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**An Improved Method for Contouring
on Isoparametric Surfaces**

W. H. Gray
J. E. Akin

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AN IMPROVED METHOD FOR CONTOURING ON ISOPARAMETRIC SURFACES

W. H. Gray

and

J. E. Akin

Associate Professor

Department of Engineering Science and Mechanics
The University of Tennessee
Knoxville, Tennessee 37916

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SUMMARY

A general nonlinear interpolation procedure for contouring on any isoparametric surface was presented in a previous article. This method used standard isoparametric interpolation functions and a predictor method for tracing element contour lines. The method presented here extends the previous work by using a predictor-corrector method to trace element contour lines, thereby making the contouring algorithm more accurate.

1. INTRODUCTION

Contour plotting on two- or three-dimensional (2- or 3-D) isoparametric surfaces is a problem facing many finite element code developers. Most procedures use some type of linear interpolation to approximate the contour locations.¹ In general, the use of linear interpolation to locate contour lines on higher order isoparametric finite elements destroys much of the interelement information contained within the results of an analysis. Without adequate means of visually showing the results of higher ordered finite element calculations, numerous developers of finite element codes have been reluctant to include these elements in their element libraries.

In a previous paper,² the authors presented a general nonlinear interpolation procedure for contouring on any isoparametric finite element surface. This procedure is based upon the isoparametric interpolation function itself and as such does not destroy or invent any information that was not already contained within the results. The work presented here extends the procedure with regard to accuracy in following the contour lines.

2. THEORY

Reviewing the theory expressed in Reference 2, consider any isoparametric element formulated in local coordinates, R and S , as shown in Figure 1. At any local point the value of the quantity of interest is³

$$V(R,S) = [H(R,S)]\{V^e\} \quad (1)$$

where $[H]$ and $\{V^e\}$ denote the interpolation functions and the nodal values, respectively. If a contour of V can be defined in the local space, then it can easily be converted to the global space.

Assume that the contour is given by $V = K$ where K is a known constant, and also assume that the local coordinates (R_0, S_0) of one point on the contour are known. The equation of such a curve is given by $dV = 0$. In local coordinates, this becomes

$$0 = \frac{\partial V}{\partial R} dR + \frac{\partial V}{\partial S} dS \quad (2)$$

where dR and dS are components of a displacement dL which is tangent to the contour. Assume that the value of dL , the contour trace step size, is a known constant. As shown in Figure 2, if the contour segment makes an angle of θ with respect to the R axis, then $dR = dL \cos \theta$ and $dS = dL \sin \theta$. Clearly, the value of $\tan \theta$ can be obtained from equation (2) using the values of $\partial V/\partial R$ and $\partial V/\partial S$, which are easily obtained for any isoparametric element by utilizing the local derivatives of equation (1). That is,

$$\partial V/\partial R = [\partial H/\partial R]\{V^e\} \quad (3)$$

$$\partial V/\partial S = [\partial H/\partial S]\{V^e\} \quad (4)$$

or symbolically

$$\{\partial_{\ell} V\} = [DH]\{V^e\} \quad (5)$$

where the subscript ℓ denotes local derivatives. Thus, given a starting point on an element contour line, all one needs to trace the line through the element are the nodal values of the function, the local coordinate derivatives of the interpolation equations, and an assumed step increment dL .

Using this assumption, the formulas which predict the position of the contour line's next (or new) location with respect to the previous (or old) location are

$$\nabla = \sqrt{\left(\frac{\partial V}{\partial R}\right)^2 + \left(\frac{\partial V}{\partial S}\right)^2} \quad (6)$$

$$R_{\text{new}} = R_{\text{old}} + \left(\frac{dL}{\nabla}\right) \frac{\partial V}{\partial S} \quad (7)$$

$$S_{\text{new}} = S_{\text{old}} - \left(\frac{dL}{\nabla}\right) \frac{\partial V}{\partial R} \quad (8)$$

Clearly, the accuracy and cost of such a procedure depend on the size of the local increment dL . This procedure will tend to deviate from the true contour path because of the numerical errors involved. That is, at the end of a single step the new contour value is not exactly equal to the one which was supposed to be followed. The gradient of the new contour will be used to calculate another position which is more inaccurate than the previous one, etc. In practice, however, this accumulation of error is not visually perceptible except when dealing with a closed contour. Because of the above inaccuracies, the contour will not close; instead it will spiral until an element boundary is reached or the maximum number of allowable points upon a contour has been exceeded.

The above procedure can be modified to make the accumulated error acceptably small without excessive increase in computational cost. It has been pointed out⁴ that a simple correction step normal to the contour line will reduce the amount of deviation. In our terminology, the corrected local coordinates may be calculated from the equations

$$R_{\text{cor}} = R_{\text{new}} - \left(\frac{1}{\nabla}\right)^2 \frac{\partial V}{\partial R} [V(R_{\text{new}}, S_{\text{new}}) - V_{\text{cor}}]$$

$$S_{\text{cor}} = S_{\text{new}} - \left(\frac{1}{\nabla}\right)^2 \frac{\partial V}{\partial S} [V(R_{\text{new}}, S_{\text{new}}) - V_{\text{cor}}]$$

where V_{cor} is the correct contour value. This simple correction produces contour lines which are in most cases more accurate than it is possible to record on a graphics display device.

To terminate the contour, one checks the coordinates at the end of each new segment to see if they remain within the element. For higher order elements it is likely that some contours will be closed loops, and in this case the test would fail to stop the calculations. Thus, it is necessary to have a maximum number of allowable segments on any one contour. The required value is $\text{MAX} \leq P/dL$.

Once a contour has been completely traced in the 2-D local space, all points on the contour are converted to the corresponding 2-D or 3-D global coordinates and returned for plotting. The 3-D global values would generally be transformed again for isometric or perspective plotting.

The selection of the local coordinate starting point can involve two options: one for conveying quick and inexpensive engineering information and another for detailed quality plots of specific contour values. In the first case, one could plot contours beginning at specific points

instead of those which have specific values. For example, one could plot all contours beginning at the mid- or third points of each edge of each element. This would give contour segments that are continuous across two elements and then terminate. This eliminates the need for expensive contour locating logic but is not desirable for final reports.

The application of the second and more common procedure is more expensive. One must test each element to determine if a specified contour value lies within the element. The local coordinates of a contour intersecting the edge of a linear, quadratic, or cubic element are easily found. However, a given curve will usually intersect more than one edge. Thus, to avoid plotting such curves twice, it is necessary to compare the calculated terminal point of one curve to see if it lies within a distance of dL of any other initial point on other edges of the element. For quadratic and cubic elements, it is necessary to test for closed loops not intersecting the edge. This is more difficult. One could check the value of V on lines of $R = \text{const}$ and $S = \text{const}$ that pass through the centroid of the element to determine an internal starting point in local coordinates.

3. RESULTS

Figure 3 shows a subroutine, LCONTC, for tracing the contour curve in a single element. It calls subroutine SHAPE to extract the interpolation functions $[H]$, subroutine DERIV to extract the local derivatives $[DH]$ of $[H]$, and a standard matrix multiplication subroutine MMULT. Figure 4 shows typical results of the application of subroutine LCONTC to contour calculation in a quadratic triangle. For comparison, Figure 5

shows a similar problem except that the method presented in Reference 2 was used. Notice that in Figure 5 the interior contour line spirals, while in Figure 4 the contour line closes upon itself, graphically demonstrating the difference between contour line calculation without and with a correction step normal to the contour line, respectively.

Figure 6 shows typical results obtained from a quadratic quadrilateral. This figure demonstrates that subroutine LCONTC can successfully calculate contours when the nodal contour function contains a separatrix. Two continuous curves were drawn by subroutine LCONTC to represent the separatrix. The first starts at the right-hand midpoint node and proceeds to the bottom midpoint node. The second starts at the left-hand midpoint node and proceeds to the top midpoint node.

NOMENCLATURE

<u>Symbol</u>	<u>Description</u>
R, S	element local coordinates
$V(R,S)$	contour variable
$H(R,S)$	isoparametric interpolation function
$\{V^e\}$	node contouring values
$\frac{\partial V}{\partial R}$	variation of the contour with respect to the local R coordinate
$\frac{\partial V}{\partial S}$	variation of the contour with respect to the local S coordinate
∇	$\sqrt{\left(\frac{\partial V}{\partial R}\right)^2 + \left(\frac{\partial V}{\partial S}\right)^2}$
R_{old}, S_{old}	old local coordinates on the element contour
R_{new}, S_{new}	new local coordinates on the element contour
R_{cor}, S_{cor}	corrected local coordinates on the element contour
P	element perimeter in local coordinate units
dL	length of a step along the contour line
MAX	maximum number of allowable points on a contour line

REFERENCES

1. J. L. Meek and G. Beer, 'Contour Plotting of Data Using Isoparametric Element Representation', Int. J. Numer. Methods Eng. 10, 954 (1976).
2. J. E. Akin and W. H. Gray, 'Contouring on Isoparametric Surfaces', Int. J. Numer. Methods Eng. 11, 1893 (1977).
3. R. H. Gallagher, *Finite Element Analysis Fundamentals*, Prentice-Hall, Inc., New Jersey, 1975.
4. Jonas T. Holdeman, Jr. (Oak Ridge National Laboratory), private communication, October 13, 1977.

FIGURE CAPTIONS

- Figure 1. Typical element contours.
- Figure 2. Marching along a contour.
- Figure 3. Contouring routine.
- Figure 4. Contours drawn on a quadratic triangle using the predictor-corrector method presented in this paper. Notice the closed loop contour on the interior of the triangle.
- Figure 5. Contours drawn on a quadratic triangle using the method presented in Reference 2. Notice the spiraling contour on the interior of the triangle.
- Figure 6. Contours drawn on a quadratic quadrilateral using the predictor-corrector method presented in this work.

(a) GLOBAL

(b) LOCAL

Fig. 1.

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Fig. 2.

```

C      SUBROUTINE LCONTC (RINOUT,SINOUT,V,COORD,XYZ,N,NSPACE,
C      1      KOUNT,H,DH,LTYPE)
C
C      SUBROUTINE LCONTC
C
C      PURPOSE:
C
C      TO CALCULATE THE COORDINATES OF POINTS ON A CONTOUR
C      ON AN ISOPARAMTERIC SURFACE USING A PREDICTOR-CORRECTOR
C      METHOD.
C
C      DIMENSIONING:
C
C      PXYZ-   NSPACE
C      XYZ-    MAX,NSPACE
C      R,S-    MAX
C
C      ARGUMENTS:
C
C      RINOUT,SINOUT-  LOCAL COORDINATES OF FIRST ( ON INPUT ) OR
C                      LAST ( ON RETURN ) POINT.
C      V-            NODAL VALUES OF THE QUANTITY TO BE CONTOURED.
C      COORD-        GLOBAL COORDINATES OF THE ELEMENT NODES.
C      XYZ-          GLOBAL COORDINATE ARRAY FOR CONTOUR POINTS.
C      N-            NUMBER OF NODES PER ELEMENT.
C      NSPACE-       DIMENSIONING OF GLOBAL SPACE, EITHER 2 OR 3.
C      KOUNT-        NUMBER OF POINTS ON A CONTOUR CURVE.
C      H-            ELEMENT INTERPOLATION FUNCTIONS.
C      DH-           LOCAL COORDINATE DERIVATIVES OF H
C      LTYPE-        EQUAL 0 IF QUADRILATERAL OR 1 IF TRIANGLE
C
C      LOCAL VARIABLES:
C
C      MAX-         MAXIMUM NUMBER OF CONTOUR POINTS.
C      DL-          LOCAL COORDINATE LENGTH OF A CONTOUR SEGMENT.
C      R,S-         LOCAL COORDINATE ARRAYS FOR CONTOUR POINTS.
C      PXYZ-        GLOBAL COORDINATES FOR A SINGLE CONTOUR POINT
C      VIN-         INITIAL CONTOUR VALUE.
C
C      DIMENSION COORD(N,NSPACE), V(N), H(N), DH(2,N),VS(1)
C      DIMENSION PXYZ(3), XYZ(300,NSPACE), R(300), S(300), DER(2)
C
C      EQUIVALENCE (PXYP(1),DER(1),DVDR), (DER(2),DVDS)
C
C      DEFINE MAX AND DL
C      DATA MAX,DL / 298, 0.01 /
C      KOUNT = 1
C
C      LOCAL COORDINATE CALCULATIONS
C      R(1) = RINOUT
C      S(1) = SINOUT
C
C      CALCULATE THE INITIAL VALUE OF THE CONTOUR
C      CALL SHAPE(R(1),S(1),H)
C      CALL MMULT(H,V,VS,1,N,1)
C      VIN = VS(1)
C
C      MARCH ALONG CONTOUR
C      CONTINUE

```

Fig. 3.

```

C FORM SHAPE FUNCTION LOCAL DERIVATIVES
  CALL DERIV (R(KOUNT),S(KOUNT),DH)
C
C FORM LOCAL DERIVATIVE OF VARIABLE, DER = DH*V
  CALL MMULT (DH,V,DER,2,N,1)
  GRAD = SQRT( DVDR*DVDR + DVDS*DVDS )
C
C FIND LOCAL COORD. OF SEGMENT END
  RNEW = R(KOUNT) + DL*DVDS/GRAD
  SNEW = S(KOUNT) - DL*DVDR/GRAD
C
C USE CORRECTOR TO CORRECT POSITION
  CALL SHAPE(RNEW,SNEW,H)
  CALL MMULT(H,V,VS,1,N,1)
  VHERE = VS(1)
C
C CHECK FOR A SEPARATRIX
  IF ( GRAD .LE. 1.0E-3 ) GO TO 70
  GRADD = - (VHERE-VIN)/(GRAD*GRAD)
  RNEW = RNEW + GRADD*DVDR
  SNEW = SNEW + GRADD*DVDS
70 CONTINUE
C
C IS NEXT POINT IN THE ELEMENT
  IF ( LTYPE.EQ.0 ) GO TO 10
C
C TRIANGLE (UNIT COORDINATES)
  IF ( RNEW.LT.0.0 .OR. SNEW.LT.0.0 .OR.
    1 (RNEW+SNEW).GT.1.0 ) GO TO 20
  GO TO 15
C
C QUADRILATERAL (-1 TO +1)
10 IF ( ABS(RNEW).GT.1.0 .OR. ABS(SNEW).GT.1.0 ) GO TO 20
C
C ADD POINT TO CONTOUR LIST
15 KOUNT = KOUNT + 1
  R(KOUNT) = RNEW
  S(KOUNT) = SNEW
  IF ( KOUNT.EQ.MAX ) GO TO 20
  GO TO 5
C
C LINE COMPLETED IN LOCAL COORDINATES
20 CONTINUE
C
C RETURN LOCAL COORD. OF LAST POINT
  RINOUT = R(KOUNT)
  SINOUT = S(KOUNT)
C
C CONVERT TO GLOBAL COORDINATES
  DO 25 I = 1,KOUNT
C
C EVALUATE SHAPE FUNCTIONS
  CALL SHAPE (R(I),S(I),H)
C
C EVALUATE GLOBAL COORDINATES, XYZ = H*COORD
  CALL MMULT (H,COORD,PXYZ,1,N,NSPACE)
  XYZ(1,1) = PXYZ(1)
  XYZ(1,2) = PXYZ(2)
  IF ( NSPACE.EQ.3 ) XYZ(1,3) = PXYZ(3)
25 CONTINUE

C
C CONTOUR FINISHED, RETURN FOR PLOTTING
  RETURN
  END

```

Fig. 3. (continued)

Quadratic Triangle

Fig. 4.

Quadratic Triangle

Fig. 5.

Quadratic Quadrilateral

Fig. 6.

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