varphi_\alpha = 0$. Equations (20) reduce to

$$\langle C^*u',\varphi_\alpha\rangle \quad \langle g - f,\varphi_\alpha\rangle \;, \quad \alpha=1,\ldots,N \qquad (23)$$

which is Trefftz method for non-symmetric operators [Herrera, 1984c].

FINITE DIFFERENCES

As an illustration of boundary methods in the extended sense, consider the case when $P:D\to D^*$ is associated with an ordinary differential equation. Thus

$$\langle Pu,v\rangle = \int_0^1 v\,\mathcal{L}u\,dx \qquad (24)$$

where $\mathcal{L}$ is an ordinary differential operator which is linear. The interval $[0,1]$ has been taken for definiteness. Let $\mathcal{L}^*$ be the formal adjoint of $\mathcal{L}$. Then

$$\langle Qu,v\rangle = \int_0^1 v\,\mathcal{L}^*u\,dx \qquad (25)$$

The results of the analysis for arbitrary differential operators will be presented elsewhere [Herrera, 1984a]. Here, attention is restricted to second order equations. Thus, we take

$$\mathcal{L}u = \frac{d^2u}{dx^2} + a_1\frac{du}{dx} + a_2u \;;\; \mathcal{L}^*u = \frac{d^2u}{dx^2} - \frac{d}{dx}(a_1u) + a_2u \qquad (26)$$

The operators B and C^* depend on the boundary conditions to be prescribed. For definiteness it is here assumed that $u(0)$ and $u(1)$ are prescribed, in which case suitable boundary operators are

$$\langle Bu,v\rangle = u(0)\left[\frac{dv}{dx}(0) - a_1 v(0)\right] - u(1)\left[\frac{dv}{dx}(1) - a_1 v(1)\right] \tag{27a}$$

and

$$\langle C^*u,v\rangle = v(0)\frac{du}{dx}(0) - v(1)\frac{du}{dx}(1) \tag{27b}$$

Consider a partition of the unit interval $[0,1]$, such that the nodes $\{x_0,x_1,\dots,x_E\}$ satisfy $0=x_0<x_1<\dots x_E=1$.

Then

$$\langle Ju,v\rangle = \sum_{i=1}^{E-1}\{[u]_i \frac{d\dot{v}_i}{dx} - \dot{v}_i\left[\frac{du}{dx}\right]_i - a_1 v_i, u_i\} \tag{28a}$$

and

$$\langle K^*u,v\rangle = \sum_{i=1}^{E-1}\{[v]_i \frac{d\dot{u}_i}{dx} - \dot{u}_i\left[\frac{dv}{dx}\right]_i + a_1\dot{u}_i[v]_i\} \tag{28b}$$

where

$$2\dot{u}_i = u(x_i+) + u(x_i-) \quad , \quad [u]_i = u(x_i+) - u(x_i-) \tag{29}$$

and similarly for the derivatives.

Application of the results of Section 5 allows obtaining the exact values of the solution at the nodes. Indeed, consider the boundary value problem

$$\mathcal{L}u = f \quad ; \quad u(0) - g_0 \ , \quad u(1) = g_1 \tag{30}$$

where $\mathcal{L}$ is given by (26), f is a prescribed function in (0,1) and g_0, g_1 are given numbers. If no continuity restriction is imposed at the nodes, then a T-complete system $\{\varphi_1,\dots,\varphi_N\}$ is made of 2E functions (i.e. N=2E), because the differential operator $\mathcal{L}$ is second order. In view of equations (27b) and (28b), the system

$$\langle C^*u,\varphi_\alpha\rangle + \langle K^*u,\varphi_\alpha\rangle = \langle g-f,\varphi_\alpha\rangle \ , \quad \alpha=1,\dots,2E \tag{31}$$

involve 2E unkowns; these are, the values of u at the E+1 nodes and the values of du/dx at E-1 interior nodes.

If we are not interested on the derivative, it may be convenient to eliminate it from the system of equations. This is achieved by imposing additional conditions on the test functions. Let us require $\langle C^*u,\varphi_\alpha\rangle = \langle C\varphi_\alpha,u\rangle = 0$; i.e. $C\varphi_\alpha=0$. Hence $\varphi_\alpha(0)=\varphi_\alpha(1)=0$. In addition, let φ_α be continuous. Then a T-complete system is made E-1 functions, only, and by inspection it is seen that system (31) involves only the values of u at the interior nodes.

In order to illustrate the procedure just explained we consider three specific cases. These correspond to the choices $a_1 = 0$ with $a_2 = 0$ (Case 1), $a_2 = -1$ (Case 2) and $a_2 = 1$ (Case 3). In addition $x_{i+1} - x_i = h = b$, is independent of i.

TABLE 1

Case	$x_{\alpha-1} < x < x_\alpha$	$x_\alpha < x < x_{\alpha+1}$
1	$\varphi_\alpha = x - x_{\alpha-1}$	$\varphi_\alpha = (x_{\alpha+1} - x)$
2	$\varphi_\alpha = \sinh(x - x_{\alpha-1})$	$\varphi_\alpha = \sinh(x_{\alpha+1} - x)$
3	$\varphi_\alpha = \sin(x - x_{\alpha-1})$	$\varphi_\alpha = \sin(x_{\alpha+1} - x)$

The system of equations (31), become:

Case 1

$$\frac{u_{\alpha+1} + u_{\alpha-1} - 2u_\alpha}{h^2} = \frac{1}{h^2} \int_{x_{\alpha-1}}^{x_{\alpha+1}} f_\Omega \varphi_\alpha dx \quad ; \quad \alpha = 2, \ldots, N-1 = E-2 \qquad (32a)$$

$$\frac{u_2 - 2u_1}{h^2} = \frac{1}{h^2} \int_0^h f_\Omega \varphi_0 dx - g_0/h^2 \; ; \quad \frac{u_N - 2u_{N+1}}{h^2} = \frac{1}{h^2} \int_{1-h}^{1} f_\Omega \varphi_N dx - $$

$$- g_1/h^2 \qquad (32b)$$

Notice that these are central differences.

Case 2

$$\frac{u_{\alpha+1} + u_{\alpha-1} - 2u_\alpha \cosh b}{b^2} = \frac{1}{b^2} \int_{x_{\alpha-1}}^{x_{\alpha+1}} f_\Omega \varphi_\alpha dx \; ; \quad \alpha = 2, \ldots, N-1 = E-2 \qquad (33a)$$

$$\frac{u_2 - 2u_1 \cosh b}{b^2} = \frac{1}{b^2} \int_0^b f_\Omega \varphi_0 dx - g_0/b^2 \; ; \quad \frac{u_N - 2u_{N+1}}{b} =$$

$$= \frac{1}{b^2} \int_{1-b}^{1} f_\Omega \varphi_N dx - g_1/b^2 \qquad (33b)$$

where we have written $b = h$, for clarity.

Case 3

$$\frac{u_{\alpha+1} + u_{\alpha-1} - 2u_\alpha \cos b}{b^2} = \frac{1}{b^2} \int_{x_{\alpha-1}}^{x_{\alpha+1}} f_\Omega \varphi_\alpha dx \; ; \quad \alpha = 2, \ldots, N-1 = E-2 \qquad (34a)$$

$$\frac{u_2 - 2u_1 \cos b}{b^2} = \frac{1}{b^2} \int_0^b f_\Omega \varphi_0 dx - g_0/b^2 \; ; \quad \frac{u_N - 2u_{N+1}}{b^2} =$$

$$= \frac{1}{b^2} \int_{1-b}^{1} f_\Omega \varphi_N dx - g_1/b^2 \qquad (34b)$$

In a similar fashion one can derive finite difference schemes which would yield the exact values of the derivative at prescribed nodes only or as a matter of fact the exact values of the solution at some nodes and the exact values of the derivative at other ones. For illustrations and more thorough discussion of such construction the reader is referred to [Herrera, 1984 a,d].

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