76

PROCEDINGS OF THE SECOND INTERNATIONAL CONFERENCE ON VARIATIONAL METHODS IN ENGINEERING SOUTHAMPTON, ENGLAND 17-19 JULY, 1985.

GENERAL VARIATIONAL PRINCIPLES FOR NUMERICAL METHODS

Ismael Herrera

Instituto de Geofísica, U.N.A.M., Apdo. Postal 21-524, 04000 México, D.F. MEXICO.

ABSTRACT

Three of the most powerful numerical procedures for partial differential equations are finite elements, finite differences and boundary element methods. In this paper a general variational theory of such methods is presented. The approach is quite general, since it is applicable to any linear operator, symmetric or non-symmetric, regardless of its type. In particular, the theory includes steady state and time dependent problems. In general there are two alternatives but equivalent variational principles associated with any linear problem. The first one is in terms of "prescribed data" while the second one is in terms of "sought information". The latter variational principle is quite useful for analyzing the relation between the exact solution and any approximate one. The general development of such variational principles depends on the availability of Green's formulas for operators defined in discontinuous fields. The systematic development of Green's formulas for operators defined in discontinuous fields has been carried out recently by the author.

1. INTRODUCTION

Variational principles for problems formulated in discontinuous functions are essential for the understanding of numerical methods for partial differential equations. This has been recognized since long by some authros (see for example [1,2]). However, a systematic development of this subject has been lacking.

Recently, the author has presented a unifying theory of Numerical Methods [3-5], whose fundamental ingredients are general variational principles for problems formulated in discontinuous functions (or, more generally, discontinuous fields). This paper is devoted to present an outline at that theory, which is completely general, since it is applicable to any linear boundary value problem, regardless of the type of the operator or of the boundary condition. In particular, the variational principles here given are applicable to steady state and time dependent problems.

2. PRELIMINARY NOTIONS AND NOTATIONS

Denote by F the field of real or complex numbers. Let D be a linear space over the field F, whose elements will be called scalars. Elements of D will be denoted by u,v,..., and will be said to be admissible functions. Write D* for the linear space of linear functionals defined on D; i.e. D* is the algebraic dual of D. Hence, any element $\alpha \in D^*$ is a function $\alpha : D \to F$ which is linear. Given $v \in D$, the value of the function α at v will be denoted by

$$\alpha(v) = \langle \alpha, v \rangle \in F \tag{2.1}$$

In this work, functional-valued operators $P:D \to D^*$ will be extensively used. Given $u \in D$, the value $P(u) \in D^*$ is itself a linear functional. According to (2.1), given any $v \in D$, $\langle P(u),v \rangle \in F$ will be the value of this linear functional at v. When the operator P is itself linear, $\langle P(u),v \rangle$ is linear in u when v is kept fixed. Therefore, as it is costumary, we write

$$\langle Pu,v \rangle = \langle P(u),v \rangle \in F \tag{2.2}$$

for this value. We shall be concerned, exclusively, with functional valued operators that are linear.

On the other hand, let $D^2 = D \oplus D$ be the space of pairs $\{u,v\}$ with $u \in D$ and $v \in D$. We may consider functions $\beta : D^2 \to F$. The value of such function on a pair $\{u,v\} \in D^2$, will be written as $\beta(u,v)$. Such function is said to be a bilinear functional if it is linear in u when $v \in D$ is kept fixed and conversely, it is linear in v when u is kept fixed. There is a one-to-one correspondence between bilinear functionals and functional-valued operators which are linear. This is given by

$$\beta(u,v) = \langle Pu,v \rangle \tag{2.3}$$

In what follows, operators $P:D \to D^*$ will be defined by giving the corresponding bilinear functional.

Given $P:D \to D^*$, let equation (2.3) be satisfied, the notation $P^*:D \to D^*$ will be used for the operator associated with the transposed bilinear functional; thus

$$\langle P^*u,v\rangle = \beta^*(u,v) = \beta(v,u) = \langle Pv,u\rangle \qquad (2.4)$$

Here, β^* is the transposed of β and $P^*:D \to D^*$ will be called transposed of $P:D \to D^*$. Observe that the transposed operator is well defined whenever $P:D \to D^*$ is given.

3. BOUNDARY VALUE PROBLEMS

Boundary value problems formulated in discontinuous functions can be formulated by means of three operators: $P:D \to D^*$, $B:D \to D^*$ and $J:D \to D^*$ associated with the differential operator $\mathcal{L}$, the boundary conditions and the prescribed jumps, respectively. The systematic construction of these operators was presented in [3]. Usually, but this is not essential, $P:D \to D^*$ is defined by

$$\langle Pu,v\rangle = \int_\Omega v\,\mathcal{L}u\,d\underset{\sim}{x} \qquad (3.1)$$

Then the boundary value problem with prescribed jumps is

$$Pu = f\ ,\quad Bu = g\ ,\quad Ju = j \qquad (3.2)$$

where f, g and j are prescribed functionals. When f, g and j are in the ranges of P, B and J, respectively, the three equations (3.2) are equivalent to the variational principle

$$\langle (P - B - J)u,v\rangle = \langle f - g - j,v\rangle \quad \forall\ v \in D \qquad (3.3)$$

4. GREEN'S FORMULAS FOR OPERATORS IN DISCONTINUOUS FUNCTIONS

In the systematic analysis of discrete methods (e.g. finite elements, finite differences and boundary methods) the use of Green's formulas for operators defined in discontinuous fields, is essential. Such formulas were developed in [3] for arbitrary linear operators.

It is convenient to define the space of admissible functions as the product space $D = D_I \oplus D_{II}$, where D_I and D_{II} are two linear spaces. In applications the elements of D_I and D_{II} will be functions defined on two neighboring regions Ω_I and Ω_{II} (Fig. 1), respectively. Thus, the elements of D are pairs $u = \{u_I,u_{II}\}$, where $u_I \in D_I$ and $u_{II} \in D_{II}$. Usually, we start from a Green's formula $P - B = Q^* - K^*$ satisfied by smooth functions. When discontinuous functions are considered, this

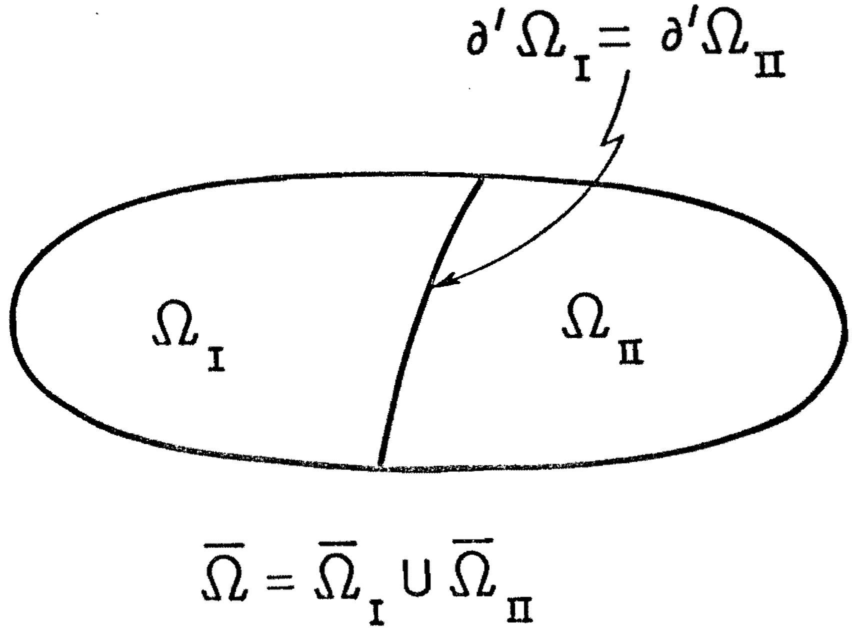

Figure 1.

relation no longer holds, and one can define $R = P - B - (Q - K)^*$; i.e. the operator R is the residue. Generally, the operator $R: D \rightarrow D^*$ satisfies

$$\langle Ru, v\rangle = \langle R_I u_I, v_I\rangle + \langle R_{II} u_{II}, v_{II}\rangle \qquad (4.1)$$

where $R_I: D_I \rightarrow D_I^*$ and $R_{II}: D_{II} \rightarrow D_{II}^*$ are associated with the values at each one of the sides of the connecting boundary $\partial'\Omega_I = \partial'\Omega_{II}$ (Fig. 1).

The notion of jump and its numerical value, is dependent on the smoothness criterium considered. Usually the set of smooth functions constitutes a linear subspace of D, to be denoted by $S \subset D$. In order to achieve complete generality, it is necessary to introduce a second smoothness criterium. Thus, two linear subspaces $\{S^\ell, S^r\}$ of smooth functions are considered, associated with each of one of the smoothness criteria. Even more, they will be assumed to be conjugate; by this we mean that

$$\langle Ru, v\rangle = 0 \quad \forall\ u \in S^\ell \ \ \& \ \ v \in S^r \qquad (4.2)$$

Then the jump operator $J: D \rightarrow D^*$ and the generalized averages $K^*: D \rightarrow D^*$, are defined by [3]:

$$\langle Ju, v\rangle = -\langle R_I [u]^\ell, \dot{v}^r\rangle \text{ while } \langle K^* u, v\rangle = \langle R_I \dot{u}^\ell, [v]^r\rangle \qquad (4.3)$$

Here, the square brackets stand for the jumps and the dot for the averages. These depend on the smoothness criteria used.

With these definitions the "General Green's Formula for Problems in Discontinuous Functions"

$$P - B - J = Q^* - C^* - K^* \qquad (4.4)$$

holds.

5. THE VARIATIONAL PRINCIPLES

There are <u>two variational principles</u> applicable to any linear boundary value problem, whose explicit expressions are given in this article. The first one is in terms of the "prescribed data".

$$\langle Pu,v\rangle - \langle Bu,v\rangle - \langle Ju,v\rangle = \langle f,v\rangle - \langle g,v\rangle - \langle j,v\rangle \qquad \forall \ v \in D \qquad (5.1)$$

while the second one is in terms of the "sought information"

$$\langle Q^*u,v\rangle - \langle C^*u,v\rangle - \langle K^*u,v\rangle = \langle f,v\rangle - \langle g,v\rangle - \langle j,v\rangle \qquad \forall \ v \in D \qquad (5.2)$$

Here $f \in D^*$, $g \in D^*$ and $j \in D^*$ are the prescribed values of the operator Pu associated with the differential operator, the boundary operator Bu and the jump operator Ju. The definition of these operators is given explicitly by the theory and it is dependent on the differential operator, the kind of boundary conditions and the smoothness requirements, considered, respectively. The equivalence between (5.1) and (5.2) is granted by the Green's formula (4.4). If Ω (Figure 1) is the region of definition of the problem one usually defines - but this is not essential - the operators P and Q^* by

$$\langle Pu,v\rangle = \int_\Omega v\mathcal{L}u\,dx \quad \text{and} \quad \langle Q^*u,v\rangle = \int_\Omega u\,\mathcal{L}^*v\,dx \qquad (5.3)$$

where $\mathcal{L}$ is a differential operator defined in Ω and $\mathcal{L}^*$ its formal adjoint. Observe that knowing Q^*u is tantamount to know the function u in the interior of Ω. The "complementary boundary values" C^*u are here illustrated by means of examples; thus, for Dirichlet problem of Laplace equation in which u is prescribed on the boundary $\partial\Omega$, the complementary boundary values are the normal derivatives $\partial u/\partial n$, there. For problems of Elasticity, the prescribed and complementary boundary values, may be the displacements and the tractions, respectively. The average values of the exact solution across the surface Γ (Fig. 2), where Γ is the surface on which discontinuities of the functions may occur, constitute the third component of the sought information and are characterized by K^*u. The operators J and K^* in a region like the one illustrated in Figure 2 is constructed by a processes which generalizes the results of Section 4 and explained in detail in [4].

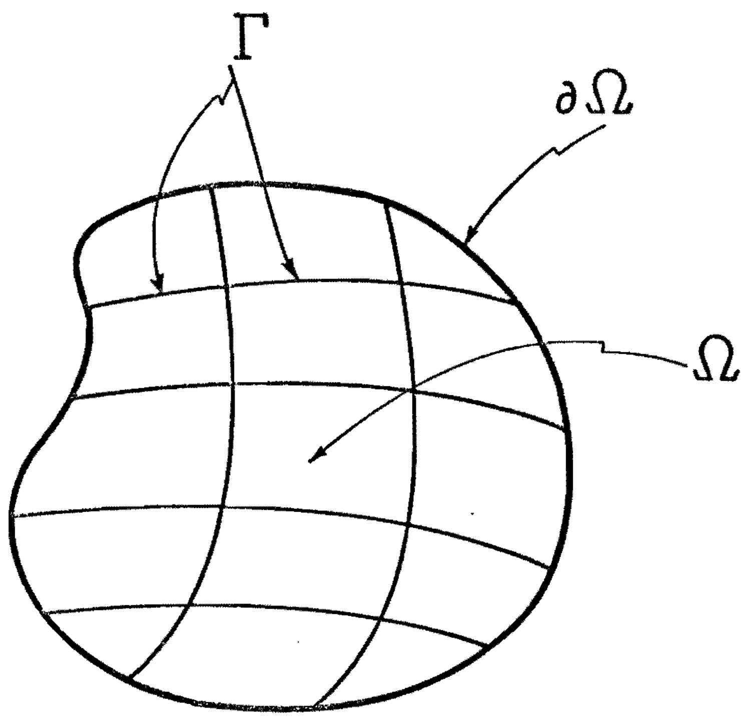

Figure 2.

It must be emphasized that the integrals in (5.3) are understood in an elementary sense; thus, the theory of distributions is not applied, because in this manner greater generality is achieved. Generally, the admissible functions may possess as many continuous derivatives as required by the order of the differential operator $\mathcal{L}$, in the interior of the subregions $\overline{\Omega}_e$ in which the region Ω is decomposed (Fig. 2). Hence, the integral $\int_{\Omega_e} v\mathcal{L}u dx$ is well defined for every subregion Ω_e. Then, the integral over Ω is understood as the sum over all the subregions and the resulting theory allows greater generality than the theory of distributions, in some respects.

In order to illustrate this point, consider the differential operator $\mathcal{L}u \equiv d^2u/dx^2$ which will be applied to functions defined on the unit interval (0,1). When these functions are reqired to possess second order continuous derivatives in the closed interval, the operator is well-defined. To extend it to functions with a jump discontinuity at an interior point, the theory of distributions yields a definition of $\mathcal{L}u$ such that $\int_0^1 v\mathcal{L}u dx$ is well defined only when v is continuous and possesses a continuous first derivative at x=1/2. For example if u=x-H(x-1/2), where H is Heaviside unit step function (Fig. 2), then $\mathcal{L}u = -\delta'(x-1/2)$ where δ' is the derivative of Dirac's delta function. Then, $\int_0^1 v\mathcal{L}u dx = dv/dx\ (1/2)$, when v has a continuous first order derivative at x=1/2. However, if v is discontinuous, $\int_0^1 v\mathcal{L}u dx$ is not defined. On the other hand, when v is discontonuous at x=1/2, $\int_0^1 v\delta'\ (x-1/2)\ dx = \int_0^1 v\mathcal{L}u dx$ is not defined.

In the theory that has just been published by the author [3-5], the operator $\mathcal{L}u$ is extended to be P-J, which is given by

$$\langle (P-J)u,v\rangle = \int_0^1 v\ d^2u/dx^2\ dx + \left(\dot{v}\ [du/dx] - [u]\, d\dot{v}/dx\right)_{x=1/2} \tag{5.4}$$

Here, the square brackets [ ] and the dots, stand for the jump and the average of the functions involved, whose definition depends on the smoothness criterion adopted. The usual smoothness condition associated with a second order differential operator requires that a function and its derivative be continuous at x=1/2, in order to be smooth. In this case the jump of a functions is defined as the limit from the right minus the limit from the left and the average as one half of the sum of this quantities. Thus, if u=x-H(x-1/2), then equation (5.4) yields

$$\langle (P-J)u,v\rangle = (d\dot{v}/dx)_{x=1/2} \tag{5.5}$$

This is well defined even if v and its derivative are discontinuous. Observe that in particular, when v and its derivative are continuous, this reduces to dv/dx(1/2) which is the result given by the theory of distributions.

ACKNOWLEDGEMENT.

This work was supported by a grant from CONACYT (Consejo Nacional de Ciencia y Tecnología) México.

REFERENCES

1 Prager, W. (1967) Variational Principles of Linear Elastodynamics for Discontinuous Displacements, Strains, and Stressess, in Recent Progress in Applied Mechanics, in The Folke-Odqvist Volume, eds. Broberg, B., Hult, J. & Niordson, F. (Almgvist and Wiksell, Stockholm), 463-474.

2 Nemat-Nasser, S. (1972) On Variational Methods in Finite and Incremental Elastic Deformation Problems with Discontinuous Fields. Q. Appl. Math. 30, 2:143-156.

3 Herrera, I. (1985) Unified Approach to Numerical Methods. Part 1. Green's Formulas for Operators in Discontinuous Fields. Numerical Methods for Partial Differential Equations, 1, 1:12-37.

4 Herrera, I. (1985) Unified Approach to Numerical Methods. Part 2. Finite Elements, Boundary Methods and its Coupling. Numerical Methods for Partial Differential Equations, in press.

5 Herrera, I. (1985) Unified Approach to Numerical Methods. Part 3. Finite Differences. Numerical Methods for Partial Differential Equations, in press.