2 SINGULAR FINITE ELEMENTS

2.1 Isoparametric, Quadratic Singular Elements

A fundamental difficulty when modeling Linear Elastic Fracture Mechanics (LEFM) problems using the finite element method is that the polynomial basis functions used for most conventional elements cannot represent the singular crack-tip stress and strain fields predicted by the theory. This means that as the mesh is refined the finite element solution will initially begin to converge to the theoretical solution, but eventually will diverge. This difficulty was recognized and demonstrated relatively early in the development of the finite element method (Chan, 1970). A number of researchers investigated special finite element formulations that incorporate singular basis functions or stress intensity factors as nodal variables (e.g., Byskov, 1970; Tracey, 1971; Tong, 1973; Papaioannou, 1974; Atluri, 1975; and Benzley, 1974). While successful, these special purpose elements are not available in most general-purpose finite element programs and thus are used very infrequently.

A significant advancement in the use of the finite element method for LEFM problems was the simultaneous, and independent, development of "quarter-point" elements by Henshell and Shaw (1975) and Barsoum (1976). These researchers showed that the proper crack-tip displacement, stress, and strain fields are modeled by standard quadratic order isoparametric finite elements if one simply moves the element's mid-side node to the position one quarter of the way from the crack tip to the far end of the element. This procedure introduces a singularity into the mapping between the element's parametric coordinate space and Cartesian space.

Henshell and Shaw described a quadrilateral quarter-point element, illustrated in Figure 1a. Barsoum proposed collapsing one edge of the element at the crack tip. This is shown in Figure 1b, where the crack-tip nodes (1, 4, 8) are constrained to move together. The discovery of quarter-point elements was a significant milestone in the development of finite element procedures for LEFM. With these elements standard and widely available, finite element programs can be used to model crack tip fields accurately with only minimal preprocessing required. The remainder of this section will focus exclusively on quarter-point elements in their various forms.

2.2 One-Dimensional Quarter-Point Elements

The effect of moving the side node of a quadratic element to the quarter-point position can be best illustrated with a one-dimensional element. Although these elements are not practically very useful, the algebra is much simpler than with two- and three-dimensional elements, and is same in principle for the higher dimensionality elements. A 1-D quadratic order element is illustrated in Figure 2. Figure 2a shows the parametric space of the element. Figure 2b shows the element in the Cartesian space, with the location of the center node controlled by the value of the parameter α, and the "crack-tip" is located at $r = 0$.

The displacement, u, at any point within the element is determined by interpolating the nodal displacements, u_i, using the standard Lagrange second order shape functions,

$$u=\sum_{i=1}^{3} N_i u_i=\tfrac{1}{2}\xi(\xi-1)u_1+(1-\xi^2)u_2+\tfrac{1}{2}\xi(\xi+1)u_3 \qquad (1)$$

or, regrouping in powers of ξ,

$$u=u_2+\tfrac{1}{2}(u_3-u_1)\xi+(\tfrac{1}{2}(u_1+u_3)-u_2)\xi^2\,. \qquad (2)$$

Using an isoparametric formulation, the same shape functions are used to interpolate the geometry of the element:

$$r=\sum_{i=1}^{3} N_i r_i=\alpha l+\tfrac{1}{2}l\xi+l(\tfrac{1}{2}-\alpha)\xi^2. \qquad (3)$$

First consider the case where the center node is located at the mid-point of the element. That is, $\alpha=\frac{1}{2}$, and $\xi=\dfrac{2r}{l}-1$. Substituting this expression for ξ into equation 2 yields the expected quadratic expression in *r* for the displacements:

$$u=u_1+(-3u_1+4u_2-u_3)\frac{r}{l}+2(u_1-2u_2+u_3)\frac{r^2}{l^2}\,. \qquad (4)$$

Differentiating this expression yields the expected linear expression in *r* for the strains in the element:

$$\varepsilon = \frac{du}{dr} = (-3u_1 + 4u_2 - u_3)\tfrac{1}{l} + 4(u_1 - 2u_2 + u_3)\tfrac{r}{l^2}. \qquad (5)$$

Under linear elastic conditions, the stresses are linearly related to the strains so the stress distribution will be linear in *r* also.

Now consider the case where the middle node is moved to the quarter-point position. For this case $\alpha = \frac{1}{4}$ and $\xi = \frac{2\sqrt{lr}}{l} - 1$. Substituting this expression for ξ into equation 2 and differentiating yields the following expressions for the displacements and strains in the element:

$$u = u_1 + 2(u_1 - 2u_2 + u_3)\tfrac{r}{l} + (-3u_1 + 4u_2 + u_3)\frac{\sqrt{lr}}{l} \qquad (6)$$

$$\varepsilon = \frac{du}{dr} = 2(u_1 - 2u_2 + u_3)\tfrac{1}{l} + (-\tfrac{3}{2}u_1 + 2u_2 - \tfrac{1}{2}u_3)\frac{1}{\sqrt{lr}} \qquad (7)$$

One can clearly see that the three terms in the displacement expression model a constant value, a linear variation in *r*, and the square root variation in *r*. This corresponds to the leading terms in the LEFM expressions for the near crack-tip displacement. The expression for the strains contains a constant term and a term a singular term that varies as $r^{-1/2}$, the form of lead term in the LEFM stress and strain expansions.

2.2.1 Isoparametric, cubic-order singular elements

The "quarter-point" singular mapping is not unique to quadratic order elements. Consider a cubic order isoparametric element with Lagrange shape functions. The expression for the displacement in the element is

$$\begin{aligned} u = {} & \tfrac{1}{16}(-1+\xi+9\xi^2-9\xi^3)u_1 + \tfrac{9}{16}(1-3\xi-\xi^2+3\xi^3)u_2 + \\ & \tfrac{9}{16}(1+3\xi-\xi^2-3\xi^3)u_3 + \tfrac{1}{16}(-1-\xi+9\xi^2+9\xi^3)u_4 \end{aligned} \tag{8}$$

If the locations of the middle nodes are parameterized by α and β, the expression that interpolates geometry within the element is:

$$\begin{aligned} r = {} & \tfrac{9\alpha l}{16}(1-3\xi-\xi^2+3\xi^3) + \tfrac{9\beta l}{16}(1+3\xi-\xi^2-3\xi^3) + \\ & \tfrac{l}{16}(-1-\xi+9\xi^2+9\xi^3) \end{aligned} \tag{9}$$

If one selects $\alpha = \frac{1}{9}$ and $\beta = \frac{4}{9}$ then, similar to the quarter-point quadratic element, $\xi = \dfrac{2\sqrt{lr}}{l} - 1$. Substituting this into the displacement expression and differentiating yields:

$$\begin{aligned} u = {} & u_1 + 9(u_1 - \tfrac{5}{2}u_2 + 2u_3 - \tfrac{1}{4}u_4)\tfrac{r}{l} + (-\tfrac{11}{2}u_1 + 9u_2 - \tfrac{9}{2}u_3 + u_4)\tfrac{\sqrt{lr}}{l} + \\ & \tfrac{9}{2}(-u_1 + 3u_2 - 3u_3 + u_4)\tfrac{r\sqrt{lr}}{l^2} \end{aligned} \tag{10}$$

and

$$\varepsilon = \frac{du}{dr} = 9(u_1 - \tfrac{5}{2}u_2 + 2u_3 - \tfrac{1}{2}u_4)\frac{1}{l} + \tfrac{1}{2}(-\tfrac{11}{2}u_1 + 9u_2 - \tfrac{9}{2}u_3 + u_4)\frac{1}{\sqrt{lr}} + \\ \tfrac{27}{4}(-u_1 + 3u_2 - 3u_3 + u_4)\frac{r}{l\sqrt{lr}} \tag{11}$$

When compared to the quadratic order element, there is an additional $r^{3/2}$ term in the displacement fields and an $r^{1/2}$ term in the strain fields. As discussed in Volume 2, Chapter 3, the expression for the series solution for the near crack-tip strain field is

$$\varepsilon = \frac{B_1}{\sqrt{r}} + \sum_{n=1}^{\infty} B_n r^{(n-1)/2} \; . \tag{12}$$

The strain terms in the cubic element correspond to the first three terms in this expansion. Additional terms in the expansion can be modeled by using elements with higher order basis functions.

2.2.2 Hierarchical singular elements

The preceding discussion regarding cubic isoparametric elements is largely of academic interest because cubic elements are not widely used in practice. A related topic of more practical interest is elements with hierarchical basis functions. These elements are typically used with the "p-version" of the finite element method (Szabo, 1991).

There are a number of different ways to formulate hierarchical finite elements. One popular way is to start with linear Lagrange shape functions that interpolate the displacements of the element's corner nodes. To these are added higher order shape functions based on Legendre polynomials. The higher order shape functions are "nodeless", meaning that they are associated with generalized displacements not associated with the physical displacement of any particular location in the element.

In general, hierarchical elements are not isoparametric. That is, different orders, and potentially different families, of basis functions are used for interpolating the element's geometry and the displacements within the element.

To develop a singular hierarchical element we can use second order Lagrange shape functions with the center node located at the quarter-point to interpolate the geometry of the element. This means that the relationship between the element's parametric space and the Cartesian space will be:

$$\xi = \frac{2\sqrt{lr}}{l} - 1. \tag{13}$$

Other schemes for geometry interpolation can be used providing they result in a similar relationship between the geometry mappings in the element's parametric and Cartesian space (e.g., cubic Lagrange polynomials with the center nodes position at the 1/9-th and 4/9-th positions).

The first order basis functions for interpolating displacements within the element are:

$$u^{h1} = -\tfrac{1}{2}(\xi - 1)u_1 + \tfrac{1}{2}(\xi + 1)u_2 \tag{14}$$

The superscript *h*1 here indicate that this is the first-order hierarchical term. Substituting Equation 13 into 14 gives the following expression for the displacement variation in the element:

$$u^{h1} = u_1 + (-u_1 + u_2)\frac{\sqrt{lr}}{l}\,. \tag{15}$$

The corresponding strain variation is

$$\varepsilon^{h1} = \tfrac{1}{2}(-u_1 + u_2)\frac{1}{\sqrt{lr}} \tag{16}$$

that is the first term of equation 12.

Higher order elements are developed by adding "nodeless" basis function based on Legendre polynomials to the linear interpolation. For example, the second order displacement and strain variations are:

$$u^{h2} = u^{h1} + (\xi^2 - 1)a_3 = u^{h1} + 4a_3\left(-\frac{\sqrt{lr}}{l} + \frac{r}{l}\right) \tag{17}$$

and

$$\varepsilon^{h2} = \varepsilon^{h1} + 4a_3\left(-\frac{2}{\sqrt{lr}} + \frac{1}{l}\right) . \tag{18}$$

That is, the second order basis functions generate expressions associated with the first two terms of equation 12.

The expression for the third order elements is:

$$u^{h3} = u^{h2} + 2(\xi^3 - \xi)a_4 = u^{h2} + 8a_4\left(\frac{\sqrt{lr}}{l} - 3\frac{r}{l} + 2\frac{r\sqrt{lr}}{l^2}\right) \tag{19}$$

and

$$\varepsilon^{h3} = \varepsilon^{h2} + 4a_4\left(\frac{1}{\sqrt{lr}} - 6\frac{1}{l} + 4\frac{r}{l\sqrt{lr}}\right) , \tag{20}$$

that adds terms associated with the first three terms of equation 12. This pattern continues when higher order Legendre polynomials are used in the element. For example, the expressions for the fourth order element are:

$$\begin{aligned} u^{h4} &= u^{h3} + \frac{3}{4}(5\xi^4 - 6\xi^2 + 1)a_5 \\ &= u^{h3} + 12a_4\left(-\frac{\sqrt{lr}}{l} - 6\frac{r}{l} + 10\frac{r\sqrt{lr}}{l^2} + 5\frac{r^2}{l^2}\right) \end{aligned} \tag{21}$$

and

$$\varepsilon^{h4} = \varepsilon^{h3} + 6a_4\left(-\frac{1}{\sqrt{lr}} + 12\frac{1}{l} - 30\frac{r}{l\sqrt{lr}} + 20\frac{r}{l^2}\right) \qquad (22)$$

In summary, provided the mapping of geometry in a hierarchical element is similar to that given equation 13, as higher polynomial orders are used to interpolate the displacements in the element, higher order terms in the theoretical crack-tip displacement, stress, and strain fields will be modeled.

2.3 Two-Dimensional Quarter-Point Elements

Expression 7 demonstrates that the quarter-point elements shown in Figure 1 have the desired strain (and stress) singularities along the quarter-point element edges (edges 1-5-2 and 1-7-4). However, this may not necessarily be the case for all rays through the element emanating from the crack tip.

For the collapsed triangular form, Figure 1b, Barsoum (1977) showed that the proper singular form is obtained along all rays provided that the side node on the edge opposite the crack tip (node 6) is placed at the mid-point between the two corner nodes (nodes 2 and 3). Freese and Tracy (1976) showed that the $r^{-1/2}$ singularity holds along paths of constant parametric coordinate η, (see Figure 3a). When the opposite side node is mid-way between the corner nodes, lines of constant η map into straight rays emanating from the crack tip in the Cartesian space (Figure 3b). However, when the node is moved from the center position, lines of constant η map into quadratic curves in the Cartesian space (Figure 3c). The $r^{-1/2}$ singularity holds along these curves but not along straight rays.

Freese and Tracey (1976) have shown that the, so called, natural triangle quarter-point element, Figure 4, reproduces the $r^{-1/2}$ singularity along all rays emanating from the crack tip regardless of the placement of the node opposite the crack front.

Another triangular quarter point element is a collapsed 9-noded element. Manu (1985) showed that this element produces square root behavior along all rays provided the far side node is mid-way between the far corner points and that the central node is also moved to the quarter-point position.

The quadrilateral quarter-point element shown in Figure 1a has been used less frequently in practice than the triangular versions. This may in part be because fewer of these elements can be placed conveniently around a crack tip. With fewer elements, the (trigonometric) circumferential variation of the stress and displacement fields about a crack tip may be less accurately represented than in the triangular case where more elements can be used.

The unpopularity may also be due in part to a note published by Hibbitt (1977) that claimed that the element's strain energy, and hence stiffness, was unbounded. This assertion has since been demonstrated not to be true (Ying, 1982; Banks-Sills, 1984).

Banks-Sills and Bortman (1984) demonstrated that this element has a square root singularity along all rays emanating from the crack tip, but only in a small neighborhood near the tip (shown schematically in Figure 5), and only if the element has a rectangular shape (Banks-Sills, 1987). Banks-Sills and Einav (1985) show that the region of singular stresses is slightly larger for 9-noded quadrilateral elements providing the central node is suitably positioned (at a location on the diagonal between the crack-tip and the far corner, 11/32nds of the distance from the crack-tip).

2.4 Three-Dimensional Quarter-Point Elements

Three-dimensional quarter-point elements can be created by extruding the 2-D forms along the crack front. Barsoum (1976) discussed the use of a collapsed 20-noded brick element as a natural extension of the collapsed 8-noded quadrilateral. He considered straight-sided elements were all three element faces were rectangles.

Hussain, *et. al.* (1981), Manu (1983), and Koers (1989) considered collapsed 20-noded elements with curved crack fronts. Manu gives constraints on node positioning that must be observed to insure the proper square root singularity on all rays emanating from the crack front. With respect to Figure 6a, the constraints one might expect are

$$\begin{array}{lll} x_1 = x_4 = x_{12} & x_{17} = x_{20} & x_5 = x_8 = x_{16} \\ x_{10} = (x_1 + x_3)/2 & x_{14} = (x_6 + x_7)/2 & x_9 = (x_1 + x_2)/4 \\ x_{11} = (x_1 + x_3)/4 & x_{13} = (x_5 + x_6)/4 & x_{15} = (x_5 + x_7)/4 \end{array} \tag{23a}$$

In addition, the less obvious conditions

$$x_{18} = (-x_1 + x_2 - x_5 + x_6 + 2x_{17})/2 \qquad x_{19} = (-x_1 + x_3 - x_5 + x_7 + 2x_{17})/2 \tag{23b}$$

must be enforced. Similar conditions hold for the *y* and *z* coordinates of the nodes.

Manu (1985) showed that square root singular behavior holds for 21-noded elements provided node placements similar to those given by equation 23 are followed. However, this result is primarily of academic interest as 21-noded elements are used only infrequently in practice.

The 15-noded natural wedge element shown in Figure 6b is of practical interest. If the following node placement rules, similar to equation 23, are observed,

$$\begin{aligned} x_7 &= (x_1 + x_2)/4 \qquad & x_9 &= (x_1 + x_3)/4 \\ x_{10} &= (x_4 + x_5)/4 \qquad & x_{12} &= (x_4 + x_6)/4 \end{aligned} \tag{24}$$
$$x_{14} = (-x_1 + x_2 - x_4 + x_5 + 2x_{13})/2$$
$$x_{15} = (-x_1 + x_3 - x_4 + x_6 + 2x_{13})/2$$

it is easily shown that the determinant of the Jacobian mapping matrix is singular along the crack front, a necessary condition for square root singular behavior. However, the authors are not aware of a published proof of square root singular behavior along all rays emanating from the crack front. Given Freese and Tracey's (1976) results for the natural triangle it is likely that such behavior exits. The authors' experience is that these elements work well in practice.

Koers showed that if a 20-noded element is further collapsed to a pyramid, Figure 7a, a square root singularity is found along all rays emanating from the collapse node.

It is relatively straightforward to show that similar behavior is obtained in the quarter-point version of a natural 10-noded tetrahedral element, Figure 7b. However, the practical use of these element forms is somewhat limited because the singular behavior is seen at only one point in the element. A potential situation where these elements could be used is modeling a crack front meeting a free surface at a relatively large or relatively small angle.

The behavior of hexahedral crack-front elements has been studied by Banks-Sills (1988) and Banks-Sills and Sherman (1989). They show that for a straight crack front, Figure 8, if the nodes are placed so that the element forms a rectangular parallelepiped then square root singularity is reproduced on all rays emanating from the crack front in each cross-section perpendicular to the front. The square root behavior is seen in a small neighborhood near the crack front similar to that illustrated in Figure 5.

For circular crack fronts they show that square root behavior is observed in all planes perpendicular to the crack front provided the element edges on and parallel to the crack front are curved to form an arc of a circle, Figure 9a. A trapezoidal, straight-sided version of this element, Figure 9b exhibits square root singularity only on the element faces, not on all cross sections. Similarly, they showed that for elliptical crack fronts, if the side faces form hyperbolic surfaces locally normal to the front, as in Figure 10, then a square root singularity is observed on all hyperbolic surfaces perpendicular to the crack front.

As a practical matter, if the size of the crack front elements is small relative to the crack front curvature, the difference in geometry between the circular and elliptical/hyperbolic elements and the trapezoidal approximation would be small, and one might expect that the performance of the trapezoidal elements would be acceptable. Their use seems reasonable for the more general case where one does not have an analytical description of the crack front shape.

2.4 Summary

In this section it was shown that the LEFM-predicted stress, strain, and displacement fields can be accurately modeled with standard, second-order, isoparametric elements, provided that the side nodes are moved to the quarter-points. In addition, it was shown that if the quarter-point geometry mapping is used for hierarchical elements, then as terms are added to the polynomial order of the element, additional terms of the LEFM crack-tip fields are modeled. A number of different two- and three-dimensional quarter-point configurations were presented.