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NUMERICAL QUADRATURE IN THE FINITE ELEMENT METHOD

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ABSTRACT

The Finite Element method requires the numerical evaluation of integrals over one, two- or three-dimensional domains. The integrals are usually evaluated in a local system of curvilinear coordinates, where the domain of integration has a simple geometry. The integrands are usually sums of products of functions of the global coordinates by shape functions and/or their global derivatives of different orders. When the shape functions are given in terms of the local curvilinear coordinates, their global derivatives depend on the coordinate transformation and have to be evaluated numerically.

In this report we present the basic formulation and discuss the computational strategies requires to perform the calculations.

RESUMEN

Para el método de Elementos Finitos se requiere la evaluación numérica de integrales sobre dominios de una, dos o tres dimensiones. Las integrales se evalúan habitualmente en un sistema local de coordenadas curvilíneas donde el dominio de integración tiene una geometría simple. Los integrandos suelen ser sumas de productos de funciones de las coordenadas globales por funciones de forma y/o sus derivadas globales de diversos órdenes. Cuando las funciones de forma están dadas en términos de las coordenadas curvilíneas locales, sus derivadas globales dependen de la transformación de coordenadas y deben ser evaluadas numéricamente.

En este informe presentamos la formulación básica y discutimos las estrategias computacionales requeridas para realizar los cálculos.

I. INTRODUCTION

An integral is specified when both the integrand function and the domain of integration are given. In the Finite Element method the domain of integration Ω is an element, either finite or infinite, and in either one, two or three dimensions. Suitable domains of integration are also facets of edges of three-dimensional elements, and sides of two-dimensional elements.

The integrand may be a scalar quantity, a vector quantity consisting of a set of functions identified by an index i, or a matrix quantity consisting of a set of functions identified by two indexes i and j. Matrices with more indexes may also arise and can be dealt with using the same techniques to be described. The indexes i and j are associated with the shape functions N_i of the element.

In some cases, both the integrand and the domain are simple enough for an analytic integration to be possible. This simplicity can certainly be exploited, but the resulting computer programs will be limited to the simplest situations. On the other hand, since distorted elements are usually obtained from simple geometric shapes by coordinate transformations, the integral can be solved over the original domain Ω° using $Jd\Omega^\circ$ instead of $d\Omega$, where J is the Jacobian determinant of the transformation. The integral can then be calculated by numerical quadrature over the

original simple domain, no matter how complex are the integrand or the function J. Truly automatic computer programs can be written using these techniques. Coordinate transformations of the type employed in the Finite Element method are described in Section 2 of this report.

The integrands which appear in the Finite Element method usually involve the shape functions N_i and their derivatives with respect to the system of global coordinates. The functions N_i are usually given in terms of the local coordinates of the element and can only be derived with respect to the global coordinates when the derivatives of the local with respect to the global coordinates have been calculated. Such a calculation requires again numerical techniques, since the coordinate transformation is defined giving the global in terms of the local coordinates, and in most cases of interest can not be explicitly inverted. Section 3 of this report describes the calculation of global first and second derivatives of shape functions.

Finally in Section 4 we describe the transformation of the line, surface and volume integrals in three dimensions to local coordinates. In section 5, the transformation of two-dimensional line and surface integrals is discussed. In all cases, the transformation formulas given are written in a form suitable for direct computation in the Finite Element method.

II. COORDINATE TRANSFORMATIONS

The coordinate transformation between the local coordinates ξ_β of an element and the global system of coordinates x_α is based on a set of points called the geometric nodes, which belong to the boundary or the interior of the element, and is given in terms of the set of geometric shape functions $\hat{N}_i$. Greek indexes such as α and β run over the dimensions of the domain (e.g. 1,2 for two-dimensional elements, or 1,2,3 for three-dimensional elements). Latin indexes i, j, etc, run over the nodes of the element under consideration. We will apply the Einstein summation convention: a summation is implied in any expression containing the same index twice (e.g. $a_i\, b_i \equiv \sum_i a_i\, b_i$).

The geometric shape function $\hat{N}_i$ is equal to 1 at the geometric node i, to 0 at all the remaining geometric nodes, and is usually given by some simple function of the local variables ξ_β over the element. The coordinate transformation is defined as follows:

$$x_\alpha = \hat{N}_i\, X_{i\alpha} \tag{1}$$

where $X_{i\alpha}$ is the global α-coordinate of the geometric node i, a summation over all values of i is implied, and (1) is valid for each value of α. The dependence on the local coordinates ξ_β is given by the $\hat{N}_i$, which are functions of

the ξ_β. The transformation (1) maps a simple geometric figure in the ξ_β system onto a distorted figure in the x_α system. Note that $x_\alpha = X_{i\alpha}$ when the local coordinates of the geometric node i are substituted in (1).

The Jacobian matrix $J_{\alpha\beta}$ of the transformation (1) is defined by:

$$J_{\alpha\beta} = \frac{\partial x_\beta}{\partial \xi_\alpha} \tag{2}$$

The elements of $J_{\alpha\beta}$ can be explicitly obtained by derivation of (1).

The Jacobian matrix of the inverse transformation is

$$H_{\alpha\beta} = \frac{\partial \xi_\beta}{\partial x_\alpha} \tag{3}$$

and fulfils the relations

$$J_{\alpha\beta}\ H_{\beta\gamma} = \delta_{\alpha\gamma} \tag{4}$$

and

$$H_{\alpha\beta}\ J_{\beta\gamma} = \delta_{\alpha\gamma} \tag{5}$$

Each matrix is thus the inverse of the other. $H_{\alpha\beta}$ can be obtained either by derivation of the inverse of the transformation (1), when this inverse is explicitly known, or by inversion of $J_{\beta\gamma}$. This last procedure has the advantage

that the resulting computer program is not restricted to coordinate transformations for which the inverse transformation be explicitly known. The complete matrix $J_{\beta\gamma}$ is evaluated at each sampling point of the element (since values of the integrand are required only at the sampling points) and then numerically inverted to obtain $H_{\alpha\beta}$. $J_{\beta\gamma}$ is a small matrix, 2x2 in two dimensions or 3x3 in three dimensions, and the computation of its inverse is cheap. As a side product, when $J_{\beta\gamma}$ is inverted, its determinant J is also obtained at all the sampling points:

$$J = \text{Det } (J_{\beta\gamma}) \tag{6}$$

The values of J are necessary when the integral over the distorted domain Ω is to be calculated over the original domain Ω°, using the well-known property that:

$$d\Omega = Jd\Omega^\circ \tag{7}$$

where Ω is expressed in terms of the global coordinates x_α, while Ω° is expressed in terms of the local coordinates ξ_β.

III. GLOBAL DERIVATIVES OF SHAPE FUNCTIONS.

When the Finite Element method is used to solve a problem, what is obtained in fact is an approximation to the solution given by a polyhedral function, say ϕ. The definition of this function in each element is based on a set of points called the functional nodes, which belong to the boundary or the interior of the element, and is given in terms of a set of functional shape functions N_i and of the values ϕ_i of ϕ at the functional nodes:

$$\phi = N_i \phi_i \tag{8}$$

The functional shape function N_i is equal to 1 at the functional node i, to 0 at all remaining nodes, and is usually given by some simple function of the local coordinates ξ_β over the element. An element is called isoparametric when the geometric and functional nodes are the same. Isoparametric elements have their functional and geometric shape functions identical: $\tilde{N}_i = N_i$. In all other cases, even when all geometric and all functional nodes, less one, are identical, the two sets N_i and $\tilde{N}_i$ are different. In particular, infinite elements are never isoparametric, since they have necessarily functional nodes at infinity which may not be used as geometric nodes.

As explained in the introduction, the integrands of the integrals which appear in the F.E. method contain products

of the functions N_i and/or their derivatives with respect to the global coordinates x_α. These derivatives can only be obtained implicitly, since in all but the simplest cases the functions N_i are given in terms of the local coordinates ξ_β. For the first global derivatives:

$$\frac{\partial N_i}{\partial x_\alpha} = \frac{\partial N_i}{\partial \xi_\beta} \frac{\partial \xi_\beta}{\partial x_\alpha} \tag{9}$$

or, using (3):

$$\frac{\partial N_i}{\partial x_\alpha} = \frac{\partial N_i}{\partial \xi_\beta} H_{\alpha\beta} \tag{10}$$

where $H_{\alpha\beta}$ is obtained by numerical inversion of $J_{\alpha\beta}$ at the sampling points of the element, as discussed in Section (2). The derivatives $\partial N_i/\partial x_\alpha$ can thus be numerically evaluated at the sampling points of the element. It is important to note here that, while $H_{\alpha\beta}$ is "element dependent" because the nodal coordinates $X_{i\alpha}$ in (1) are required for its evaluation, the $\partial N_i/\partial \xi_\beta$ are not because they depend only on the element topology and on the sampling points (given in terms of the local coordinates). We say that all elements having the same topology and the same set of sampling points in the domain Ω° are of the same type. The derivatives $\partial N_i/\partial \xi_\beta$ depend only on the type of the element and not on its geometry and have to be evaluated only once for each type of element present in the problem.

The calculation of the second global derivatives is done along the same lines. If we consider the N_i to be functions of the global coordinates, we may write:

$$\frac{\partial N_i}{\partial \xi_\lambda} = \frac{\partial N_i}{\partial x_\alpha} \frac{\partial x_\alpha}{\partial \xi_\lambda} \tag{11}$$

(11) is implicitly derived with respect to ξ_μ to obtain:

$$\frac{\partial^2 N_i}{\partial \xi_\lambda \partial \xi_\mu} = \frac{\partial}{\partial \xi_\mu}\left(\frac{\partial N_i}{\partial x_\alpha}\right)\frac{\partial x_\alpha}{\partial \xi_\lambda} + \frac{\partial N_i}{\partial x_\alpha}\frac{\partial}{\partial \xi_\mu}\left(\frac{\partial x_\alpha}{\partial \xi_\lambda}\right) \tag{12}$$

$$= \frac{\partial^2 N_i}{\partial x_\alpha \partial x_\beta}\frac{\partial x_\alpha}{\partial \xi_\lambda}\frac{\partial x_\beta}{\partial \xi_\mu} + \frac{\partial N_i}{\partial x_\alpha}\frac{\partial^2 x_\alpha}{\partial \xi_\lambda \partial \xi_\mu}$$

Multiplying (12) by $(\partial \xi_\lambda / \partial x_\gamma)(\partial \xi_\mu / \partial x_\varepsilon)$ and solving for $\partial^2 N_i / \partial x_\alpha \partial x_\beta$:

$$\frac{\partial^2 N_i}{\partial x_\gamma \partial x_\varepsilon} = \left(\frac{\partial^2 N_i}{\partial \xi_\lambda \partial \xi_\mu} - \frac{\partial N_i}{\partial x_\alpha}\frac{\partial^2 x_\alpha}{\partial \xi_\lambda \partial \xi_\mu}\right)\frac{\partial \xi_\lambda}{\partial x_\gamma}\frac{\partial \xi_\mu}{\partial x_\varepsilon} \tag{13}$$

In (13), the local derivatives $\partial^2 N_i / \partial \xi_\lambda \partial \xi_\mu$ depend only on the type of element and are evaluated at each sampling point of each type of element existing in the problem. $\partial N_i / \partial x_\alpha$ are given by (10), and are element dependent. $\partial^2 x_\alpha / \partial \xi_\lambda \partial \xi_\mu$ are easily evaluated from the coordinate transformation (1), and are also element dependent. The remaining derivatives are elements of the matrix $H_{\beta\gamma}$, the inverse of the Jacobian matrix, and are element dependent.

IV. VOLUME, SURFACE AND LINE ELEMENTS IN THREE-DIMENSIONAL SPACE

The solution of a three- dimensional problem by the FE method frequently requires the evaluation of line, surface or volume integrals. For volume integrals, the domain of integration Ω is an element, and when the integral is calculated over the undistorted domain Ω° in the local coordinates ξ, η, ζ, the element of volume is:

$$dV = J d\xi d\eta d\zeta \tag{14}$$

where J is given by (6).

Let $\vec{r}$ be the position vector of a point in the element under consideration, and $\vec{R}_i$ the position vectors of its geometric nodes. Then (1) can be written:

$$\vec{r} = \hat{N}_i \vec{R}_i \tag{15}$$

Equation (15) gives $\vec{r}$ as a function of the local coordinates ξ, η, ζ:

$$\vec{r} = \vec{r}\ (\xi, \eta, \zeta) \tag{16}$$

The expression of an element of line is obtained by differentiation of (16):

$$\vec{dr} = \frac{\partial \vec{r}}{\partial \xi} d\xi + \frac{\partial \vec{r}}{\partial \eta} d\eta + \frac{\partial \vec{r}}{\partial \zeta} d\zeta \tag{17}$$

If ξ, η, ζ are interpreted as curvilinear coordinates in three-dimensional space, then equation (17) shows that $\partial\vec{r}/\partial\xi$ is a vector tangent to the ξ-coordinate line (a line with constant η and ζ), pointing in the direction of increasing ξ. Thus, $(\partial\vec{r}/\partial\xi)d\xi$ is the element of line in the ξ direction. In the same way, we can prove that $(\partial\vec{r}/\partial\eta)d\eta$ and $(\partial\vec{r}/\partial\zeta)d\zeta$ are elements of line along the η and ζ lines, respectively. Note that the cartesian components of the elements of line are the $J_{\alpha\beta}$ already discussed, multiplied by the corresponding differentials of the local coordinates.

Usually line integrals in 3-D will be calculated along element edges. In particular, consider an edge along the ζ direcion, given by $\xi = \xi_o$, $\eta = \eta_o$, where ξ_o and η_o are constants. The components of the element of line $(\partial\vec{r}/\partial\zeta)d\zeta$ for this ζ-edge are:

$$\frac{\partial x}{\partial\zeta}d\zeta \ , \ \frac{\partial y}{\partial\zeta}d\zeta \text{ and } \frac{\partial z}{\partial\zeta}d\zeta \tag{18}$$

or:

$$J_{31}d\zeta, \ J_{32}d\zeta \quad \text{and } J_{33}d\zeta \tag{19}$$

and a line integral is transformed as follows:

$$\int_{\zeta\text{-edge}} \vec{A} \cdot \vec{d\ell} = \int_{\text{line } \xi = \xi_o,\ \eta = \eta_o} (A_x J_{31} + A_y J_{32} + A_z J_{33})d\zeta \tag{20}$$

Similarly:

$$\int_{\xi\text{- edge}} \vec{A} \cdot \vec{d\ell} = \int_{\text{line } \eta=\eta_o,\zeta=\zeta_o} (A_x J_{11} + A_y J_{12} + A_z J_{13}) d\xi \qquad (21)$$

$$\int_{\eta\text{- edge}} \vec{A} \cdot \vec{d\ell} = \int_{\text{line } \xi=\xi_o,\zeta=\zeta_o} (A_x J_{21} + A_y J_{22} + A_z J_{23}) d\eta \qquad (22)$$

For a surface integral, the domain of integration will be usually an element facet. Consider an element facet defined by $\xi = \xi_o$. The elements of line on such a facet are $(\partial\vec{r}/\partial\eta)d\eta$ and $(\partial\vec{r}/\partial\zeta)d\zeta$, and thus the element of surface is:

$$\vec{ds}_\xi = \left(\frac{\partial\vec{r}}{\partial\eta}\right) \times \left(\frac{\partial\vec{r}}{\partial\zeta}\right) d\eta d\zeta \qquad (23)$$

The cartesian components of $\vec{ds}$ can be obtained from the usual determinantal expression of the vector product:

$$\vec{ds}_\xi = \begin{vmatrix} \vec{i} & \vec{j} & \vec{k} \\ \partial x/\partial\eta & \partial y/\partial\eta & \partial z/\partial\eta \\ \partial x/\partial\zeta & \partial y/\partial\zeta & \partial z/\partial\zeta \end{vmatrix} d\eta d\zeta \qquad (24)$$

or:

$$\vec{ds}_\xi = \begin{vmatrix} \vec{i} & \vec{j} & \vec{k} \\ J_{21} & J_{22} & J_{23} \\ J_{31} & J_{32} & J_{33} \end{vmatrix} d\eta d\zeta \qquad (25)$$

If ξ, η, ζ is a right-handed system, then $\vec{ds}$ will point in the direction of increasing ξ. Note that this is not necessarily the direction of the "outward normal" as required by most surface integrals. Similarly:

$$\vec{ds}_\eta = \begin{vmatrix} \vec{i} & \vec{j} & \vec{k} \\ J_{31} & J_{32} & J_{33} \\ J_{11} & J_{12} & J_{13} \end{vmatrix} d\xi d\zeta \tag{26}$$

$$\vec{ds}_\zeta = \begin{vmatrix} \vec{i} & \vec{j} & \vec{k} \\ J_{11} & J_{12} & J_{13} \\ J_{21} & J_{22} & J_{23} \end{vmatrix} d\xi d\eta \tag{27}$$

A surface integral over an element facet normal to the ξ direction, for example, transforms as follows:

$$\int_{\xi=\text{facet}} \vec{A} \cdot \vec{ds}_\xi = \int_{\xi=\xi_o} \text{Det} \begin{vmatrix} A_x & A_y & A_z \\ J_{21} & J_{22} & J_{23} \\ J_{31} & J_{31} & J_{33} \end{vmatrix} d\eta d\zeta \tag{28}$$

using the well-known determinantal expression of the triple product. Similar expressions can be written for surface integrals over η- and ζ-facets.

V. SURFACE AND LINE ELEMENTS IN TWO-DIMENSIONAL SPACE

The solution of two-dimensional problems by the FE method frequently requires the evaluation of line and surface integrals. If $\vec{r}$ is the position vector of a point in an element under consideration, and ξ, η are the local coordinates.

$$\vec{r} \equiv \vec{r}\ (\xi, \eta) = \tilde{N}_i\ \vec{R}_i \tag{29}$$

where $\vec{R}_i$ are the position vectors of the geometric nodes of the element and $\tilde{N}_i$ the geometric shape functions. The general element of line is obtained by differentiation of (29):

$$d\vec{r} = \frac{\partial \vec{r}}{\partial \xi}\, d\xi + \frac{\partial \vec{r}}{\partial \eta}\, d\eta \tag{30}$$

which shows that $(\partial \vec{r}/\partial \xi)d\xi$ and $(\partial \vec{r}/\partial \eta)d\eta$ are line elements tangent to the ξ and η coordinate directions, respectively. These line elements point in the direction of increasing ξ and η, respectively. If the Jacobian matrix is defined in the usual way by eq.(2), the element of surface is:

$$ds = J\, d\xi d\eta \tag{31}$$

where $J = \text{Det}\ (J_{\alpha\beta})$. Equation (31) is used to transform a surface integral over a distorted element Ω, to the undistorted domain Ω° in the coordinates ξ, η, where it can be numerically evaluated.

For line integrals in two-dimensions, the domain of integration will be usually an element side. Consider an element side defined by $\xi=\xi_o$. The element of line on such a side is

$$\vec{d\ell}_\xi = \frac{\partial \vec{r}}{\partial \eta} d\eta \tag{32}$$

which has components:

$$\vec{d\ell}_\xi = \left(\frac{\partial x}{\partial \eta} d\eta \quad , \quad \frac{\partial y}{\partial \eta} d\eta \right) \tag{33}$$

The left-normal $\vec{n}_\xi$ to the side $\xi=\xi_o$ is defined in such a way that the vector $\vec{n}_\xi d\ell$ has components

$$\vec{n}_\xi d\ell = \left(- \frac{\partial y}{\partial \eta} d\eta \quad , \quad \frac{\partial x}{\partial \eta} d\eta \right) \tag{34}$$

$\vec{n}_\xi$ is a unit vector normal to the side $\xi=\xi_o$ at the point where it is evaluated, which points to the left for an observer who is on the side and faces the direction of increasing η. Line integrals are thus transformed as follows:

$$\int_{\text{edge } \xi=\xi_o} \vec{A} \cdot \vec{d\ell} = \int_{\xi=\xi_o} \left(A_x \frac{\partial x}{\partial \eta} + A_y \frac{\partial y}{\partial \eta} \right) d\eta \equiv \int_{\xi=\xi_o} \left(A_x J_{21} + A_y J_{22} \right) d\eta \tag{35}$$

$$\int_{\text{edge } \xi=\xi_o} \vec{A} \cdot \vec{n}\, d\ell = \int_{\xi=\xi_o} \left(-A_x \frac{\partial y}{\partial \eta} + A_y \frac{\partial x}{\partial \eta} \right) d\eta \equiv \int_{\xi=\xi_o} \left(-A_x J_{22} + A_y J_{21} \right) d\eta \tag{36}$$

Similarly:

$$\int_{\text{edge}} \vec{A} \cdot \vec{d\ell} = \int_{\eta=\eta_o} \left(A_x \frac{\partial x}{\partial \xi} + A_y \frac{\partial y}{\partial \xi} \right) d\xi \equiv \int_{\eta=\eta_o} \left(A_x J_{11} + A_y J_{12} \right) d\xi \qquad (37)$$

$$\int_{\text{edge}} \vec{A} \cdot \vec{n}\, d\ell = \int_{\eta=\eta_o} \left(-A_x \frac{\partial y}{\partial \xi} + A_y \frac{\partial x}{\partial \xi} \right) d\xi = \int_{\eta=\eta_o} \left(-A_x J_{12} + A_y J_{11} \right) d\xi \qquad (38)$$

Note that in expressions (36) and (38), $\vec{n}$ is the left-normal to the side. The "outward normal" required by many integrals may be equal to either $\vec{n}$ or $-\vec{n}$.

VI. COMPUTATIONAL DETAILS

In the FE method, the integrand of an integral is usually a sum of terms, each term being a product of a few factors. The factors may be a known function of the global coordinates and/or functional shape functions and their global derivatives of first, second, etc., order. The integrand I must be evaluated at each sampling point h of the element and multiplied by the weight W_h which corresponds to that point and by the determinant J_h of the Jacobian evaluated at the same point, and the results accumulated in order to obtain the value of the integral, e.g.:

$$\int_{\Omega} I dV = \int_{\Omega^\circ} IJ d\xi d\eta d\zeta \tilde{=} \sum_{h} I_h J_h W_h \qquad (39)$$

The computational strategy for programming eq.(39) consists of evaluating and storing first all quantities which depend on the type of element, for all types which exist in the problem to be solved. Next, the program runs over the elements and evaluates all quantities which depend on each particular element. For linear problems, these last quantities do not have to be stored; instead, they can be immediately used to obtain the values of the required integrals for each element; the integrals are then conveniently assembled and stored, and the integrand values are discarded.

When the problem is to be solved iteratively, (non-linear problems or time-dependent problems in which time steps are performed), it may be convenient to store all iteration-independent information, which includes both type-dependent and element-dependent quantities. However, the storage requirements for the element-dependent quantities may be very large.

The type dependent quantities are:

1 - Local coordinates of the sampling points and the associated weights: ξ_h, η_h, ζ_h, W_h.

2 - Geometric and functional shape functions $\tilde{N}_i$ and N_i evaluated at the sampling points, necessary for the

evaluation of integrands and of the coordinate transformation (1).

3 - Local derivatives of any order of the geometric and functional shape functions, evaluated at the sampling points, necessary for eq.(10) and eq.(13).

The element-dependent quantities are:

1 - Global coordinates $X_{i\alpha}$ of the nodes, necessary for eq. (1) and eq.(2).

2 - Global coordinates x_α of the sampling points, obtained from eq.(1) and necessary for the evaluation of known functions.

3 - The Jacobian matrix $J_{\alpha\beta}$, inverse $H_{\alpha\beta}$ and determinant J, important quantities necessary for almost all calculations.

4 - The global derivatives of shape functions, such as $\partial N_i/\partial x_\alpha$ obtained from eq.(10) and $\partial^2 N_i/\partial x_\alpha \partial x_\beta$ obtained from eq.(13), necesary for the evaluation of integrands.

5 - Second derivatives of global with respect to local coordinates, such as $\partial^2 x_\alpha/\partial \xi_\beta \partial \xi_\gamma$, necessary for eq.(13).

Some computations may not necessitate all the above mentioned quantities, e.g.second derivatives of any kind are used only if elements higher than linear are involved in the problem. On the other hand, each group of quantities is required complete or not required at all, e.q., either all possible derivatives $\partial N_i/\partial x_\alpha$ are required, or none is required.