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THREE-DIMENSIONAL ANALYSIS OF ELASTIC SOLIDS—I ANALYSIS PROCEDURE†

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Abstract—A method of analysis of nonhomogeneous elastic solids involving general three-dimensional states of stress is presented. The displacement equations of equilibrium based on the finite-element variational procedure are derived in the usual manner. The element shape considered is a tetrahedron with linear displacement approximations.

The main feature of this paper is the method of solution of the equilibrium equations. This method, called the alternating component iterative method, belongs to the class of block iterative schemes and is particularly suited for problems involving several dependent variables such as the ones encountered in elasticity. The method is presented in a form sufficiently general to permit the utilization of higher-order displacement approximations in the tetrahedral elements.

The alternating component iterative method is discussed in detail with respect to the following aspects: the general procedure, convergence criterion, refinement of the solution, and convergence acceleration procedure.

INTRODUCTION

THE analysis of elastic solids that involve three-dimensional stress fields has been the object of increasing concern in recent years. The development of the finite-element method as a new application of variational procedures in elasticity provided an effective tool for the analysis of a large class of problems in solid mechanics. The literature is quite extensive on this subject and it would be prohibitive to list all previous contributions [1–14].

In the general application of the finite-element variational methods, the displacement formulation of the problem is better suited for automatic computation than is the stress or the mixed formulation. By employing the variational principle of minimum total potential energy in which the element displacement field is varied consistently with the constraints on it, the displacement equations of equilibrium of the element are derived. The complete set of equilibrium equations of the entire system of elements is obtained through the superposition of the individual element relations.

The use of polynomial functions to express the element displacement patterns has been the accepted approach to this method of analysis. The choice of the number of terms in those polynomial functions is governed, with very limited degree of arbitrariness, by the kinematic characteristics of the element and by admissibility conditions of the displacement field.

In the present discussion, we are concerned with the computational problem only. To maintain completeness, however, the equilibrium equations are derived first, following the standard finite-element variational procedure. We then give a method of solution of the equilibrium equations (called the alternating component iterative method) and discuss its

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application to the three-dimensional problem at hand. In Part II [15], we deal with the influence of roundoff on the computed solution and with the convergence properties of the iterative process.

DISPLACEMENT EQUATIONS OF EQUILIBRIUM

Consider an elastic continuum occupying a region R with boundary Σ, having displacements u_i, strains ε_{ij}, stresses σ_{ij}, and body forces f_i in R. The surface tractions S_i may be prescribed over Σ_s, and on Σ_u the displacements may be known. If the relations

$$\sigma_{ij} = \left(\varepsilon_{kk} - \frac{1+\nu}{\nu}\alpha T\right)\lambda\delta_{ij} + 2\mu\varepsilon_{ij} \tag{1}$$

and

$$\varepsilon_{ij} = \frac{1}{2}\left(\frac{\partial u_i}{\partial x_j} + \frac{\partial u_j}{\partial x_i}\right) \tag{2}$$

hold in R, and the relation

$$S_i = \sigma_{ij} n_j \tag{3}$$

holds on Σ_s, then the principle of minimum potential energy can be defined by the following formula:

$$\delta\frac{1}{2}\int_R \varepsilon_{ij}\sigma_{ij}\,\mathrm{d}R = \delta\left(\int_R f_i u_i\,\mathrm{d}R + \int_\Sigma S_i u_i\,\mathrm{d}\Sigma\right). \tag{4}$$

Here

λ, μ Lamé's constants,
ν Poisson's ratio,
α the coefficient of linear thermal expansion,
T the temperature change,
δ_{ij} the Kronecker delta, and
n the unit vector normal to the surface.

The above is restricted to isotropic material behavior. If we adopt matrix notation, equations (1) and (2), respectively, can be rewritten as

$$\{\sigma\} = \frac{E}{3(1-2\nu)}[J_1](\{\varepsilon\} - \alpha T\{\delta\}) + \frac{E}{3(1+\nu)}[J_2]\{\varepsilon\} \tag{5}$$

and

$$\{\varepsilon\} = [L]\{u\}, \tag{6}$$

where $\{\sigma\}$, $\{\varepsilon\}$ and $\{u\}$ are column vectors whose components, respectively, are stresses σ_{ij}, strains ε_{ij}, and displacements u_i; $[L]$ is a matrix differential operator given in the Appendix; E and ν are Young's modulus and Poisson's ratio, respectively; $[J_1]$ and $[J_2]$ are symmetric matrices given in the Appendix; and $\{\delta\}$ is the Kronecker delta written as a column vector.

If we write the body forces f_i and the surface tractions S_i as column vectors $\{f\}$ and $\{S\}$, respectively, and substitute (5) and (6) into (4), we obtain

$$\delta\left(\int_R \left\{ \frac{E}{6(1-2\nu)} \{\varepsilon\}^T [J_1](\{\varepsilon\} - 2\alpha T\{\delta\}) + \frac{E}{6(1+\nu)} \{\varepsilon\}^T [J_2] \{\varepsilon\} \right\} \mathrm{d}R \right.$$
$$\left. - \int_R \{u\}^T \{f\} \, \mathrm{d}R - \int_\Sigma \{u\}^T \{S\} \, \mathrm{d}\Sigma \right) = 0, \tag{7}$$

where the superscript T indicates the transpose of the quantity in question.†

The only unknown quantity in equation (7) is u, which, through the strain–displacement relations, gives rise to ε. We restrict the vector field u to be continuous and in C^1 over any finite subregion ΔR. Different subregions, designated in the literature as "finite elements," can in general have different material properties and different temperature distributions.

If the body can be sufficiently closely subdivided into a number of such ΔR's, then a displacement field that satisfies the continuity and differentiability conditions stated above will converge to the limit solution as ΔR's go to zero. The shape of each element is arbitrary, provided the original geometric continuity of the body is preserved.

Our purpose is to express the equilibrium state of each individual subregion ΔR as a relation between two generalized force and displacement vectors, defined only for a particular ΔR. By means of coordinate transformations these individual relations can be expressed in a common coordinate system and then superposed to obtain the equilibrium equations of the entire system.

Consider a typical element ΔR whose displacements $u_i(x)$ can be expressed in terms of coordinate functions $\phi_{i\alpha}(x)$ and the generalized coordinates b_α as follows:

$$u_i(x) = \phi_{i\alpha}(x) b_\alpha \qquad i = 1, 2, 3$$
$$\alpha = 1, 2, \ldots, r. \tag{8}$$

If we use matrix notation, equation (8) can be written as

$$u = \Phi b, \tag{9}$$

where u is a column vector function of three components, ϕ is a $3 \times r$ rectangular matrix function, and b is a vector of dimension r. From (2) and (9), the strain–displacement relations can be written as

$$\varepsilon = \psi b, \tag{10}$$

where ψ is defined in the Appendix. Substitution of (9) and (10) into (7) yields

$$\delta\left\{ \frac{E}{6(1-2\nu)} b^T \left(\int_R \psi^T J_1 \psi \, \mathrm{d}R \right) b + \frac{E}{6(1+\nu)} b^T \left(\int_R \psi^T J_2 \psi \, \mathrm{d}R \right) b \right.$$
$$\left. - \frac{E\alpha T}{3(1-2\nu)} b^T \int_R \psi^T J_1 \delta \, \mathrm{d}R - b^T \int_R \Phi^T f \, \mathrm{d}R - b^T \int \Phi^T S \, \mathrm{d}\Sigma \right\} = 0. \tag{11}$$

† To avoid crowded notation we will dispense wherever possible with the use of brackets to identify matrices.

Upon carrying out the variation in (11) we obtain

$$B = (k_1 + k_2)b, \tag{12}$$

where

$$\left.\begin{aligned} B &= \int_R \Phi^T f \, dR + \int_\Sigma \Phi^T S \, d\Sigma + \frac{E\alpha T}{3(1-2v)} \int_R \psi^T J_1 \delta \, dR, \\ k_1 &= \frac{E}{3(1-2v)} \int_R \psi^T J_1 \psi \, dR, \\ k_2 &= \frac{E}{3(1+v)} \int_R \psi^T J_2 \psi \, dR. \end{aligned}\right\} \tag{13}$$

Equation (12) expresses the equilibrium of one element ΔR in terms of generalized forces B and the generalized displacements b. In order to make further use of (12) it is necessary to transform this equation to a coordinate system common to all elements. The coordinate transformation that does this depends on the geometry and the deformation patterns of ΔR. Of all possible shapes, the tetrahedron seems to offer the best choice from the point of view of simplicity and its adaptability to irregular geometry.

The deformation field of each tetrahedron ΔR is expressed as a continuous relation between the displacements of a finite number of points (nodes) located at the surface of the tetrahedron and shared by adjacent tetrahedra. The displacements of all the nodes in the solid together with the individual element relations fully define the displacement field of the entire solid.

By evaluating equation (9) at the nodes of tetrahedron ΔR we get

$$v = \Phi_0 b, \tag{14}$$

in which v is the nodal displacement vector, and Φ_0 is a nonsingular matrix $(r \times r)$ whose elements are functions of the coordinates of the nodes. Corresponding to the nodal displacement vector v there exists a nodal force vector f that satisfies the inner product:

$$v^T f = b^T B. \tag{15}$$

In view of (14) and (15),

$$B = \Phi_0^T f \tag{16}$$

and

$$b = \Phi_0^{-1} v. \tag{17}$$

Substituting (16) and (17) into (12), we obtain

$$f = kv, \tag{18}$$

where

$$k = (\Phi_0^{-1})^T (k_1 + k_2) \Phi_0^{-1}. \tag{19}$$

By superposition of equations of type (18) we obtain the equilibrium equations of the entire solid as follows:

$$\sum_{j=1}^{J} F_l^{(j)} = \sum_{j=1}^{J} \sum_{t=1}^{r} k_{lt}^{(j)} v_t^{(j)} \qquad l = 1, 2, \ldots, N, \tag{20}$$

where the summation is taken on all elements $j = 1, 2, \ldots, J$ that contribute to node l, r is the number of displacement unknowns of each element, and N is the total number of displacement unknowns. More compactly, equation (20) can be written as

$$F = KV. \tag{21}$$

The explicit forms of the individual element relations are given in the Appendix.

SOLUTION OF EQUILIBRIUM EQUATIONS

Methods for solving systems of linear algebraic equations are often divided into direct and iterative. Combinations of both methods or versions of each method are well-known techniques [16]. Matrix inversion being excluded as a suitable technique for solving large systems, two of the most commonly used methods are Gaussian elimination and the over-relaxation iterative method, sometimes referred to as the accelerated Gauss–Seidel method. Both techniques are subject to certain limitations that seriously limit their application to three-dimensional problems. For example, although the point Gauss–Seidel method always converges for positive definite symmetric matrices (a property of K), its rate of convergence can be hopelessly small. Whereas point iteration methods may be effective for well-conditioned systems of order 1000 or less arising from two-dimensional analysis, they are not suited for three-dimensional problems. On the other hand, Gaussian elimination for symmetric band matrices is restricted to relatively small band widths (of order 400 on a 32,000-word computer) [17]. This is considered too small for three-dimensional problems.

The solution scheme presented here belongs in principle to the general class of block iterative methods. It resembles such methods in the sense that one deals with iteration on subvectors and the direct solution of lower order systems; however, it differs from these methods in certain basic ideas that will become apparent in a later discussion. The method, called here the alternating component iterative method, is primarily intended for systems of three or more dependent variables.

The alternating component iterative method

Equation (21) can be written in the following form:

$$f_i(p) = \sum_{j=1}^{m} \sum_{q=1}^{n} k_{ij}(p, q) v_j(q) \qquad \begin{matrix} p = 1, 2, \ldots, n \\ i = 1, 2, \ldots, m, \end{matrix} \tag{22}$$

where p is a field point, q is a source point, n is the number of mesh points, m is the number of dependent variables (components), and i and j refer to the dependent variables. For the special case where only the displacements are the unknowns, i and j refer to the coordinate directions 1, 2, and 3. In partitioned form, equation (22) can be written as

$$F_i(P) = \sum_{j=1}^{m} K_{ij}(P, Q) V_j(Q) \qquad i = 1, 2, \ldots, m. \tag{23}$$

In matrix notation, this equation has the form

$$\begin{Bmatrix} F_1(P) \\ F_2(P) \\ \vdots \\ F_m(P) \end{Bmatrix} = \begin{bmatrix} K_{11}(P,Q) & K_{12}(P,Q) \dots K_{1m}(P,Q) \\ K_{21}(P,Q) & K_{22}(P,Q) \dots K_{2m}(P,Q) \\ \vdots & \vdots \quad\quad \vdots \\ K_{m1}(P,Q) & K_{m2}(P,Q) \cdots K_{mm}(P,Q) \end{bmatrix} \begin{Bmatrix} V_1(Q) \\ V_2(Q) \\ \vdots \\ V_m(Q) \end{Bmatrix}. \tag{24}$$

In this equation, P and Q denote the complete lists of field and source points, respectively. The terms $F_i(P)$, $V_i(Q)$, and $K_{ij}(P,Q)$ are of order n. The partitioned matrix in (24) is symmetric; i.e. $K_{ji}(P,Q) = K_{ij}(P,Q)^T$, where T indicates matrix transpose. The subscript m denotes the number of components; i.e. in the case where the nodal values of displacement components $u_1(x)$, $u_2(x)$, and $u_3(x)$ are the primary unknowns, $m = 3$.

It should be noted that equations (23) and (24), although sparse, are not, in the form indicated, band systems. If the list of mesh points P can be partitioned into point groups $P_1, P_2, \dots, P_M$, where coupling of one group extends to the two adjacent groups only, equation (24) can be partitioned further as follows:

$$F_i(P_\alpha) = \sum_{j=1}^{m} \sum_{\beta=1}^{M} K_{ij}(P_\alpha, Q_\beta) V_j(Q_\beta) \qquad \begin{matrix} \alpha = 1, 2, \dots, M \\ i = 1, 2, \dots, m. \end{matrix} \tag{25}$$

In this form, the component matrices $K_{ij}(P,Q)$ in equation (24) are block-tridiagonal; i.e. $K_{ij}(P_\alpha, Q_\beta)$ are null matrices for $(\alpha+1) < \beta < (\alpha-1)$. If we dispense temporarily with the use of the symbols P and Q to identify lists of field and source points, a single-matrix equation of (24) can be written as

$$F_i = \sum_{j=1}^{i-1} K_{ij} V_j + K_{ii} V_i + \sum_{j=i+1}^{m} K_{ij} V_j; \tag{26}$$

no summation on i is implied. If we solve for V_i from (26), we have

$$V_i = K_{ii}^{-1} \left[F_i - \sum_{j=1}^{i-1} K_{ij} V_j - \sum_{j=i+1}^{m} K_{ij} V_j \right]. \tag{27}$$

Applying the Gauss–Seidel iteration procedure to (27), we obtain

$$V_i^{(s+1)} = K_{ii}^{-1} \left[F_i - \sum_{j=1}^{i-1} K_{ij} V_j^{(s+1)} - \sum_{j=i+1}^{m} K_{ij} V_j^{(s)} \right], \tag{28}$$

where s refers to the sth cycle in the iteration sequence. Rather than using equation (28) to evaluate the $(s+1)$th vector iterate, we use the following equation:

$$V_i^{(s+1)} = V_i^{(s)} + \omega \Delta V_i^{(s+1)}, \tag{29}$$

where ω is a positive number between unity and two, referred to in the literature as the over-relaxation factor, and $\Delta V_i^{(s+1)}$ is obtained from (28) by subtracting $V_i^{(s)}$ from both sides of the equation,

$$\Delta V_i^{(s+1)} = K_{ii}^{-1}\left[F_i - \sum_{j=1}^{i-1} K_{ij}V_j^{(s+1)} - \sum_{j=i}^{m} K_{ij}V_j^{(s)}\right]. \tag{30}$$

The matrices in equation (30) are of order n that for problems of practical interest exceed 3000. Therefore, equation (30) would seem rather useless since it contains the inverse of a matrix of order 3000. The explicit inverses of the K_{ii}'s will not be required, however.

Defining a residual load vector

$$R_i^{(s+1)} = F_i - \sum_{j=1}^{i-1} K_{ij}V_j^{(s+1)} - \sum_{j=i}^{m} K_{ij}V_j^{(s)}, \tag{31}$$

and combining equations (30) and (31) leads to

$$R_i^{(s+1)} = K_{ii}\Delta V_i^{(s+1)}. \tag{32}$$

In each step we deal with the direct solution of m symmetric systems, each of which is of order N/m. The unknowns are the changes in displacements $\Delta V_i^{(s)}$ that result from the load vectors $R_i^{(s)}$ $(i = 1, 2, \ldots, m)$. For the total system, we have

$$\begin{Bmatrix} R_1 \\ R_2 \\ \vdots \\ R_m \end{Bmatrix}^{(s+1)} = \begin{Bmatrix} F_1 \\ F_2 \\ \vdots \\ F_m \end{Bmatrix} - \begin{bmatrix} 0 & & & \\ K_{21} & 0 & & \\ \vdots & \ddots & \ddots & \\ K_{m1} & \cdots & K_{m,m-1} & 0 \end{bmatrix} \begin{Bmatrix} V_1 \\ \cdot \\ \vdots \\ V_m \end{Bmatrix}^{(s+1)} - \begin{bmatrix} K_{11} & \cdots & K_{1m} \\ 0 & K_{22} \cdots & K_{2m} \\ \vdots & & \vdots \\ 0 & \cdots & K_{mm} \end{bmatrix} \begin{Bmatrix} V_1 \\ V_2 \\ \vdots \\ V_m \end{Bmatrix}^{(s)} \tag{33}$$

or

$$R^{(s+1)} = F - K_L V^{(s+1)} - (K_D + K_U)V^{(s)}, \tag{34}$$

where K_D, K_L, and K_U, respectively, are block-diagonal, strictly lower-triangular, and strictly upper-triangular matrices defined by (33). The changes in displacements are the solution of the following block-diagonal system:

$$\begin{Bmatrix} R_1 \\ \vdots \\ R_m \end{Bmatrix}^{(s+1)} = \begin{bmatrix} K_{11} & & \\ & \ddots & \\ & & K_{mm} \end{bmatrix} \begin{Bmatrix} \Delta V_1 \\ \vdots \\ \Delta V_m \end{Bmatrix}^{(s+1)} \tag{35}$$

or

$$R^{(s+1)} = K_D \Delta V^{(s+1)}. \tag{36}$$

The diagonal blocks K_{ii} are symmetric band matrices that can be partitioned into block tridiagonal matrices of the form

$$\begin{Bmatrix} R(P_1) \\ R(P_2) \\ \cdot \\ \cdot \\ \cdot \\ \cdot \\ \cdot \\ R(P_M) \end{Bmatrix}_i^{(s+1)} = \begin{bmatrix} K(P_1,Q_1) & K(P_1,Q_2) & 0 & \cdot & \cdot & \cdot & \cdot & 0 \\ K(P_2,Q_1) & K(P_2,Q_2) & K(P_2,Q_3) & 0 & \cdot & \cdot & \cdot & \cdot \\ 0 & K(P_3,Q_2) & K(P_3,Q_3) & K(P_3,Q_4) & 0 & \cdot & \cdot & \cdot \\ \cdot & 0 & \cdot & \cdot & \cdot & \cdot & \cdot & \cdot \\ \cdot & \cdot & 0 & \cdot & \cdot & \cdot & 0 & \cdot \\ \cdot & \cdot & \cdot & 0 & \cdot & \cdot & \cdot & 0 \\ \cdot & \cdot & \cdot & \cdot & \cdot & \cdot & \cdot & K(P_{M-1},Q_M) \\ 0 & \cdot & \cdot & \cdot & \cdot & 0 & K(P_M,Q_{M-1}) & K(P_M,Q_M) \end{bmatrix}_{ii} \begin{Bmatrix} \Delta V(Q_1) \\ \Delta V(Q_2) \\ \cdot \\ \cdot \\ \cdot \\ \cdot \\ \cdot \\ \Delta V(Q_M) \end{Bmatrix}_i^{(s+1)} \tag{37}$$

where P_α and Q_α are the lists of field and source points in the αth block. In the above

$$K_{ii}(P_\alpha, Q_\beta) = K_{ii}(P_\beta, Q_\alpha). \tag{38}$$

The triangular decomposition of (37) yields the following pair of equations:

$$L_i R_i^{*(s+1)} = R_i^{(s+1)} \tag{39}$$

and

$$U_i \Delta V_i^{(s+1)} = R_i^{*(s+1)}, \tag{40}$$

from which we obtain

$$\Delta V_i^{(s+1)} = U_i^{-1} L_i^{-1} R_i^{(s+1)}. \tag{41}$$

U_i and L_i are given by

$$U_i = \begin{bmatrix} K^*(P_1,Q_1) & K(P_1,Q_2) & 0 & \cdot & \cdot & \cdot & 0 \\ 0 & K^*(P_2,Q_2) & K(P_2,Q_3) & 0 & \cdot & \cdot & 0 \\ 0 & 0 & \cdot & \cdot & 0 & \cdot & \cdot \\ 0 & 0 & 0 & \cdot & \cdot & 0 & \cdot \\ 0 & & & 0 & \cdot & \cdot & 0 \\ 0 & & & & 0 & \cdot & \cdot \\ 0 & \cdot & \cdot & \cdot & \cdot & 0 & K^*(P_M,Q_M) \end{bmatrix} \tag{42}$$

and

$$L_i = \begin{bmatrix} I & 0 & \cdot & \cdot & & & \cdot & 0 \\ K(P_2,Q_1)K^*(P_1,Q_1)^{-1} & I & & & & & & \\ 0 & K(P_3,Q_2)K^*(P_2,Q_2)^{-1} & I & 0 & & & \cdot & 0 \\ \cdot & 0 & \cdot & \cdot & & & 0 & \cdot \\ \cdot & \cdot & 0 & \cdot & & & \cdot & 0 \\ 0 & \cdot & \cdot & 0 & K(P_M,Q_{M-1})K^*(P_{M-1},Q_{M-1})^{-1} & & & I \end{bmatrix} \tag{43}$$

where I is the identity matrix and the $K^*_{ii}(P_\alpha, Q_\alpha)$ are given by

$$K^*_{ii}(P_\alpha, Q_\alpha) = K_{ii}(P_\alpha, Q_\alpha) - K_{ii}(P_{\alpha-1}, Q_\alpha)^T \cdot K^*_{ii}(P_{\alpha-1}, Q_{\alpha-1})^{-1} \cdot K_{ii}(P_{\alpha-1}, Q_\alpha). \tag{44}$$

Although U_i and L_i are sparse block-upper and block-lower triangular matrices, their inverses are full block-triangular matrices; therefore, it is impractical to use equation (41) to determine $\Delta V_i^{(s+1)}$. Instead, we first solve for $R_i^{*(s+1)}$ from (39) and then determine $\Delta V_i^{(s+1)}$ from equation (40). The procedure is thus reduced to the solution of two triangular systems. The solution of (39) is effected through the successive application of the following recursion formula:

$$R_i^*(P_\alpha)^{(s+1)} = R_i(P_\alpha)^{(s+1)} - K_{ii}(P_{\alpha-1}, Q_\alpha)^T \cdot K^*_{ii}(P_{\alpha-1}, Q_{\alpha-1})^{-1} \cdot R_i^*(P_{\alpha-1})^{(s+1)} \tag{45}$$

$$1 \leq \alpha \leq M$$

Similarly, from equation (40),

$$\Delta V_i(Q_\alpha)^{(s+1)} = K^*_{ii}(P_\alpha, Q_\alpha)^{-1} \left[R_i^*(P_\alpha)^{(s+1)} - K_{ii}(P_\alpha, Q_{\alpha+1}) \cdot \Delta V_i(Q_{\alpha+1})^{(s+1)}\right] \quad 1 \leq \alpha \leq M, \tag{46}$$

which, together with equation (29), determines the $(s+1)$th vector iterate.

Convergence criterion

Returning to equations (28) and (29), we can combine the two into a single equation as follows:

$$K_{ii}V_i^{(s+1)} = K_{ii}V_i^{(s)} + \omega\left\{F_i - \sum_{j=1}^{i-1} K_{ij}V_j^{(s+1)} - \sum_{j=i+1}^{m} K_{ij}V_j^{(s)} - K_{ii}V_i^{(s)}\right\}. \tag{47}$$

Using previous notation,

$$(K_D + \omega K_L)V^{(s+1)} = [(1-\omega)K_D - \omega K_U]V^{(s)} + \omega F, \tag{48}$$

where K_L, K_U, and K_D are given by equations (33) and (35). Introducing the following definition for the sth error vector,

$$\varepsilon^{(s)} = V^{(s)} - V, \tag{49}$$

and substituting (49) into (48), we obtain, after some simple manipulation,

$$\varepsilon^{(s+1)} = A\varepsilon^{(s)}, \tag{50}$$

where

$$A = [I + \omega K_D^{-1}K_L]^{-1}[(1-\omega)I - \omega K_D^{-1}K_U]. \tag{51}$$

It follows that by successive substitution in (50) we have

$$\varepsilon^{(s)} = A^s\varepsilon^{(0)}. \tag{52}$$

This system converges for any $\varepsilon^{(0)}$ provided

$$\lim_{s\to\infty} A^s = 0. \tag{53}$$

It is well known that (53) holds if, and only if, the eigenvalues of A are of modulus less than unity. This condition is guaranteed by a theorem of Ostrowski [18], which can be stated as

follows: Let $K = K_D + K_L + K_U$ be an $n \times n$ Hermitian matrix, where K_D is Hermitian and positive definite and where $K_D + \omega K_L$ is nonsingular for $0 \leq \omega \leq 2$; then, $\rho(A) < 1$ if, and only if, K is positive definite and $0 < \omega < 2$. The spectral radius of A, $\rho(A)$, is defined by

$$\rho(A) = \max_{1 \leq i \leq n} |\lambda_i|, \tag{54}$$

where λ_i is an eigenvalue of A. It is obvious that all the conditions of the theorem are satisfied and therefore (52) is convergent.

From a practical standpoint we need to know when convergence has been achieved. For this we require a convergence criterion that can be expressed in terms of computed quantities. From (49) and (50) we have

$$\Delta V^{(s)} = (A - I)\varepsilon^{(s-1)}, \tag{55}$$

or in terms of $\varepsilon^{(0)}$

$$\Delta V^{(s)} = (A - I)A^{s-1}\varepsilon^{(0)}. \tag{56}$$

By virtue of (53), we have

$$\lim_{s \to \infty} \Delta V^{(s)} = 0. \tag{57}$$

In view of (36), equation (57) implies

$$\lim_{s \to \infty} R^{(s)} = 0. \tag{58}$$

In practice it is more convenient to use the following relation in place of (58):

$$\lim_{s \to \infty} \|R^{(s)}\| = 0, \tag{59}$$

where $\|R^{(s)}\|$ is a suitable norm of $R^{(s)}$. Of the three commonly known norms defined by

$$\|X\|_q = (|x_1|^q + |x_2|^q + \cdots + |x_N|^q)^{1/q} \qquad q = 1, 2, \infty, \tag{60}$$

where $\|X\|_\infty$ is interpreted as $\max|x_i|$, the 1-norm is more useful from the point of view of making a judgment on the amount of average error incurred. Condition (59) becomes

$$\lim_{s \to \infty} \|R\|_1^{(s+1)} = \sum_{i=1}^{m} \sum_{\alpha=1}^{M} \|R_i(P_\alpha)\|_1^{(s)} = 0. \tag{61}$$

In this computational procedure a zero norm is not only unattainable but also unnecessary. It is sufficient that $\|R\|^{(s+1)}$ becomes small enough that the errors in displacements and stresses are insignificant. Normally, the limit value of $\|R\|_1$ is an input quantity that must be estimated in advance.

Extrapolation procedure

Convergence of the iterative process in certain cases can be substantially improved by means of the following extrapolation procedure.

Let $X_1, X_2, \ldots, X_N$ be the eigenvectors of A corresponding to the eigenvalues $\lambda_1 > \lambda_2, \ldots, > \lambda_N$. An eigenvector expansion of $\varepsilon^{(0)}$ yields

$$\varepsilon^{(0)} = \sum_{i=1}^{N} c_i X_i. \tag{62}$$

Substitution of (56) into (62) gives

$$\Delta V^{(s+1)} = \sum_{i=1}^{N} (\lambda_i - 1)\lambda_i^s c_i X_i. \tag{63}$$

From (63) we have

$$\Delta V^{(s+1)} = \lambda_1^s \sum_{i=1}^{N} (\lambda_i - 1)\left(\frac{\lambda_i}{\lambda_1}\right)^s c_i X_i. \tag{64}$$

For sufficiently large s, the terms $(\lambda_i - 1)(\lambda_i/\lambda_1)^s$, $2 \leq i \leq N$, become small compared with $(\lambda_1 - 1)$. Hence, (64) gives

$$\Delta V^{(s+1)} \doteq \lambda_1^s(\lambda_1 - 1)c_1 X_1, \tag{65}$$

and for the jth element of $\Delta V^{(s+1)}$ we have, within first order approximation,

$$\Delta v_j^{(s+1)} \doteq \lambda_1^s(\lambda_1 - 1)c_1 x_{j1} \qquad 1 \leq j \leq N. \tag{66}$$

This recursion formula leads to

$$\frac{\Delta v_j^{(s)}}{\Delta v_j^{(s+1)}} = \left(\frac{\Delta v_j^{(r+s)}}{\Delta v_j^{(s)}}\right)^{1/r} \qquad r = 1, 2, \ldots. \tag{67}$$

After substituting (67) into (29) and performing simple manipulation, we obtain

$$v_j^{(r+s)} = v_j^{(s+1)} + \omega \Delta v_j^{(s)} \sum_{i=2}^{r} \left(\frac{\Delta v_j^{(s+1)}}{\Delta v_j^{(s)}}\right)^i \qquad \begin{matrix} 1 \leq j \leq N \\ r = 2, 3, \ldots. \end{matrix} \tag{68}$$

Equation (68) is applied to each element of the displacement vector $V = (v_1, v_2, \ldots, v_N)$.

This extrapolation formula is based on the assumption that the vector $\Delta V^{(s)}$ contains only one term [equation (65)] rather than N terms as given by equation (64). The validity of this assumption is dependent on the value of s and on the distribution and relative magnitudes of the eigenvalues of A, particularly those with the largest absolute values. Experience with this formula indicates that it can be successfully applied after only a few cycles.

Refinement of the solution

The alternating-component iterative method is intended for large systems of order 15,000 or more and of band widths that exceed 1000. For linear systems of this size, round-off becomes an important consideration, especially if the system is ill-conditioned. (The general problem of the influence of roundoff error on various aspects of this method is discussed in [15].) Here we deal with a correction procedure to reduce roundoff errors in the final solution.

We define $r_i^{(s)}$ and $\delta V_i^{(s)}$, the rounding error vectors in the computed $R_i^{(s)}$ and $\Delta V_i^{(s)}$, respectively, by the relations

$$r_i^{(s)} = \bar{R}_i^{(s)} - R_i^{(s)} \tag{69}$$

and

$$\delta V_i^{(s)} = \Delta \bar{V}_i^{(s)} - \Delta V_i^{(s)}, \tag{70}$$

where $\bar{R}_i^{(s)}$ and $\Delta\bar{V}_i^{(s)}$ are, respectively, the exact (free of roundoff) residual and incremental displacement vectors of the ith component. Substituting (69) and (70) into (35) we obtain

$$\bar{R}_i^{(s)} - r_i^{(s)} = K_{ii}\Delta\bar{V}^{(s)} - K_{ii}\delta V^{(s)}, \tag{71}$$

from which we have

$$r_i^{(s)} = K_{ii}\delta V_i^{(s)}. \tag{72}$$

We see that the rounding error vectors satisfy the same equations. Therefore, from (41) and (72) we obtain

$$\delta V_i^{(s)} = U_i^{-1}L_i^{-1}r_i^{(s)}. \tag{73}$$

A one-cycle correction will then give

$$\Delta\bar{V}_i^{(s)} = \Delta V_i^{(s)} + \delta V_i^{(s)}. \tag{74}$$

Equation (74) is valid only if no further roundoff errors are introduced in calculating $\delta V_i^{(s)}$. Since this is impossible, we may resort to an iterative procedure for further improvement. Even then, because we use the computed triangular matrices U_i and L_i, the process converges to a nonzero δV_i or r_i. Unless the problem is hopelessly ill-conditioned, however, the correction procedure works and in most cases one or two corrections are sufficient.

Since the iterative process tends to be somewhat self-correcting, this refinement need be applied only during the last one or two iterations. It should be pointed out that solutions for $\Delta V_i^{(s)}$ and $\delta V_i^{(s)}$ follow the same steps and utilize the same equations; furthermore, the triangular decompositions of the K_{ii}'s are carried out prior to the iteration, usually in singleprecision arithmetic. A one-cycle correction is therefore equivalent to carrying out one iteration in double precision using the single-precision L_i and U_i. This correction cycle is outlined as follows:

1. Compute $\bar{r}_i^{(s)}$ from the matrix equation

$$\bar{r}_i(P)^{(s)} = F_i(P) - \sum_{j=1}^{i-1}\sum_{Q=1}^{M} K_{ij}(P,Q)V_j(Q)^{(s)} - \sum_{j=i}^{M}\sum_{Q=1}^{M} K_{ij}(P,Q)V_j(Q)^{(s-1)}. \tag{75}$$

Here $\bar{r}_i(P)^{(s)}$ differs from $\bar{R}_i(P)^{(s)}$ only in that it is computed in double-precision. If infinite-precision calculations were performed, $\bar{r}_i(P)^{(s)}$ would, by definition, be equal to $\bar{R}_i(P)^{(s)}$.

2. Using the single-precision L_i, compute $\bar{r}_i^*(P)^{(s)}$ from

$$\bar{r}_i^*(P)^{(s)} = L_i^{-1}\bar{r}_i(P)^{(s)}. \tag{76}$$

3. Using the single-precision U_i, compute $\delta\bar{V}_i(P)^{(s)}$ from

$$\delta\bar{V}_i(P)^{(s)} = U_i^{-1}\bar{r}_i^*(P)^{(s)}. \tag{77}$$

Here $\delta\bar{V}_i(P)^{(s)}$ is defined in a manner similar to $\bar{r}_i(P)^{(s)}$.

4. The refined ith displacement component is then

$$\bar{V}_i^{(s)} = V_i^{(s-1)} + \omega\delta\bar{V}_i^{(s)}. \tag{78}$$

5. Repeat steps 1 through 4 for all components $i = 1, 2, \ldots, m$.

Although this procedure is recommended for the last one or two iterations it can be applied to all iterations. The arithmetic process involves only inner-product accumulation that can be performed in double-precision and then stored as single-precision numbers.

As a result of this truncation process the roundoff error in each number will not exceed $\frac{1}{2}2^{-t}$, where t is the number of binary figures in a single-precision representation. In our experience this refinement is unnecessary for well-conditioned problems with up to 10,000 unknowns.

EXAMPLES

Example 1

Figure 1 shows the geometry and the finite-element mesh of homogeneous isotropic solid analyzed for the effect of uniform temperature drop equivalent to 0·01 free contraction strain. The solid is assumed to be partially bonded to a rigid case, as shown in the figure. The geometry and material properties chosen closely represent those of a solid rocket propellant grain subjected to uniform shrinkage in the presence of partial bond failure between the grain and the case. The cylindrical structure, with a spherical head, contains a full diametrical slot which extends throughout its length. Symmetry permitted the analysis of a 90° section only. Although Fig. 1 shows only the head, the analysis extended two diameters below the head junction. Long-cylinder solution was used as the boundary condition at the base of the solid.

Stresses in the form of contour plots are given in Figs. 2, 3 and 4. The problem contained 11,100 displacement unknowns and a total bandwidth of 1050. An elastic modulus of 1000 psi and Poisson's ratio of 0·495 were used. The high Poisson's ratio caused ill-conditioning because of the large differences between the bulk and shear moduli, but satisfactory convergence was obtained in 25 cycles.

Example 2

A cantilever beam of rectangular cross section and a span-to-depth ratio of 10 was analyzed for end shear load. The applied shear stresses were distributed consistently with the three-dimensional beam theory. Although this example is of no real practical importance, it presents an interesting computational problem. It is slowly convergent; consequently, it provides a severe test for the extrapolation formula (68). To eliminate the arbitrariness of the upper limit of the series in equation (68), r is always set equal to s.

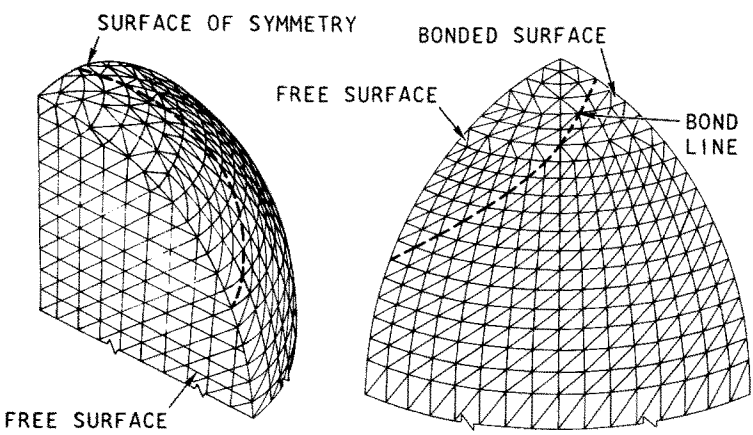

FIG. 1. Example 1, finite-element mesh.

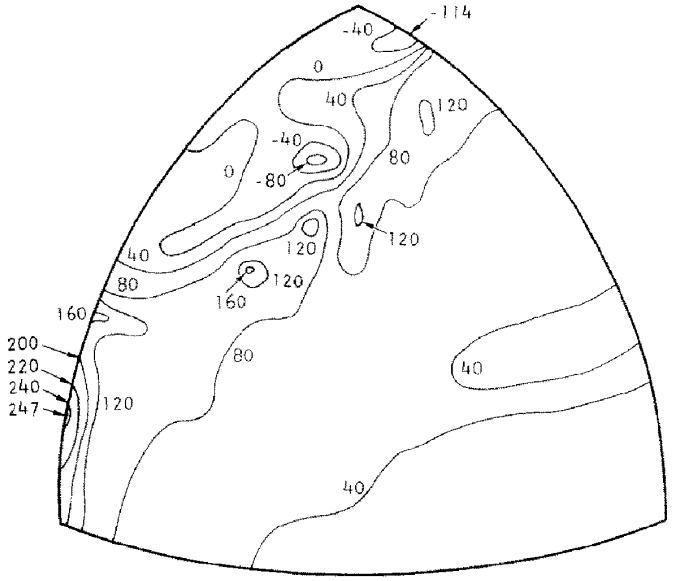

FIG. 2. Example 1, radial stresses.

The problem contains 10,530 displacement unknowns, grouped into 3 components, and has a total bandwidth of 1050. The quantities to be investigated are the following vector norms: the 1-norm of the residual vector $\|R\|_1$, the ∞-norm of the displacement vector $\|V\|_\infty$, and the ∞-norm of the displacement increment vector $\|\Delta V\|_\infty$. If we consider, for illustration purposes, that these vector norms are continuous functions of the number of iteration cycles, we may then plot these quantities as shown in Fig. 5a. Ignoring the initial

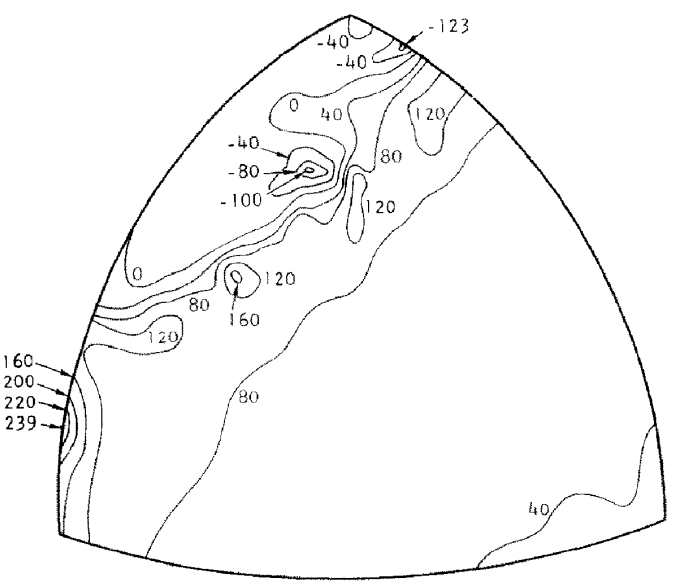

FIG. 3. Example 1, hoop stresses.

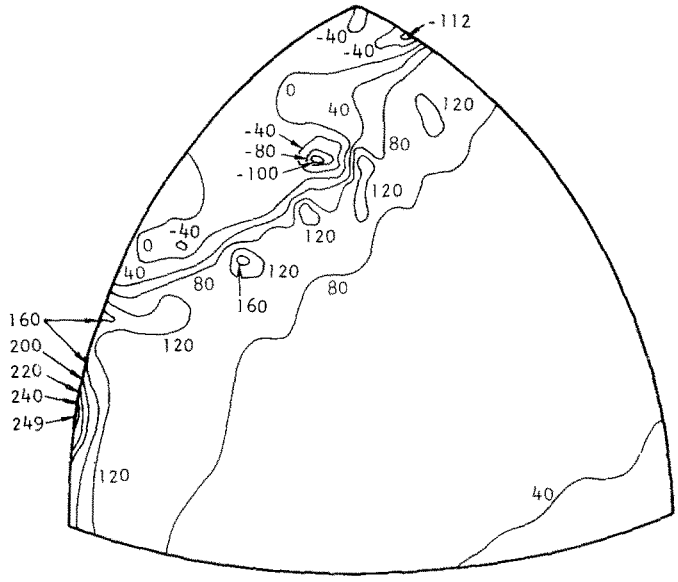

FIG. 4. Example 1, axial stresses.

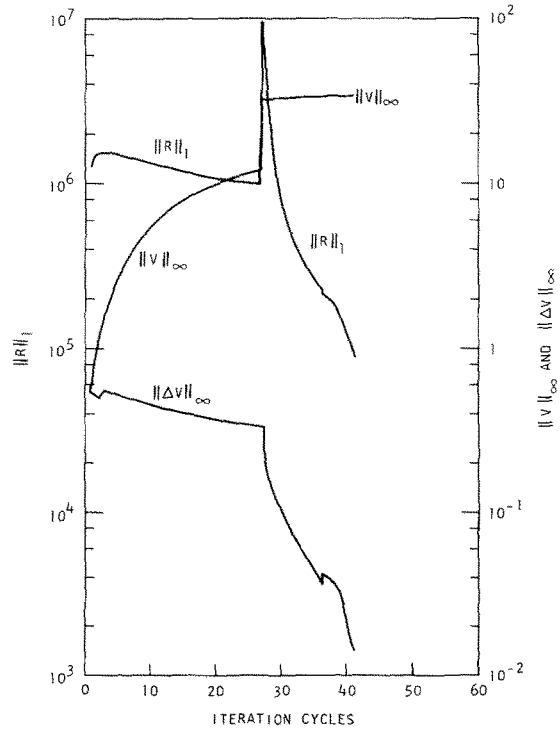

FIG. 5a. Example 2, extrapolation and convergence of the iterative solution.

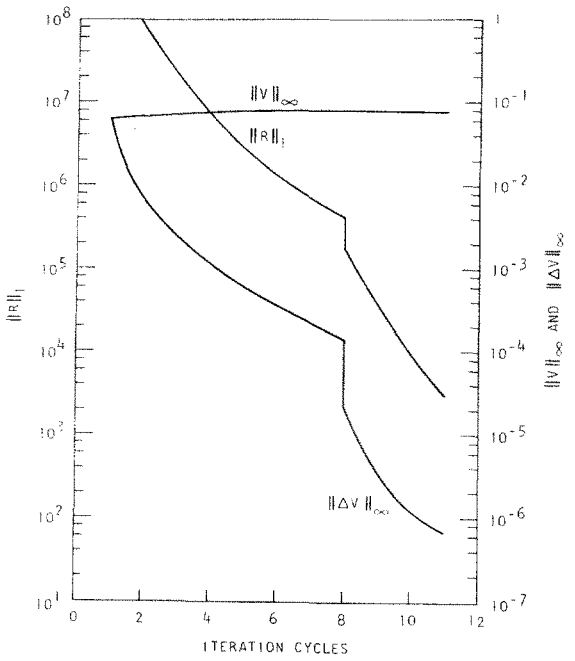

FIG. 5b. Example 3, extrapolation and convergence of the iterative solution.

apparent divergence as reflected in the curve for $\|R\|_1$, the iterative process seems to converge very slowly at a decreasing rate. At the 27th cycle, the displacement increment is of the order of 1% of the exact solution and about 3% of the computed 27th vector iterate.

By applying the extrapolation formula (68), the computed norms at the end of the first cycle after extrapolation indicated substantial improvement in the iterative process. Although the norm $\|R\|_1$ increased by more than one order of magnitude, the rapid rate of convergence that followed brought $\|R\|_1$ down to its previous value in two cycles. The computed $\|V^{(27)}\|_\infty$ increased by about three times to within 2% of the exact value. At the end of the 36th cycle, $\|V^{(36)}\|_\infty$ was brought to within 0·5% of the exact solution. The largest displacement increment $\|\Delta V\|_\infty$ was close to 0·1% of the exact solution at the end of the 36th cycle.

Further improvement of the solution was effected by carrying out cycles 37 through 41 in double precision. As expected, a slight increase in $\|\Delta V\|_\infty$ occurred, but it was reduced to a value about half of that anticipated if double precision were not used. This effect implies that at this stage a large percentage of $\|\Delta V\|_\infty$ is contributed by roundoff.

It should be pointed out that Example 2 is not a typical example. Most practical problems analyzed to date showed a much faster rate of convergence. An upper limit of 15 to 20 cycles was found to apply to the great majority of problems. This point is demonstrated in the next example, which is of more practical nature.

Example 3

This example was selected at random from many analyses of several design configurations of a prestressed concrete pressure vessel. The problem contained 7000 displacement unknowns and a maximum bandwidth of 1050. Figure 5b is a plot of the vector norms of

interest: $\|R\|_1$, $\|\Delta V\|_\infty$, and $\|V\|_\infty$. Extrapolation was applied at the 8th cycle and single-precision computation was used throughout. As can be easily seen in the figure, the iterative process was improved by extrapolation. At the end of the 11th cycle, $\|R\|_1$ was decreasing at a faster rate than $\|\Delta V\|_\infty$, but the latter was only one order of magnitude larger than the limit accuracy of single-precision computations. At that stage, $\|\Delta V\|_\infty$ and $\|R\|_1$ were judged within acceptable limits and the iterative process was terminated.

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APPENDIX

The field and equilibrium equations for a tetrahedron, namely, the stress–strain relations, the displacement approximations, the strain–displacement relations, and the equilibrium equations, are given here.

As stated earlier, in the first section, the appropriate choice of the element displacement functions that locally approximate the true displacements of the solid in the region occupied by the element is basic to this method of analysis. A second point, of equal importance, is the solution of the equilibrium equations and the degree to which it influences the choice of the primary unknowns.

The simplest form of displacement approximations is one that is linear in the three coordinate variables. This simple expansion provides twelve generalized coordinates (four for each of the three displacement components, u_1, u_2 and u_3), which can be related to the displacements of the element nodes.

Higher-order displacement approximations in the form of second- or third-degree polynomials can be used. A second-degree polynomial provides ten generalized coordinates for each displacement component. These ten coordinates can be related, through a coordinate transformation, to the ten displacements defined at ten nodes (four corners, and six at the centers of the six edges of the tetrahedron).

A third-degree polynomial in the three coordinate variables contains twenty terms. In this case, several alternate choices of the nodal displacement quantities may be found. The best choice, of course, will be the one that best utilizes the features of the alternating component iterative method. As a rule, the best set of displacement coordinates is one which is defined at a minimum number of nodal points, namely, four for a tetrahedron.

Other investigators found it more convenient to use different shape elements or to use tetrahedral elements with second-degree polynomial approximations of the displacement field. The primary unknowns in these cases were taken to be the three displacements at each node, therefore requiring that additional nodes be defined. However, the alternating-component iterative method favors the fewer-nodes scheme for the following reasons: First, the alternating-component method is limited by the number of nodes in the band, i.e. by the number B/m, where B is the band width of the total stiffness matrix and m is the number of components. In the m-component scheme, therefore, the maximum band width can be $m/3$ times larger than it is in the three-component scheme. This is quite significant in view of the fact that in three-dimensional problems the band width, not the size of the system of equations, controls the accuracy and efficiency of the solution. Second, the machine solution time of the alternating method is proportional to B^2/m; therefore, for

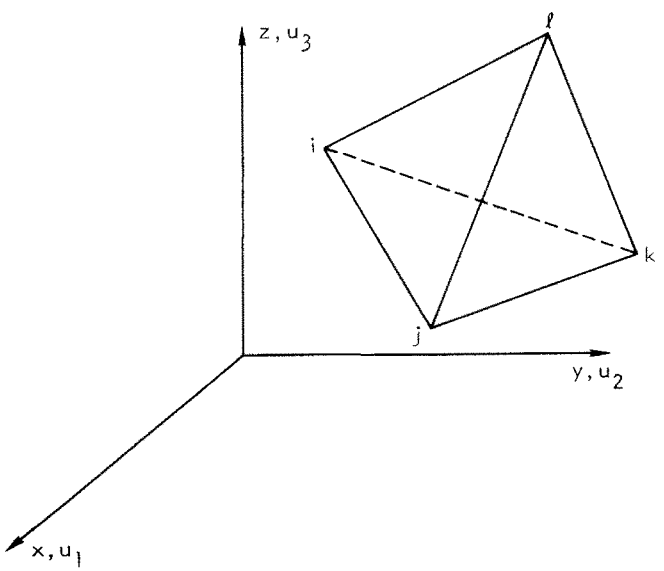

FIG. A1. Tetrahedral element.

the same number of unknowns and the same band width, a larger m is highly desirable.

It might be of interest to point out that in Gaussian elimination $m = 1$, and by the above argument Gaussian elimination is extremely inefficient for three-dimensional problems.

Although the alternating-component iterative method as presented here is valid for m components, it has only been applied to the case $m = 3$. The equations given in this Appendix are for this case only.

1. *Stress–strain relations*

The stress–strain relations [equation (5)] for the isotropic solid in Fig. A1 are explicitly given by

$$\begin{Bmatrix} \sigma_{11} \\ \sigma_{22} \\ \sigma_{33} \\ \sigma_{12} \\ \sigma_{23} \\ \sigma_{13} \end{Bmatrix} = k_0 \begin{bmatrix} 1 & 1 & 1 & 0 & 0 & 0 \\ 1 & 1 & 1 & 0 & 0 & 0 \\ 1 & 1 & 1 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 \end{bmatrix} \left[\begin{Bmatrix} \varepsilon_{11} \\ \varepsilon_{22} \\ \varepsilon_{33} \\ \varepsilon_{12} \\ \varepsilon_{23} \\ \varepsilon_{13} \end{Bmatrix} - \alpha T \begin{Bmatrix} 1 \\ 1 \\ 1 \\ 0 \\ 0 \\ 0 \end{Bmatrix} \right] + \mu_0 \begin{bmatrix} 2 & -1 & -1 & 0 & 0 & 0 \\ -1 & 2 & -1 & 0 & 0 & 0 \\ -1 & -1 & 2 & 0 & 0 & 0 \\ 0 & 0 & 0 & 3 & 0 & 0 \\ 0 & 0 & 0 & 0 & 3 & 0 \\ 0 & 0 & 0 & 0 & 0 & 3 \end{bmatrix} \begin{Bmatrix} \varepsilon_{11} \\ \varepsilon_{22} \\ \varepsilon_{33} \\ \varepsilon_{12} \\ \varepsilon_{23} \\ \varepsilon_{13} \end{Bmatrix} \tag{A1}$$

where

$$k_0 = \frac{E}{3(1-2\nu)}; \qquad \mu_0 = \frac{E}{3(1+\nu)}.$$

2. *Displacement approximations*

The displacement approximations [equation (9)] are given by

$$\begin{Bmatrix} u_1(x) \\ u_2(x) \\ u_3(x) \end{Bmatrix} = \begin{bmatrix} \phi(x) & 0 & 0 \\ 0 & \phi(x) & 0 \\ 0 & 0 & \phi(x) \end{bmatrix} \begin{Bmatrix} b_1 \\ b_2 \\ b_3 \end{Bmatrix} \tag{A2}$$

where

$$\phi(x) = [1xyz]. \tag{A3}$$

3. *Strain–displacement relations*

The strain–displacement relations [equation (6)] are explicitly given by

$$\begin{Bmatrix} \varepsilon_{11} \\ \varepsilon_{22} \\ \varepsilon_{33} \\ \varepsilon_{12} \\ \varepsilon_{23} \\ \varepsilon_{13} \end{Bmatrix} = \begin{bmatrix} \dfrac{\partial}{\partial x_1} & 0 & 0 \\ 0 & \dfrac{\partial}{\partial x_2} & 0 \\ 0 & 0 & \dfrac{\partial}{\partial x_3} \\ \dfrac{1}{2}\dfrac{\partial}{\partial x_2} & \dfrac{1}{2}\dfrac{\partial}{\partial x_1} & 0 \\ 0 & \dfrac{1}{2}\dfrac{\partial}{\partial x_3} & \dfrac{1}{2}\dfrac{\partial}{\partial x_2} \\ \dfrac{1}{2}\dfrac{\partial}{\partial x_3} & 0 & \dfrac{1}{2}\dfrac{\partial}{\partial x_1} \end{bmatrix} \begin{Bmatrix} u_1(x) \\ u_2(x) \\ u_3(x) \end{Bmatrix} \tag{A4}$$

From (A2) and (A4) we have

$$\varepsilon = \psi b, \tag{10}$$

in which

$$\psi = \begin{bmatrix} \phi_{,1} & 0 & 0 \\ 0 & \phi_{,2} & 0 \\ 0 & 0 & \phi_{,3} \\ \frac{1}{2}\phi_{,2} & \frac{1}{2}\phi_{,1} & 0 \\ 0 & \frac{1}{2}\phi_{,3} & \frac{1}{2}\phi_{,2} \\ \frac{1}{2}\phi_{,3} & 0 & \frac{1}{2}\phi_{,1} \end{bmatrix} \tag{A5}$$

where

$$\phi_{,1} = \frac{\partial \phi(x)}{\partial x_1}, \ldots \text{etc.}$$

4. *Coordinate transformation*

The coordinate transformation Φ_0[equation (14)] is obtained by evaluating (A2) at each node of the tetrahedron. This yields three matrix equations of the form

$$v_r = \phi_0 b_r \qquad r = 1, 2, 3, \tag{A6}$$

or explicitly,

$$\begin{Bmatrix} u_1^i \\ u_1^j \\ u_1^k \\ u_1^l \end{Bmatrix} = \begin{bmatrix} 1 & x_i & y_i & z_i \\ 1 & x_j & y_j & z_j \\ 1 & x_k & y_k & z_k \\ 1 & x_l & y_l & z_l \end{bmatrix} \begin{Bmatrix} b_1^1 \\ b_1^2 \\ b_1^3 \\ b_1^4 \end{Bmatrix} \tag{A7}$$

and similarly for u_2 and u_3.

Equation (14) then becomes

$$\begin{Bmatrix} v_1 \\ v_2 \\ v_3 \end{Bmatrix} = \begin{bmatrix} \phi_0 & 0 & 0 \\ 0 & \phi_0 & 0 \\ 0 & 0 & \phi_0 \end{bmatrix} \begin{Bmatrix} b_1 \\ b_2 \\ b_3 \end{Bmatrix} \tag{A8}$$

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Абстракт—Дается метод расчета неоднородных упругих тел, в общем трехмерном напряженном состоянии. Получаются, обычным способом, уравнения в перемещениях для равновесия, основанные на вариационном методе конечного элемента. Рассматривается форма элемента в виде тетраэдра с линейными приближениями для перемещений.

Главной особенностью настоящей работы является метод решения уравнений равновесия. Этот метод, называемый итерационным методом переменного компонента, принадлежит к классу блочных итерационных схем и в особенности пригоден для задач с некоторыми зависимыми переменными, которые существуют в упругости. Метод дается в достаточно общей форме, позваляющеи использовать в элементах тетраэдра приближения выших порядков для перемещений.

Обсуждается подробно итерационный метод переменного компонента по отношению к следую щим вопросам: общий процесс, критерий сходимости, обработка решения и процесс ускорения сходимости.