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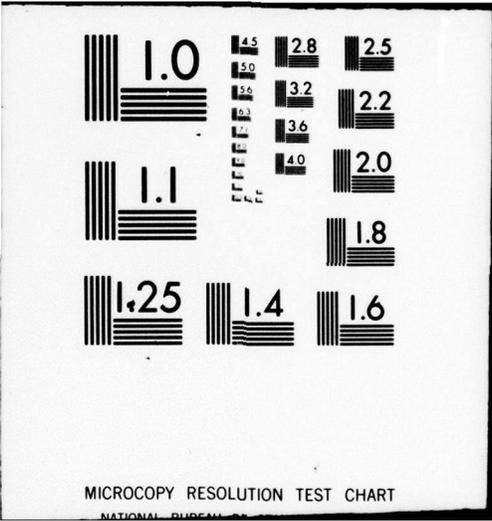
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by
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Inversion of Isoperimetric Mappings and Applications
of Computer Graphics to Three
Dimensional Finite Element Analyses

by

Charles A. Hall & Thomas A. Porosning

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RESEARCH
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DEVELOPMENT
DIVISION
JULY 1979

Institute for Computational Mathematics and Applications
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Final Scientific Report

July, 1979

INVERSION OF ISOPARAMETRIC MAPPINGS AND APPLICATIONS
OF COMPUTER GRAPHICS TO THREE DIMENSIONAL
FINITE ELEMENT ANALYSES

AFOSR CONTRACT NO. F44620-76-C-0104

June, 1976 to May, 1979

Principal Investigators: Charles A. Hall
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Graduate Research Assistants: Addison Frey *6-76 to 5-78
Frank Sledge 6-78 to 6-79

*Ph.D. in Mathematics 8-78

Thesis: "A C^1 Compatible Curved Plate Element Which Satisfies
Constant Strain".

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INVERSION OF ISOPARAMETRIC MAPPINGS AND APPLICATIONS
OF COMPUTER GRAPHICS TO THREE DIMENSIONAL
FINITE ELEMENT ANALYSES

ABSTRACT

Finite element analyses of two and three dimensional structures often require the use of curved isoparametric elements. The overall effectiveness of such analyses by large scale finite element computer programs is often handicapped by the costly and tedious job of verifying input data and the lack of a comprehensive graphical presentation of the output. This contract work involved mathematical research concerning various approaches to improving this pre- and post processing of finite element data utilizing interactive computer graphics. A key aspect of this work was the characterization of the existence of the inverses of isoparametric mappings, as well as the development of efficient algorithms for the numerical inversion of such mappings.

INVERSION OF ISOPARAMETRIC MAPPINGS AND APPLICATIONS
OF COMPUTER GRAPHICS TO THREE DIMENSIONAL
FINITE ELEMENT ANALYSES

1. INTRODUCTION

Finite element analyses of three dimensional structures with curved bounding surfaces most often require the use of curved "isoparametric brick" elements, [6]. One such brick is illustrated in Figure 1.

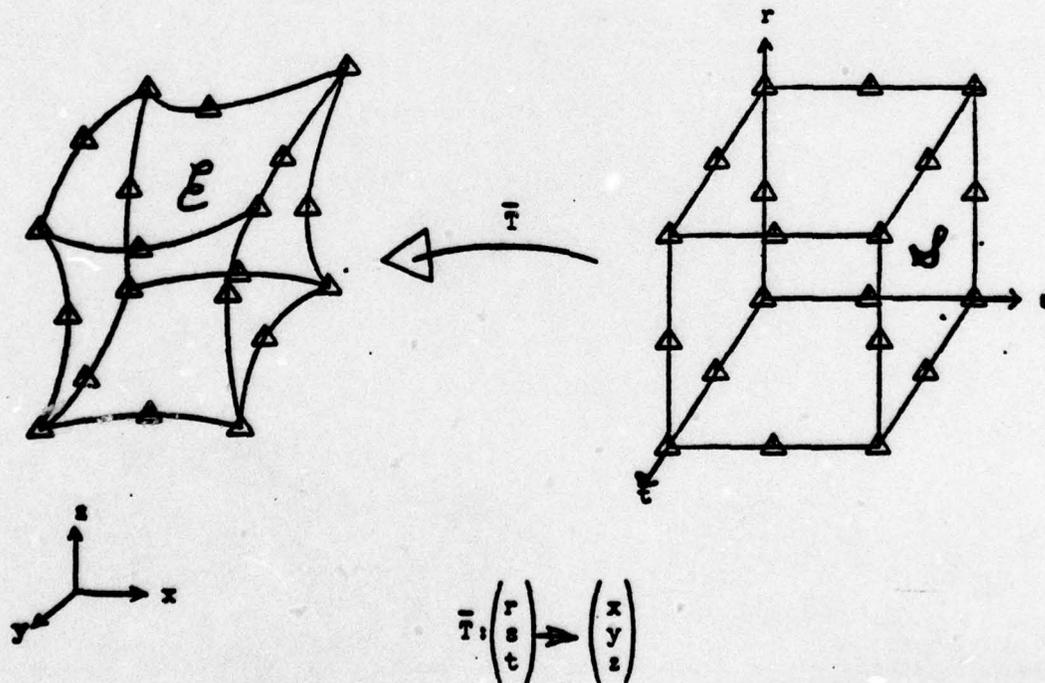


FIGURE 1. The 20-node isoparametric brick element E .

The trial functions in the finite element (or Ritz-Galerkin) method for such elements are expressed in terms of the curvilinear (or natural) coordinate system (r,s,t) and the computations of stiffness matrices, etc. are carried out in this same local system; not the global (x,y,z) system. Since the unknowns are, say, the displacements at the nodal points, there is no problem in going from the local (r,s,t) system to the global (x,y,z) system. That is, built into the transformation \bar{T} is an explicit 1-1 correspondence between the 20 nodes of \mathcal{E} and the 20 nodes of the "standard" brick $\mathcal{S}: (0,1) \times (0,1) \times (0,1)$. For example, the geometric description of \mathcal{E} includes global coordinates (x_1, y_1, z_1) of node 1 and \bar{T} associates node 1 with $(0,0,1)$ in the (r,s,t) local system. However, such an explicit relation for points other than nodes does not exist in general.

This leads to the investigation of the question of existence of an inverse mapping $\bar{T}^{-1}: \mathcal{E} \rightarrow \mathcal{S}$ as well as efficient algorithms for its evaluation. An understanding of the dependence of the invertibility of \bar{T} on the choice of nodal topology is imperative for the successful construction of finite element idealization of a given structure.

The question of the existence of an inverse itself is of interest since it is not guaranteed a priori. Heuristic techniques for checking the existence of an inverse which rely on graphics are presented in [3].

The overall effectiveness of solving three dimensional problems by multipurpose finite element computer programs is handicapped by:

(i) the costly and tedious job of setting up and verifying input data (esp. geometric data), [1,2,3,5],

(ii) the lack of a comprehensive graphical presentation of the computed stress distributions for three dimensional structures, [5,7].

By utilizing newly developed tools of numerical analysis and computer graphics, numerical methods and associated computer programs were developed which can be used in:

(i) a pre-processor mode to aid in more efficiently describing and verifying the geometric input and,

(ii) a post-processor mode to edit and plot contours of various components of stress in and perpendicular to a given plane.

We emphasize that the key to the development of such a graphics package is in fact efficient algorithms for the numerical inversion of isoparametric mappings.

2. RESULTS OF INVESTIGATION

A. PRE-PROCESSOR: VERIFICATION OF PROBLEM GEOMETRY

In preparing input for a multi-purpose finite element program the verification that the three dimensional structure has been amenably decomposed into "isoparametric" curved bricks is of utmost importance. As a means of verifying that the subdivision contains no anomalies, it is desired to have the capability of passing a given plane through the catenation of brick elements approximating the structure and viewing the resulting two-dimensional intersection.

Figure 2 illustrates the intersection of a three dimensional isoparametric brick with a plane. This figure was generated using the program PLANIT, [11,12] developed at the University of Pittsburgh. One goal of this work program was the development of computer software to plot such intersections via a CRT and/or an incremental plotter such as CALCOMP. This computer program determines the intersection of a given plane with a union of many such 20-node isoparametric elements. Cf. Figures 5 and 6.

The program PLANIT accepts as input for each element

- (1) element number,
- (11) coordinates (x_1, y_1, z_1) of the nodes,
- (111) sufficient information to determine the intersecting plane, e.g. point and normal.

The program proceeds to

- (1) determine those elements through which the plane passes;
- (11) define the curves determined by the intersection of the plane with each element from (1);

(iii) produce an orthogonal view of the region which represents the intersection of the plane with given structure;

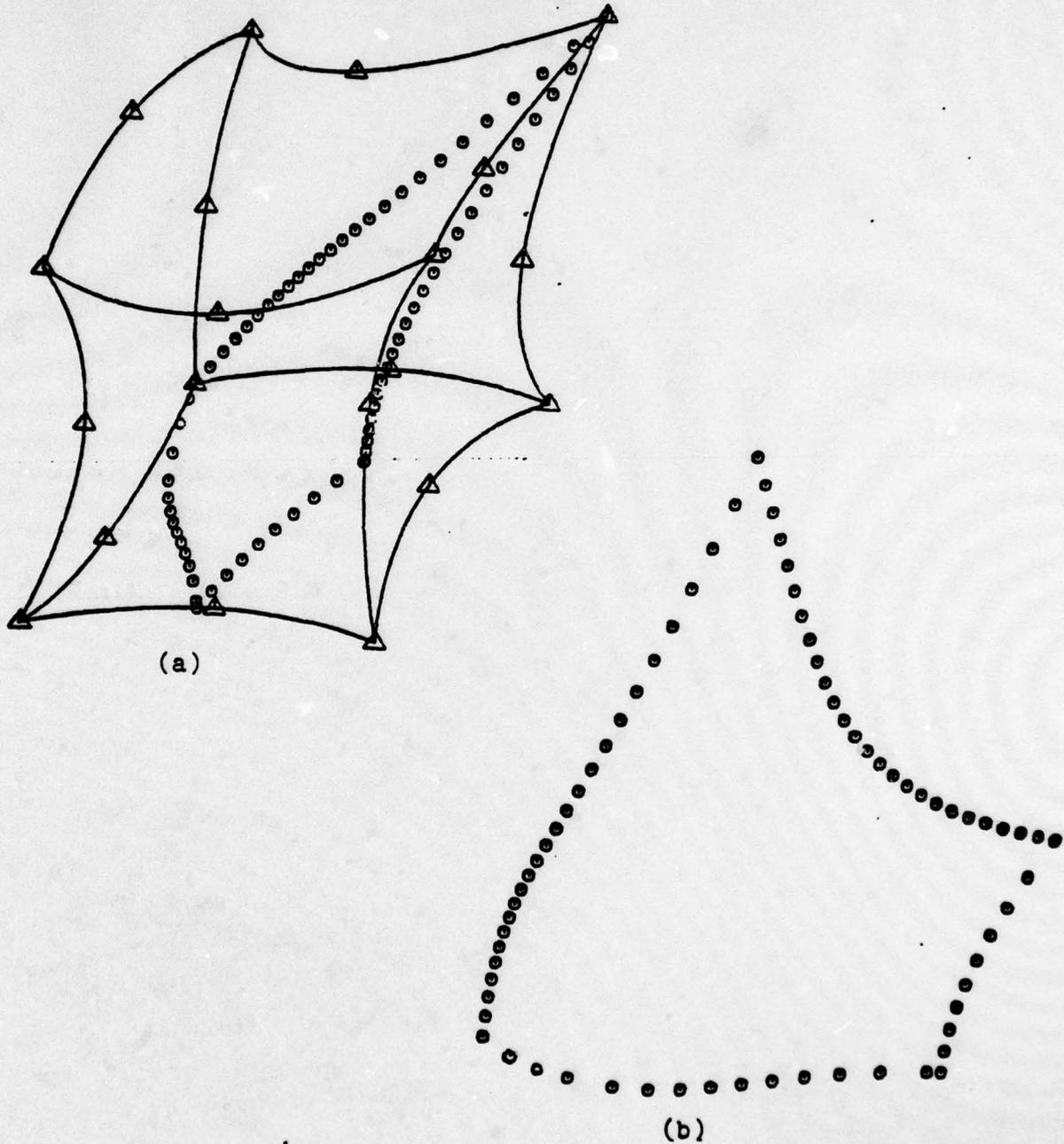


FIGURE 2

The intersection of a plane with a single 20-node brick.

(a) Isometric view. (b) View along normal to plane.

- (iv) store the information necessary to retrieve this same plane intersection (if desired) to be used in the post-processing mode to plot various stress distributions.

In order to determine the intersection of a plane

$$(1) \quad a_1x + a_2y + a_3z + a_4 = 0$$

and an element face determined by

$$(2) \quad \begin{bmatrix} X(\xi, \eta) \\ Y(\xi, \eta) \\ Z(\xi, \eta) \end{bmatrix} = \sum \phi_i(\xi, \eta) \begin{bmatrix} x_i \\ y_i \\ z_i \end{bmatrix},$$

the nonlinear equation

$$(3) \quad F(\xi, \eta) = a_1X(\xi, \eta) + a_2Y(\xi, \eta) + a_3Z(\xi, \eta) + a_4 = 0$$

is solved numerically for η as a function of ξ , say $\eta = f(\xi)$.

Given a specific value of $\xi = \xi_0$ then $F(\xi_0, \eta)$ is a quadratic in η which is easily solved. The algorithm tests if there are zero, one, or two admissible values of η . Equation (3) is obtained by substituting (2) into (1). The locus of points $(X(\xi, f(\xi)), Y(\xi, f(\xi)), Z(\xi, f(\xi)))$ determined by (3) is the desired curve \mathcal{C} in 3-space.

If \bar{n} is a unit normal to the given plane \mathcal{P} and $P_0: (X_0, Y_0, Z_0)$ is a point in the plane designated as the origin then a point $P_1: (X_1, Y_1, Z_1)$ is also in the plane \mathcal{P} if

$$\overline{(P_1 - P_0)} \cdot \bar{n} = 0.$$

(As input, \bar{n} and a point P_1 in the plane \mathcal{P} could be given, or, given three points in the plane \bar{n} could be computed.) A coordinate system is established by the orthogonal unit vectors

$$\bar{e}_1 = \frac{\overline{P_1 - P_0}}{|P_1 - P_0|}$$

$$\bar{e}_2 = \bar{n} \times \bar{e}_1$$

The curve \mathcal{C} can now be plotted in the plane \mathcal{P} relative to the established coordinate system by

$$s = (P - P_0) \cdot \bar{e}_1$$

$$t = (P - P_0) \cdot \bar{e}_2$$

where P traces over \mathcal{C} .

Figures 3 and 4 illustrate two other intersections of single bricks with a plane. As indicated, the boundary of intersection may be disjoint and the intersection may not be simply connected, i.e., it may be the union of disjoint lines or even single points. For that reason, one must be extremely careful in connecting the computed points of the boundary of the intersection by a curve. Such decisions are best made interactively by the analyst with the aid of a graphics terminal.

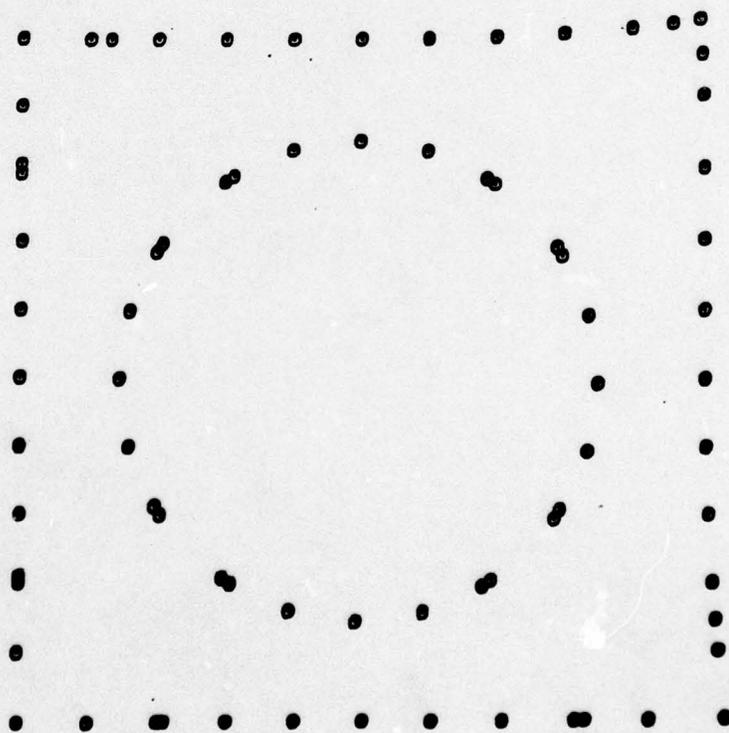
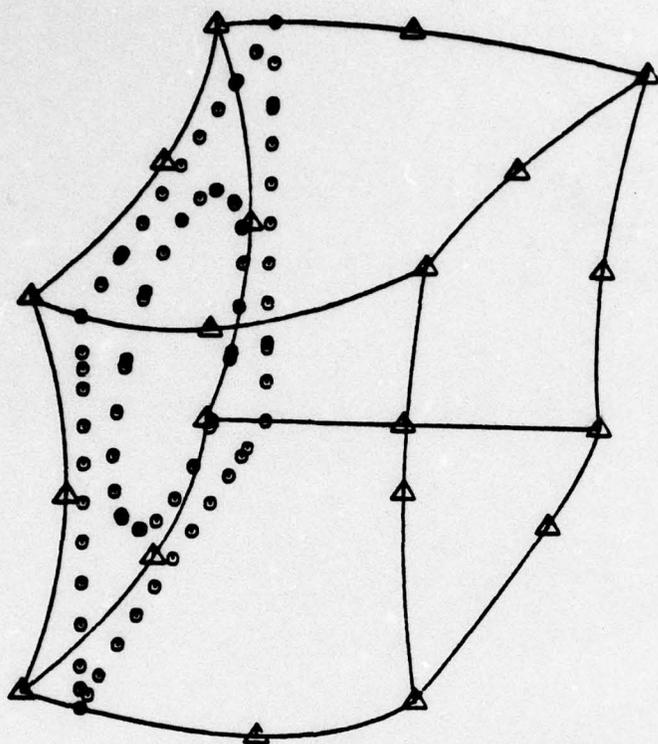


FIGURE 3

This intersection of a 20-node brick and a plane is annular in shape.

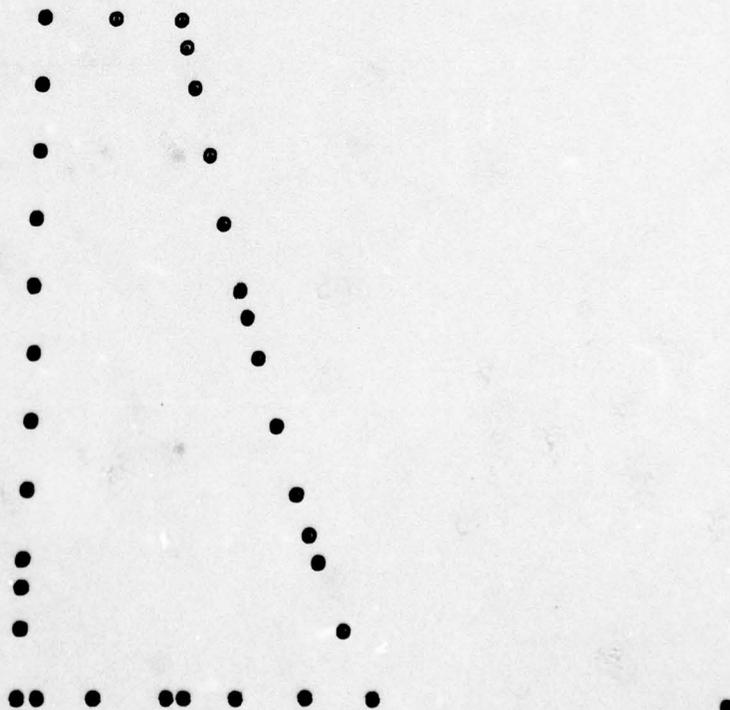
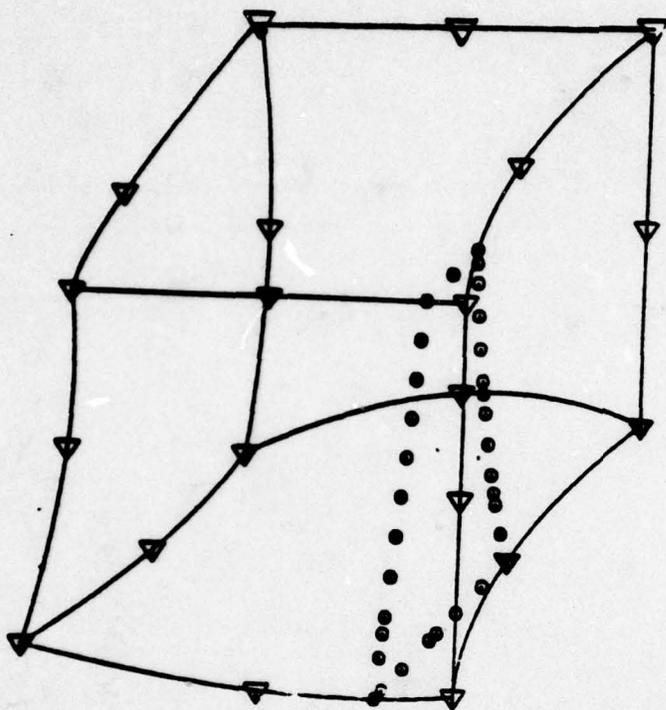


FIGURE 4

This intersection of a 20-node brick and a plane is multiply connected and one subregion is a point.

The pre-processor strategy is as follows:

- A geometry file for the proposed finite element idealization is constructed.
- The user views this idealization and chooses a cross-sectional plane of the structure for close scrutiny.
- The user specifies all or some of those brick elements he wishes to be scanned.
- The intersection of each brick with the specified plane is determined (if such exists) and displayed.
- The user labels each portion of the intersection that he desires appended to a master plot file.
- After considering the totality of bricks to be scrutinized, the master plot file is displayed. Voids between, or overlapping of elements will appear as unlabeled or multiple labeled subregions.
- The geometry file can then be scanned and corrected as needed.

Figure 5 illustrates a portion of a reactor vessel near the intersection with a 45° lateral. The finite element idealization contains 450 brick elements. This figure serves to demonstrate the seemingly impossible task of detecting anomalies in the geometric data as well as gauging the distribution of nodes. The above strategy was implemented for this structure and Figure 6 contains a plot of a plane of intersection. From this figure it is not difficult to see that an error exists in the original geometric data. Specifically, as described by this data, elements 407 and 408 are not contiguous to, but penetrate, element 206.

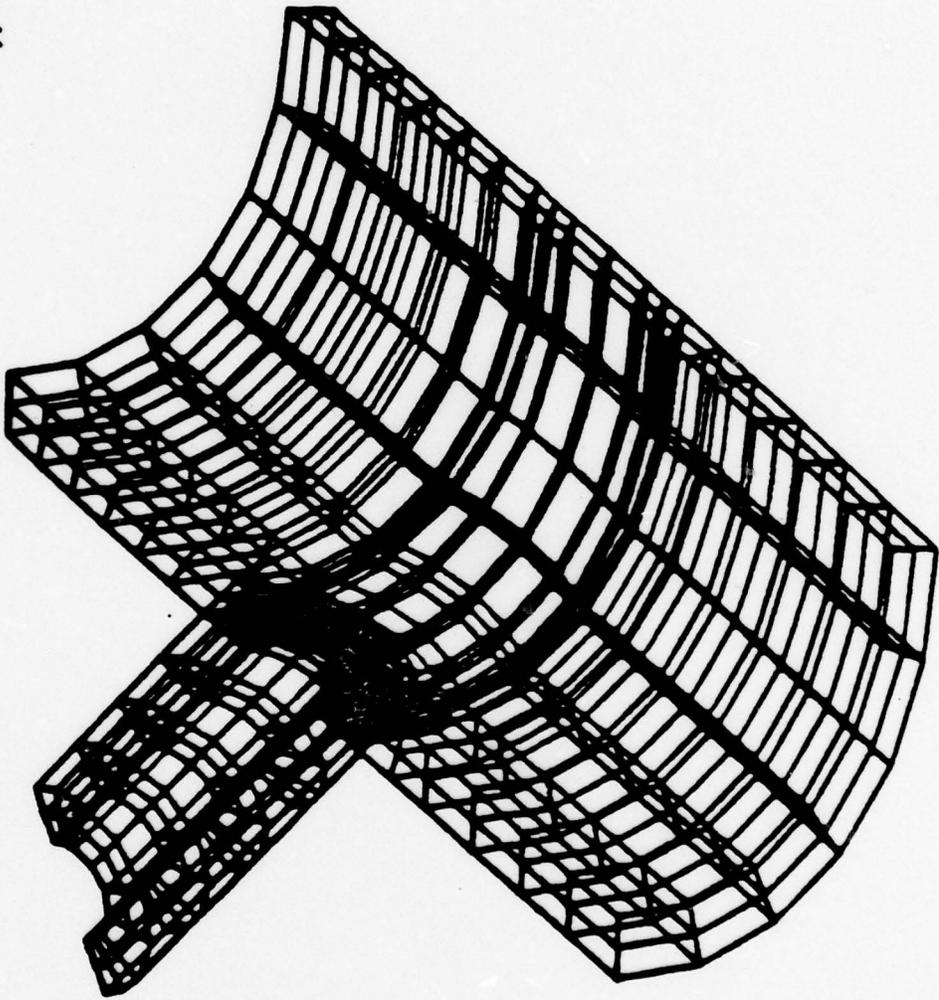


FIGURE 5. Reactor vessel near lateral nozzle

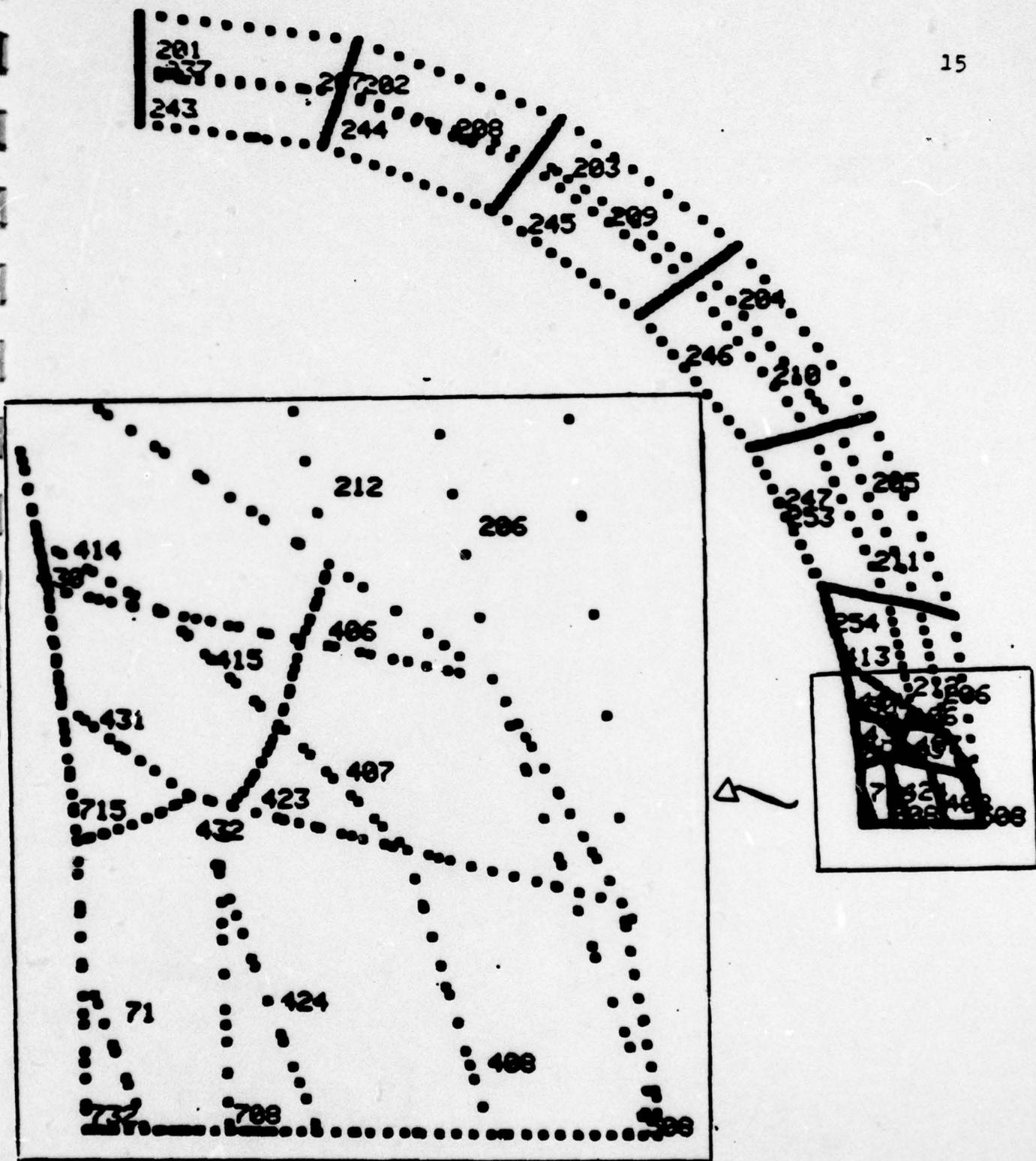


FIGURE 6. Plane of intersection and a section of that intersection which has been windowed for greater detail. Note the overlap between elements 206, 407 and 408. There are two subregions which are unlabeled and the order in which their boundaries were drawn indicates an overlap.

B. INVERSION OF TWO-DIMENSIONAL ISOPARAMETRIC MAPPINGS

The nature of two-dimensional isoparametric mappings $\bar{T}: \mathcal{J} \rightarrow \mathcal{E}$ (where $\mathcal{J} : (0,1) \times (0,1)$ and \mathcal{E} is the specified element) and in particular the existence of inverses for such mappings has been analyzed. Various results are reported in [8] and include:

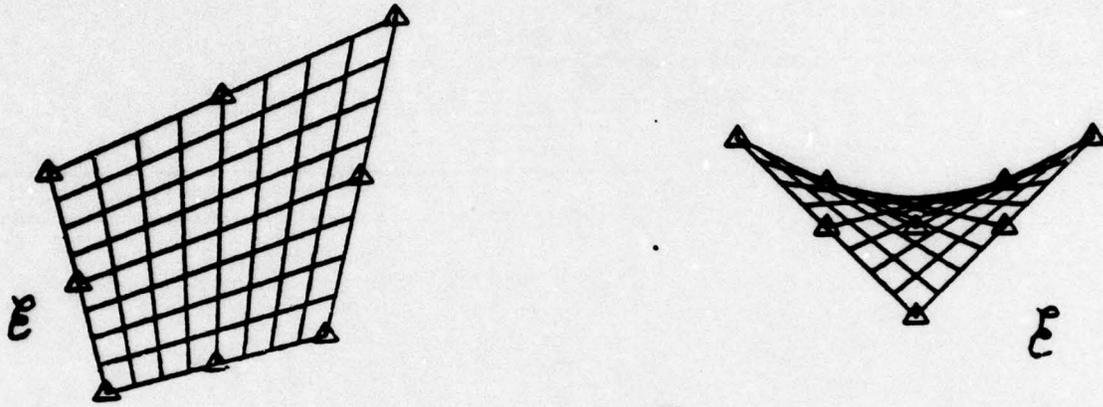
(a) The straight sided quadrilateral mapping \bar{T}_1 is bijective (one-to-one) if and only if \mathcal{E} is convex. (Cf. Figure 7).

(b) The 8-node quadratic isoparametric mapping \bar{T}_2 is bijective if its Jacobian is nonzero throughout \mathcal{J} and the mapping is one-to-one on the boundary. A class of element shapes is specified for which the Jacobian is nonzero. (Cf. Figure 8).

(c) For the 8-node quadratic isoparametric mapping \bar{T}_2 , sufficient conditions are given to guarantee that overspill cannot occur. Further, under rather weak assumptions it is proven that \bar{T}_2 is bijective if and only if overspill does not occur.

(d) Perturbation arguments are given to provide another set of sufficient conditions for the bijectivity of \bar{T}_2 .

Details of this work can be found in reference [8], Mathematics of Computations, 32, July 1978, pp. 725-749.



CONVEX ELEMENT
INVERTIBLE

NON-CONVEX ELEMENT
NON-INVERTIBLE

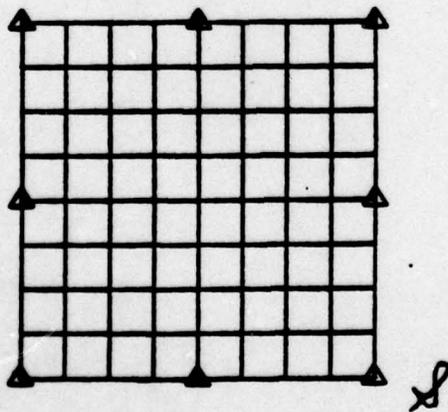
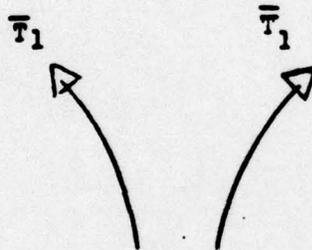


FIGURE 7.

Straight sided quadrilateral

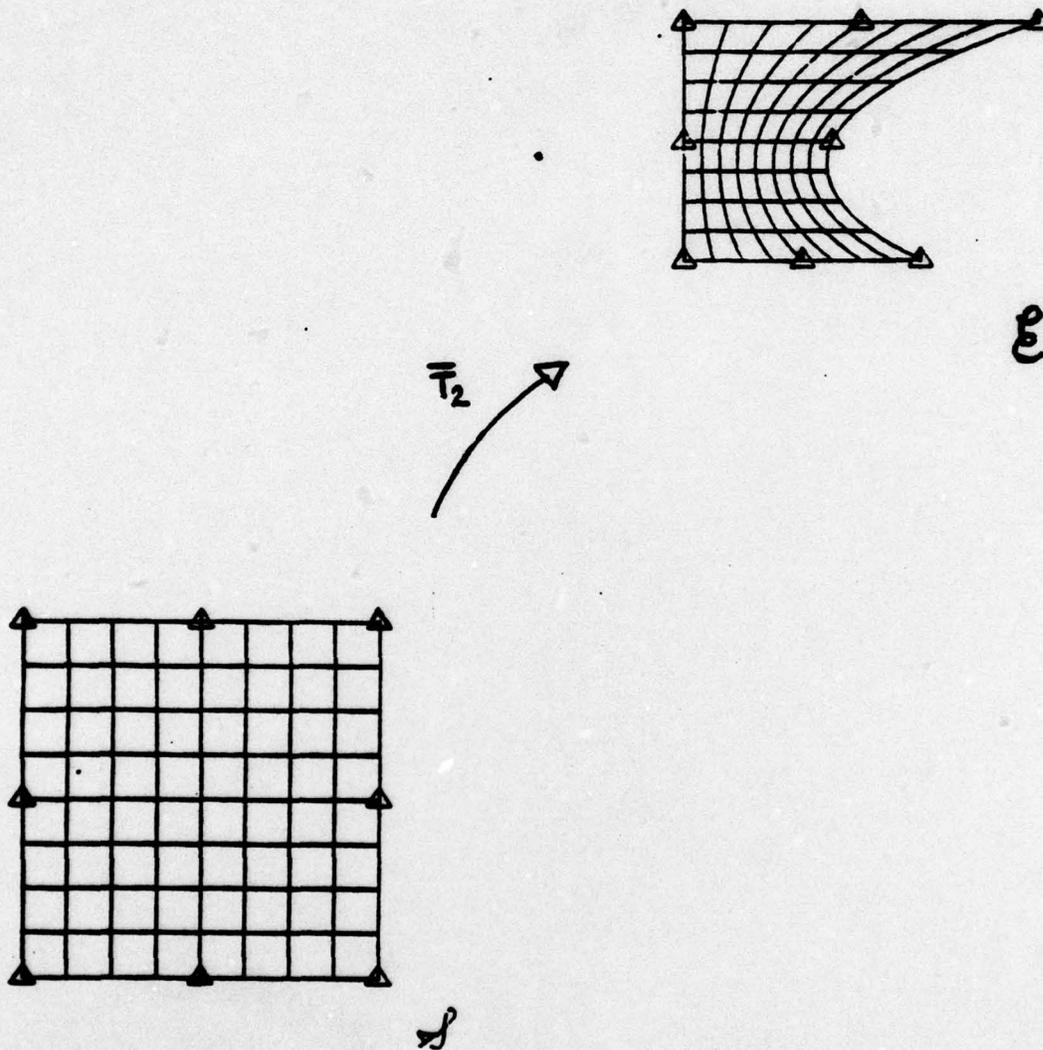


FIGURE 8. Invertible 8-node isoparametric mapping \bar{T}_2 .

An algorithm for numerically inverting the two-dimensional 8-node quadratic isoparametric mapping \bar{T}_2 has been developed. The algorithm is based on bigradients and appears to be relatively efficient. (Cf. Figure 9). This algorithm will determine all pre-images of a point in \mathcal{E} , including those which do not lie in \mathcal{S} . A program (SOLV8) which implements this algorithm was documented and submitted for publication, [10]. This paper was revised and resubmitted in June, 1979. The algorithm now includes an iterative improvement strategy based on Newton's method.

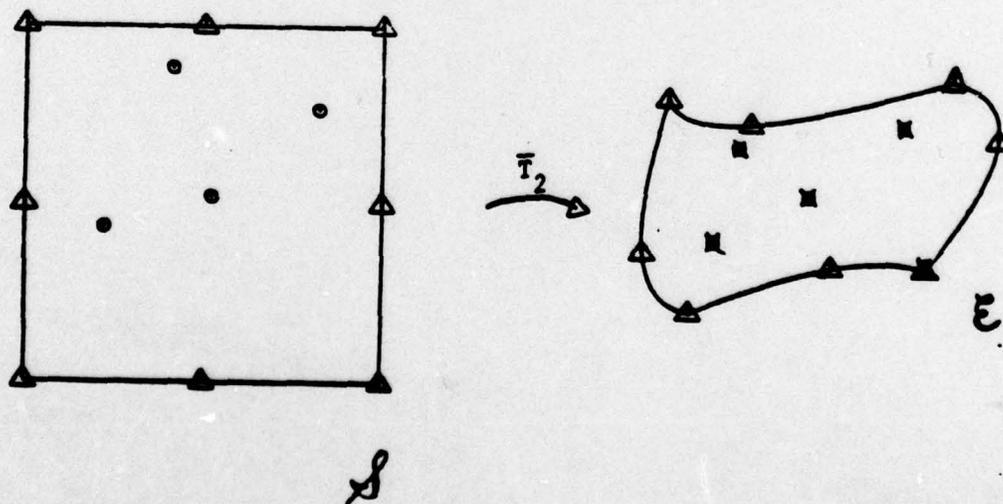


FIGURE 9

The pre-images of the points marked "x" were found to be those marked "o".

C. THE CONSTANT STRAIN CONDITION

The constant strain condition for classes of second and fourth order boundary value problems was investigated [Ph.D. Dissertation, A. E. Frey, 1978]. Results concerning the effect on the error in calculating stiffness matrices when using elements with curved boundaries include:

(a) Second Order Problems. Exact integration preserves an element's ability to satisfy the constant strain condition even when curved boundaries are introduced. For any reasonable numerical integration formula, it is shown that even though large errors may be introduced in the entries of the stiffness matrix due to rational integrands (caused by curved element boundaries) the vectors $\underline{1}$, \underline{x} and \underline{y} are in the null space of this error matrix. Hence any such numerical integration formula also preserves an element's ability to reproduce constant strain. This work is reported in [13], which has been accepted for publication.

(b) Fourth Order Problems. We were unable to find in the literature -a C^1 -compatible element which satisfies the constant strain condition for elements with curved boundaries. Using sub-parametric element mapping concepts, such an element was developed. (Paper in preparation.)

D. SUPPORT PROGRAMS

(1) Computer graphics routines BC8E2 and B20E3 were developed which graphically display the images of two and three dimensional isoparametric mappings. These were documented in [9].

(2) An algorithm PLAINT, [9] was developed which determines the intersection of a single 20-node isoparametric (3-dimensional) brick and a given plane. The necessary software for graphic representation of this intersection was also developed. (Cf. Figures 2, 3, and 4.)

(3) A conversational computer graphics program PLANIT was developed using PLAINT to plot the intersection of a given plane with a union of isoparametric bricks. Cf. Figures 5 and 6. PLANIT has been documented in [11], and was reported on at a symposium [12] and in Computers and Structures, 10, 1979, pp. 149-154.

(4) The bigradient algorithm used in [10] for the 8-node element was considered for the numerical inversion of the three dimensional 20-node isoparametric element. This does not seem to be a fruitful approach due to the complexity of the elimination process. An algorithm based on Newton's method was implemented and seems to perform reasonably well.

E. POST-PROCESSOR: PLOTTING OF STRESS DISTRIBUTIONS

A finite element program computes various components of stress in terms of the global (x,y,z) coordinate system. A program STRSIT [16] was developed which plots in a post-processing mode contours of components of stress in and perpendicular to a given plane which intersects the structure.

The input is an output file of the program PLANIT. This file contains the intersection of the plane and the finite element

idealization. In addition, the element geometry file is available. An analyst also specifies those components of in-plane and out-of-plane stresses which he desires to be plotted.

Given the mesh point displacements (u_1, v_1, w_1) determined by a finite element program, the displacement components

$$u(x,y,z) = \sum u_1 \phi_1(r,s,t)$$

$$v(x,y,z) = \sum v_1 \phi_1(r,s,t)$$

$$w(x,y,z) = \sum w_1 \phi_1(r,s,t)$$

can be reconstructed element-by-element. The displacement vector $\bar{\delta} \equiv (u,v,w)$ is independent of coordinate system and can be projected onto the given plane and a normal to the plane (cf. Figure 10). If we denote the new components of $\bar{\delta}$ relative to the (r,s,t) system, respectively,

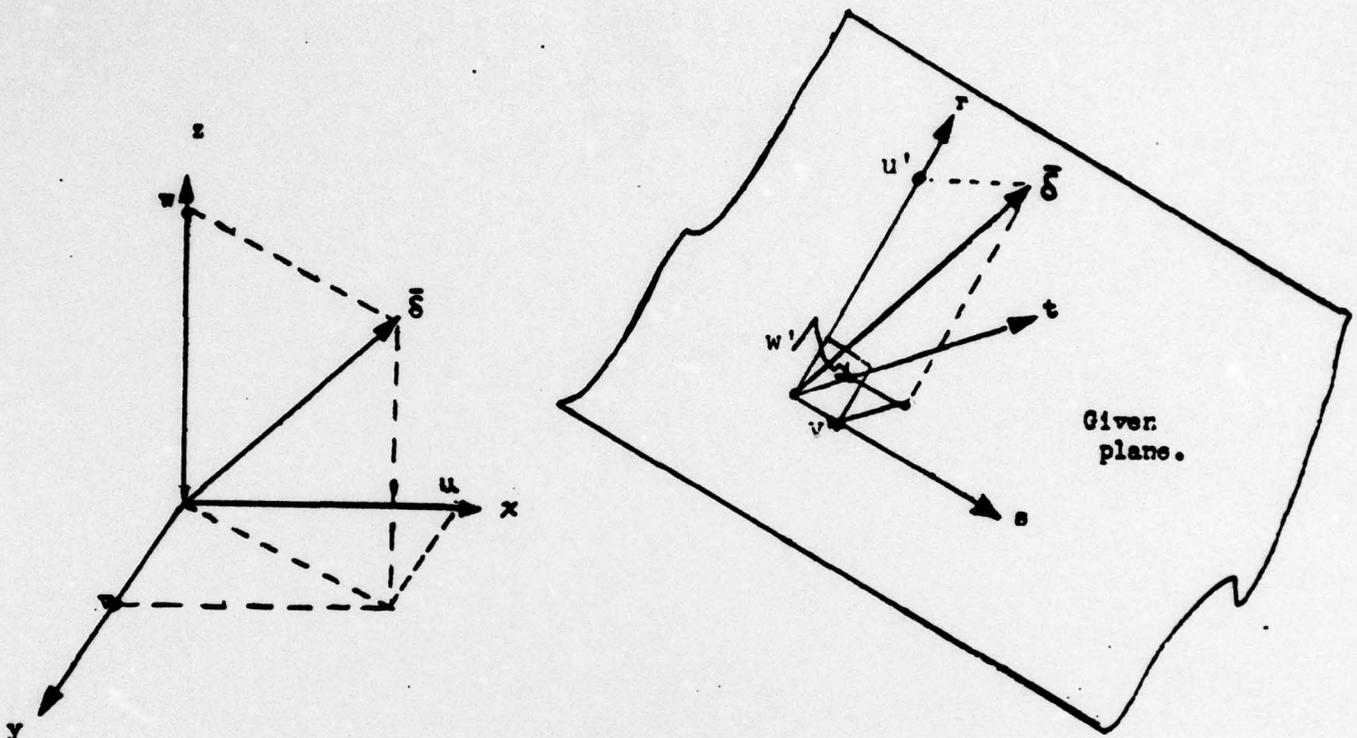


FIGURE 10

u', v', w' , then the strains relative to the (r, s, t) directions are

$$\bar{\epsilon}_{rst} \equiv \begin{bmatrix} \epsilon_r \\ \epsilon_s \\ \epsilon_t \\ \gamma_{st} \\ \gamma_{tr} \\ \gamma_{rs} \end{bmatrix} = \begin{bmatrix} \partial u' / \partial r \\ \partial v' / \partial s \\ \partial w' / \partial t \\ \partial v' / \partial t + \partial w' / \partial s \\ \partial w' / \partial r + \partial u' / \partial t \\ \partial u' / \partial s + \partial v' / \partial r \end{bmatrix}$$

These computations necessitate inverting various isoparametric maps and their associated Jacobian matrices. Via Hooke's Law the stresses are then determined as

$$\bar{\sigma}_{rst} \equiv \begin{bmatrix} \sigma_s \\ \sigma_t \\ \sigma_r \\ \tau_{st} \\ \tau_{tr} \\ \tau_{rs} \end{bmatrix} = D \bar{\epsilon}_{rst}$$

where D is the appropriate 6 × 6 elasticity matrix.

The program STRSIT (element-by-element) computes the stress state $\bar{\sigma}_{rst}$ and plots those components desired in the plane specified in the input. A sketch of such a contour plot is given in Figure 11 where the plane intersects fourteen different elements. (The program HOLES4 [15] is used to plot the contours).

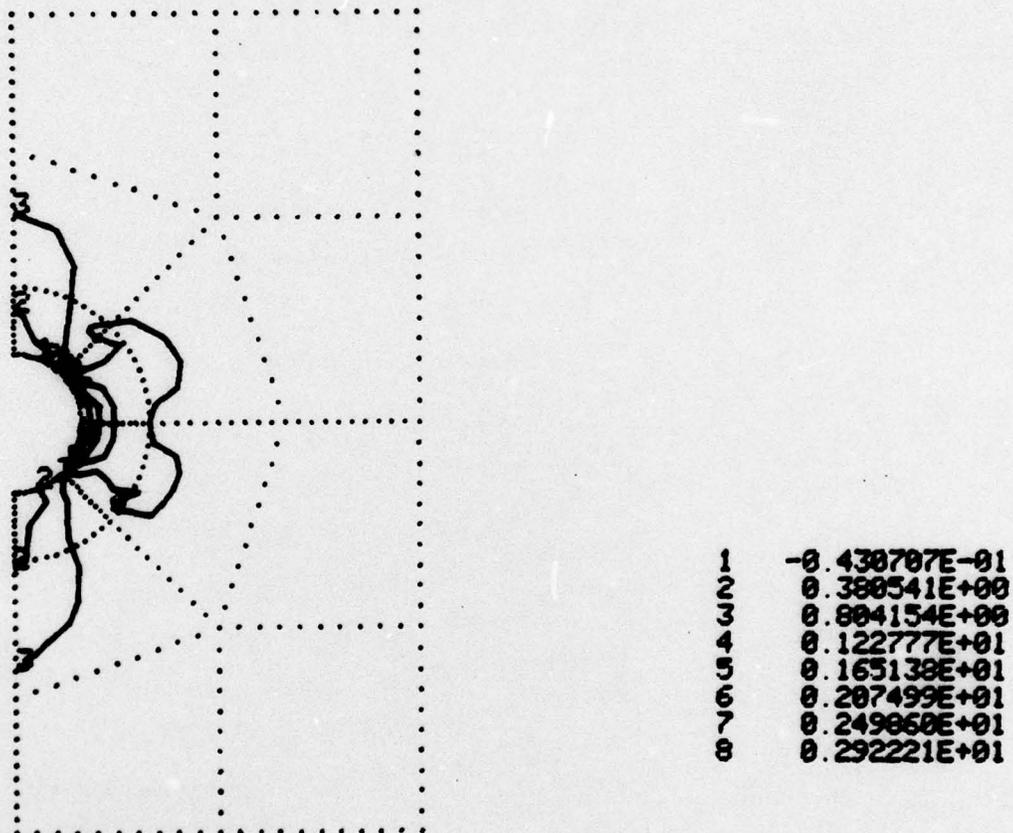


FIGURE 11

Contour plot of σ_s showing also the intersection of the plane with the fourteen bricks which contribute to the stress distribution.

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(This is a major revision of and supercedes the report "On the Bijectivity of Mappings of Compact Domains with Applications to Parametric Mappings of Finite Element Analyses," December, 1976.)
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