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On the use of quarter-point tetrahedral finite elements in linear elastic fracture mechanics

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Abstract

This paper discusses the reproduction of the square root singularity in quarter-point tetrahedral (QPT) finite elements. Numerical results confirm that the stress singularity is modeled accurately in a fully unstructured mesh by using QPTs. A displacement correlation (DC) scheme is proposed in combination with QPTs to compute stress intensity factors (SIF) from arbitrary meshes, yielding an average error of 2 – 3%. This straightforward method is computationally cheap and easy to implement. The results of an extensive parametric study also suggest the existence of an optimum mesh-dependent distance from the crack front at which the DC method computes the most accurate SIFs.

Keywords: Quarter-point tetrahedral finite element, Singular element, Stress intensity factor, Unstructured mesh, Displacement correlation.

1. Introduction

Inherent flaws and cracks exist in many materials and structures; as a result, analyzing cracks in bodies has attracted much attention in a variety of fields, including material science, structural engineering, and oil and gas reservoir engineering. In the context of Linear Elastic Fracture Mechanics (LEFM), the accurate computation of stress intensity factors (SIFs) is the first step in analyzing cracked bodies. The SIFs fully characterize the stress state adjacent to the crack, and therefore they are the key factors in the accurate estimation of the onset of crack propagation. The SIFs can be calculated analytically or experimentally only for a few simple crack configurations, and the use of numerical techniques such as the finite element (FE) method is unavoidable for more complicated crack problems. The use of the FE method to analyze crack problems, however, involves a major difficulty which lies in capturing the high stress gradient near the crack and accurately reproducing the crack tip singular stress field. This is the reason for conducting numerous investigations in the last four decades on the accurate and reliable FE methods for modeling crack problems.

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The use of FE method to solve crack problems gained great popularity in early 1970s. Soon after the poor performance of conventional elements in capturing singular stress field adjacent to the crack was identified. This is because the field variables in conventional finite elements are interpolated by polynomials which are not able to reproduce the crack tip singular stress field. Significant contributions were made by Barsoum (1976) and Henshell and Shaw (1975) who independently showed that the singularity at the crack tip can be properly modeled by placing the mid-side node near the crack tip or front at the quarter-point position. Due to a nonlinear mapping, these so-called quarter-point/singular elements reproduce square root stress singularity. The following three types of elements have been studied and used for modeling 3D cracks: collapsed quarter-point hexahedra, quarter-point pentahedrals, and quarter-point bricks. Among these, the collapsed quarter-point hexahedra have been very popular for modeling crack problems, for two main reasons: (i) these elements reproduce the singular stress field near the crack accurately. (ii) straight-forward algorithms like displacement correlation and domain integral methods have been available for these elements to extract the SIFs from the FE solution. However, the use of these elements requires the generation of a fully structured mesh around the crack front. Generating such meshes in an arbitrary cracked geometry is very difficult and cumbersome, and for complex crack and body configurations it may not be feasible.

These meshing restrictions encouraged researchers to make more use of tetrahedra in dealing with crack problems. One proposed methodology is based on the combination of hexahedral and tetrahedral elements. This takes advantage of the good performance of collapsed quarter-point hexahedral elements at the crack front region, and the efficiency of the tetrahedral elements for meshing complicated geometries. One approach is to discretize the neighborhood region of the crack by hexahedra, and remote region by tetrahedra (Bremberg and Dhondt, 2008, 2009; Bremberg and Faleskog, 2015). The major drawback is that either tie constraints or transition pyramid elements are required at the interface region between hexahedral and tetrahedral elements. This is because the node structures of these two types of elements are incompatible at their interface. In another approach, one analysis is performed to model the global structure by tetrahedra, and then by mapping the FE-solution, a sub-model is generated to solve for the near-crack fields using hexahedra (Schöllmann et al., 2003; Rabold et al., 2013; Rabold and Kuna, 2014). This approach is computationally expensive, as it requires performing two FE model analyses, and complications may arise in sub-modeling procedures. All these complications have recently encouraged the use of pure tetrahedra in an unstructured and arbitrary mesh to model the entire cracked body domain. Unlike the other types of elements, tetrahedra can be used in a fully unstructured and arbitrary mesh, such as are required to mesh dense three-dimensional fracture patterns. This methodology has been successfully applied in the context of crack propagation (Paluszny and Zimmerman, 2011) as well as fragmentation (Paluszny et al., 2013). However, the applicability, efficiency, and accuracy of tetrahedral elements for modeling crack singular fields have not been well investigated in the literature.

In order to prove the applicability and reliability of tetrahedral elements in crack problems, two major steps are required. (i) The efficiency of quarter-point tetrahedral elements for reproducing square root stress singularity must be investigated. Unlike other types of quarter-point elements, which have been addressed well enough in the literature (see Section 2), no research has evaluated the applicability and efficiency of the quarter-point tetrahedra in reproducing crack front singular

stress field. (ii) Accurate, efficient and reliable methods have to be introduced to extract the fracture parameters from the FE solution of tetrahedra. Existing methods to extract the J -integral and the SIFs using tetrahedral elements are complex, and often suffer from oscillations (Červenka and Saouma, 1997; Rajaram et al., 2000; Paluszny and Zimmerman, 2011), while others require very fine meshes near the crack front, rely on complicated numerical procedures, and are applied on arbitrary domain shapes and sizes (Okada et al., 2008; Daimon and Okada, 2014). This research discusses the behavior of quarter-point tetrahedra in reproducing the square root stress singularity at the crack front. A displacement correlation (DC) scheme is also proposed to compute very good approximations of the SIFs from unstructured meshes. The authors have recently developed a domain integral approach which computes SIFs with an average error of about 1% (Nejati et al., 2015). The results from both DC and domain integral methods provide considerable evidence on the reliability, efficiency and accuracy of the unstructured meshes by tetrahedral elements for analyzing cracked bodies.

2. A review on quarter-point finite elements

It is well known that conventional finite elements employ polynomials to interpolate field variables in the FE domain. Hence, they are not able to reproduce the crack tip square root singular stress field. Without any special formulation for the elements attached to the crack tip, a very fine mesh is required in order to obtain accurate field variables adjacent to the crack. Poor results of the FE solutions of crack problems by conventional elements were identified in the early 1970s, when many researchers suggested using special element formulations around the crack tip. These investigations mainly focused on the development of special crack tip elements (CTEs) in which the shape functions are able to reproduce the singular fields near the crack tip. These elements were used to discretize the immediate neighborhood of the crack tip, while the remainder of the domain is discretized with the conventional elements. The early development and use of CTEs for SIF computation can be found in (Byskov, 1970; Tracey, 1971, 1974; Benzley, 1974; Akin, 1976). The following are the major drawbacks that prevented CTEs to be successful: (i) the shape functions of the CTEs and conventional elements are not often compatible, and transition elements must be used to connect CTEs at the crack tip region to the conventional elements at the remote region; (ii) CTEs shape functions do not often permit constant strain and rigid body motion modes; (iii) implementation of the CTEs in commercial FE codes involves algorithmic peculiarities.

Significant development in the FE analysis of crack problems was made by Barsoum (1976) and Henshell and Shaw (1975) who proposed the idea of quarter-point elements (QPEs). They independently demonstrated that the singularity at the crack tip is properly modeled when the mid-side node near the crack tip is placed at the quarter-point position. This shift simply results in a nonlinear mapping between the natural and local coordinates by which an inverse square root stress singularity is reproduced throughout the element. With the use of QPEs, there was no need to incorporate CTEs into commercial FE codes since the entire domain of the cracked body is modeled with the same element. QPEs are simple in terms of the algorithmic implementation, the continuity of the shape functions between elements is automatically satisfied, and the rigid body motion and constant strains are included in the shape functions. These characteristics caused the QPEs to be extensively studied and used over the past four decades. Generally, the following types

of quarter-point elements have been employed for analyzing 2D and 3D crack problems:

(i) Quarter-point eight-noded quadrilateral element (Fig. 1a): This element is generated from an isoparametric eight-noded quadrilateral by shifting the mid-side nodes near the crack tip to the quarter-point position. Early investigators of the quarter-point quadrilateral elements showed some deficiencies, attributed to the incorrect assumptions that the rectangular element models the square root singularity only on the element boundaries (Barsoum, 1977), and that the strain energy of this element was incorrectly demonstrated to be unbounded (Hibbitt, 1977). However, Banks-Sills and Bortman (1984) demonstrated that stresses are square root singular at all rays emanating from the crack tip in a small region adjacent to the crack tip, expanding to the entire element along the element sides. It was also later proved that the strain energy and element stiffness is bounded in these elements (Banks-Sills and Bortman, 1984). For accurate results, the distortion of these elements from a rectangle should be minimum (Banks-Sills, 1987). Since these elements can poorly reproduce the angular distribution of stress due to the large element angle at the crack tip, they are used very rarely and they are discarded in favor of triangular elements (categories ii and iii).

[Figure 1 about here.]

(ii) Collapsed quarter-point eight-noded quadrilateral element (Fig. 1b): This element is degenerated by collapsing one side of a 8-noded isoparametric quadrilateral element to a point which is located at the crack tip, and moving the mid-side nodes near the crack tip to the quarter-point position. In LEFM application, the displacements of the nodes on the collapsed side are also coupled, to prevent blunting at the crack tip. This element models the required stress singularity at all rays emanating from the crack tip, and a group of these elements can be crafted in a fan-shape arrangement around the crack tip in order to accurately reproduce the angular variations of the crack tip fields. Any shape of this element may be used as long as the edges are straight lines (Freese and Tracey, 1976; Banks-Sills, 1987). This element has been frequently used for crack simulations, and has been implemented in several commercial FE tools (Kuna, 2013).

(iii) Quarter-point six-noded triangular elements (Fig. 1c): This element is developed by shifting the mid-side nodes near the crack tip of an isoparametric 6-noded triangular element to the quarter-point position. This QPE also reproduces square root stress singularity at all rays emanating from the crack tip. The shape makes it possible to lay many of these elements around the crack tip to represent the angular distribution of stress around the crack tip. Unlike collapsed quarter-point elements, the edge opposite to the crack tip can be curved in these elements (Freese and Tracey, 1976). Quarter-point triangular and collapsed quarter-point quadrilateral elements have been shown to be quite similar both analytically and numerically (Freese and Tracey, 1976; Wait, 1978; Lim et al., 1993).

(iv) Quarter-point twenty-noded brick elements (Fig. 1d): This element is generated from an isoparametric twenty-noded hexahedral by shifting the mid-side nodes near the crack front to the quarter-point position. Inverse square root singular fields are developed at all rays emanating from of crack front that lie in any cross-sectional orthogonal plane to the crack front. The region in which this singular behavior occurs is a small neighborhood of the crack front for the rays far from the element sides, becoming larger and expanding to the entire element along the element sides

(Banks-Sills, 1991). In the case of curved crack fronts, the mid-side nodes on the surface opposing the crack front must be moved to define a parabolic-cylindrical surface (Banks-Sills, 1991). Like quarter-point quadrilaterals, these elements are rarely used, because of the poor reproduction of angular distribution of stress due the large element angle at the crack front, and they are discarded in favour of the collapsed hexahedral and pentahedral elements (categories v and vi).

(v) Collapsed quarter-point twenty-noded brick elements (Fig. 1e): This element is generated by collapsing one face of 20-noded isoparametric brick element, which gives a wedge-shaped element, and moving the mid-side nodes near the crack to the quarter-point position. The displacements of the conformed nodes on the crack front are also constrained to model the crack sharpness in the LEFM applications (Barsoum, 1976; Koers, 1989). It reproduces the inverse square root stress singularity along all rays emanating from the crack tip. An accurate angular distribution is reproduced when a group of these elements are arranged around the crack front. In the case of curved crack fronts, the mid-side nodes of the element face opposing the crack front must be moved in a way that a parabolic-cylindrical surface is defined (Hussain et al., 1981; Manu, 1983).

(vi) Quarter-point fifteen-noded pentahedral element (Fig. 1f): This element is generated by placing the mid-side nodes near the crack front of an isoparametric fifteen-noded pentahedral at the quarter-point position. This element also reproduces square root stress singularity at all rays emanating from the crack front and lying in any cross-sectional orthogonal plane to the crack front (Kuna, 2013). An accurate angular distribution is reproduced by arranging a group of these elements around the crack front in a fan-shaped arrangement. In the case of curved crack fronts the mid-side nodes of the element face opposing the crack must also be moved to define a parabolic-cylindrical surface (Peano and Pasini, 1982).

Transition elements with appropriately placed side-nodes have also been suggested to be used along with the QPEs for more accurate computation of SIFs (Lynn and Ingraffea, 1978). These elements are placed between the QPEs and the remaining non-singular elements, resulting in more accurate stresses around the crack tip. However, the level of additional accuracy these elements offered was not high enough to make them popular. Various parameters, including the order of integration, element aspect ratio, number of elements surrounding the crack tip, use of transition elements, and the singular element length, may influence the accuracy of the FE results when using QPEs (Ingraffea and Manu, 1980; Saouma and Schwemmer, 1984; Murti and Valliappan, 1986; Jayaswal and Grosse, 1993). Ease of implementation, computational efficiency and excellent performance are the main advantages of QPEs, which has resulted in their frequent use over the past four decades.

3. Finite element formulation of tetrahedral elements

The mapping of the geometry and displacement fields of a ten-noded isoparametric tetrahedral element from the local coordinate system xyz into the natural coordinate system $\xi\eta\zeta$ ($0 \leq \xi, \eta, \zeta \leq 1$) is given by:

$$\begin{aligned} x(\xi, \eta, \zeta) &= \sum_{i=1}^{10} N_i x_i, \quad y(\xi, \eta, \zeta) = \sum_{i=1}^{10} N_i y_i, \quad z(\xi, \eta, \zeta) = \sum_{i=1}^{10} N_i z_i \\ u(\xi, \eta, \zeta) &= \sum_{i=1}^{10} N_i u_i, \quad v(\xi, \eta, \zeta) = \sum_{i=1}^{10} N_i v_i, \quad w(\xi, \eta, \zeta) = \sum_{i=1}^{10} N_i w_i \end{aligned} \quad (1)$$

in which N_i is the shape function corresponding to the node i with coordinates (x_i, y_i, z_i) in the local space, and (u_i, v_i, w_i) are the displacements of the node i in the x, y and z directions, respectively (Fig. 2). The shape functions of a ten-noded tetrahedral finite element are given by:

$$\begin{aligned} N_1 &= \lambda(2\lambda - 1), \quad N_2 = \xi(2\xi - 1), \quad N_3 = \eta(2\eta - 1), \quad N_4 = \zeta(2\zeta - 1) \\ N_5 &= 4\lambda\xi, \quad N_6 = 4\xi\eta, \quad N_7 = 4\lambda\eta, \quad N_8 = 4\lambda\zeta, \quad N_9 = 4\xi\zeta, \quad N_{10} = 4\eta\zeta \end{aligned} \quad (2)$$

[Figure 2 about here.]

where $\lambda = 1 - \xi - \eta - \zeta$. Using the infinitesimal strain theory, the Cauchy strains are obtained from the displacement fields as:

$$\boldsymbol{\varepsilon} = \begin{Bmatrix} \varepsilon_{xx} \\ \varepsilon_{yy} \\ \varepsilon_{zz} \\ \varepsilon_{xy} \\ \varepsilon_{yz} \\ \varepsilon_{xz} \end{Bmatrix} = \begin{Bmatrix} \frac{\partial u}{\partial x} \\ \frac{\partial v}{\partial y} \\ \frac{\partial w}{\partial z} \\ \frac{\partial u}{\partial y} + \frac{\partial v}{\partial x} \\ \frac{\partial w}{\partial y} + \frac{\partial v}{\partial z} \\ \frac{\partial u}{\partial z} + \frac{\partial w}{\partial x} \end{Bmatrix} = \begin{Bmatrix} \frac{\partial \mathbf{N}^T}{\partial x} \mathbf{u} \\ \frac{\partial \mathbf{N}^T}{\partial y} \mathbf{v} \\ \frac{\partial \mathbf{N}^T}{\partial z} \mathbf{w} \\ \frac{\partial \mathbf{N}^T}{\partial y} \mathbf{u} + \frac{\partial \mathbf{N}^T}{\partial x} \mathbf{v} \\ \frac{\partial \mathbf{N}^T}{\partial z} \mathbf{v} + \frac{\partial \mathbf{N}^T}{\partial y} \mathbf{w} \\ \frac{\partial \mathbf{N}^T}{\partial z} \mathbf{u} + \frac{\partial \mathbf{N}^T}{\partial x} \mathbf{w} \end{Bmatrix} \quad (3)$$

where $\mathbf{N}^T = \{N_1, \dots, N_{10}\}$ is the vector of shape functions, and $\mathbf{u}^T = \{u_1, \dots, u_{10}\}$, $\mathbf{v}^T = \{v_1, \dots, v_{10}\}$ and $\mathbf{w}^T = \{w_1, \dots, w_{10}\}$ are the vectors of nodal displacements in x, y , and z directions, respectively. The partial derivatives of the shape functions with respect to x, y and z are computed using the so-called Jacobian matrix inverse as follows:

$$\begin{Bmatrix} \frac{\partial N_i}{\partial x} \\ \frac{\partial N_i}{\partial y} \\ \frac{\partial N_i}{\partial z} \end{Bmatrix} = \mathbf{J}^{-1} \begin{Bmatrix} \frac{\partial N_i}{\partial \xi} \\ \frac{\partial N_i}{\partial \eta} \\ \frac{\partial N_i}{\partial \zeta} \end{Bmatrix}, \quad \mathbf{J} = \begin{bmatrix} \frac{\partial x}{\partial \xi} & \frac{\partial y}{\partial \xi} & \frac{\partial z}{\partial \xi} \\ \frac{\partial x}{\partial \eta} & \frac{\partial y}{\partial \eta} & \frac{\partial z}{\partial \eta} \\ \frac{\partial x}{\partial \zeta} & \frac{\partial y}{\partial \zeta} & \frac{\partial z}{\partial \zeta} \end{bmatrix} \quad (4)$$

By combining Eqs. (3) and (4), the vector of strains is given by

$$\varepsilon = \hat{\mathbf{J}}\mathbf{C} \{u_1 \ v_1 \ w_1 \ \dots \ u_{10} \ v_{10} \ w_{10}\}^T \quad (5)$$

in which

$$\hat{\mathbf{J}} = \begin{bmatrix} \mathbf{J}_{11}^{-1} & 0 & 0 & \mathbf{J}_{12}^{-1} & 0 & 0 & \mathbf{J}_{13}^{-1} & 0 & 0 \\ 0 & \mathbf{J}_{21}^{-1} & 0 & 0 & \mathbf{J}_{22}^{-1} & 0 & 0 & \mathbf{J}_{23}^{-1} & 0 \\ 0 & 0 & \mathbf{J}_{31}^{-1} & 0 & 0 & \mathbf{J}_{32}^{-1} & 0 & 0 & \mathbf{J}_{33}^{-1} \\ \mathbf{J}_{21}^{-1} & \mathbf{J}_{11}^{-1} & 0 & \mathbf{J}_{22}^{-1} & \mathbf{J}_{12}^{-1} & 0 & \mathbf{J}_{23}^{-1} & \mathbf{J}_{13}^{-1} & 0 \\ 0 & \mathbf{J}_{31}^{-1} & \mathbf{J}_{21}^{-1} & 0 & \mathbf{J}_{32}^{-1} & \mathbf{J}_{22}^{-1} & 0 & \mathbf{J}_{33}^{-1} & \mathbf{J}_{23}^{-1} \\ \mathbf{J}_{31}^{-1} & 0 & \mathbf{J}_{11}^{-1} & \mathbf{J}_{32}^{-1} & 0 & \mathbf{J}_{12}^{-1} & \mathbf{J}_{33}^{-1} & 0 & \mathbf{J}_{13}^{-1} \end{bmatrix} \quad \mathbf{C} = \begin{bmatrix} \frac{\partial N_1}{\partial \xi} & 0 & 0 & \dots & \frac{\partial N_{10}}{\partial \xi} & 0 & 0 \\ 0 & \frac{\partial N_1}{\partial \xi} & 0 & \dots & 0 & \frac{\partial N_{10}}{\partial \xi} & 0 \\ 0 & 0 & \frac{\partial N_1}{\partial \xi} & \dots & 0 & 0 & \frac{\partial N_{10}}{\partial \xi} \\ \frac{\partial N_1}{\partial \eta} & 0 & 0 & \dots & \frac{\partial N_{10}}{\partial \eta} & 0 & 0 \\ 0 & \frac{\partial N_1}{\partial \eta} & 0 & \dots & 0 & \frac{\partial N_{10}}{\partial \eta} & 0 \\ 0 & 0 & \frac{\partial N_1}{\partial \eta} & \dots & 0 & 0 & \frac{\partial N_{10}}{\partial \eta} \\ \frac{\partial N_1}{\partial \zeta} & 0 & 0 & \dots & \frac{\partial N_{10}}{\partial \zeta} & 0 & 0 \\ 0 & \frac{\partial N_1}{\partial \zeta} & 0 & \dots & 0 & \frac{\partial N_{10}}{\partial \zeta} & 0 \\ 0 & 0 & \frac{\partial N_1}{\partial \zeta} & \dots & 0 & 0 & \frac{\partial N_{10}}{\partial \zeta} \end{bmatrix} \quad (6)$$

In this equation, the so-called $\mathbf{B}$ matrix is written as the multiplication of an extended version of the Jacobian matrix inverse, $\hat{\mathbf{J}}$, by $\mathbf{C}$ which contains the derivatives of shape functions with respect to the natural coordinates ($\mathbf{B} = \hat{\mathbf{J}}\mathbf{C}$). According to Eq. (2), the shape functions are in the form of polynomials, and therefore their derivatives with respect to the local coordinates are non-singular. Therefore, as long as the Jacobian matrix determinant is non-zero, the strains are non-singular. The singularity of strains, however, occurs when the determinant of the Jacobian matrix becomes zero. Considering linear elastic behavior, and in the absence of initial strain and initial residual stress, the stress components are determined by $\sigma = \mathbf{D}\varepsilon$, where $\mathbf{D}$ is the elasticity matrix containing the material properties. Using the principle of minimum potential energy or the principle of virtual work, the element stiffness matrix is developed by integration over the element domain V as

$$\mathbf{K}^e = \int_V \mathbf{B}^T \mathbf{D} \mathbf{B} dV = \int_V \mathbf{C}^T \hat{\mathbf{J}}^T \mathbf{D} \hat{\mathbf{J}} \mathbf{C} dV \quad (7)$$

As the strains near a linear elastic crack front are square root singular, enabling the elements adjacent to the crack front to reproduce a square root strain singularity results in a more accurate finite element solution. In a standard tetrahedral element with straight edges, the components of the Jacobian matrix inverse depend only on the coordinates of the corner nodes. Therefore, the strains and stresses can only vary linearly within these elements. However, a square root singular behavior can be achieved by moving the mid-side nodes near the crack front to the quarter-point position. This shift makes the integrand in the stiffness matrix in Eq. (7) a singular function of order 1, as the strain singularity is of order 1/2.

4. Quarter-point tetrahedral finite elements

A fully unstructured mesh of a 3D cracked body mainly generates two types of tetrahedral elements surrounding the crack front: (i) tetrahedra which share a corner node with the crack

front; (ii) tetrahedra which share an edge with the crack front (see Fig. 3). Accordingly, shifting the mid-side nodes near the crack front to the quarter-point position also generates two types of quarter-point elements: (i) corner-based quarter-point tetrahedra (CQPT); and (ii) edge-based quarter-point tetrahedra (EQPT) as shown in Figs. 4a and 4b. It is noteworthy that in very coarse meshes and very curved crack fronts, some tetrahedra can share two edges with the crack front (see element iii in Fig. 3). Nevertheless, these elements are rarely generated in mesh resolutions which are fine enough to be suitable for the high stress gradients near the crack front. As these elements can barely capture properly the fields variations at the crack front, they must be degenerated into two tetrahedra in case they occur. None of these elements was observed in meshes used in Sections 6 and 7.

[Figure 3 about here.]

4.1. Corner-based quarter-point tetrahedral (CQPT)

Consider the CQPT shown in Fig. 4a in which nodes 5, 7 and 8 are moved to the quarter-point position from node 1. Considering a straight-sided tetrahedral, and assuming the corner node i is located at the position (x_i, y_i, z_i) , the positions of mid-side and quarter-point nodes are given in terms of the corner nodes coordinates as:

$$\begin{aligned} x_5 &= (3x_1 + x_2)/4, \quad y_5 = (3y_1 + y_2)/4, \quad z_5 = (3z_1 + z_2)/4 \\ x_6 &= (x_2 + x_3)/2, \quad y_6 = (y_2 + y_3)/2, \quad z_6 = (z_2 + z_3)/2 \\ x_7 &= (3x_1 + x_3)/4, \quad y_7 = (3y_1 + y_3)/4, \quad z_7 = (3z_1 + z_3)/4 \\ x_8 &= (3x_1 + x_4)/4, \quad y_8 = (3y_1 + y_4)/4, \quad z_8 = (3z_1 + z_4)/4 \\ x_9 &= (x_2 + x_4)/2, \quad y_9 = (y_2 + y_4)/2, \quad z_9 = (z_2 + z_4)/2 \\ x_{10} &= (x_3 + x_4)/2, \quad y_{10} = (y_3 + y_4)/2, \quad z_{10} = (z_3 + z_4)/2 \end{aligned} \quad (8)$$

Assume without loss of generality that the local Cartesian coordinate system xyz is located at node 1 as shown in Fig. 4a ($x_1 = y_1 = z_1 = 0$). The mapping between the natural coordinate $\xi\eta\zeta$ and the local coordinate xyz , and the polar distance from the z axis, r , are given as:

$$\begin{aligned} x &= (\xi + \eta + \zeta)(\xi x_2 + \eta x_3 + \zeta x_4) \\ y &= (\xi + \eta + \zeta)(\xi y_2 + \eta y_3 + \zeta y_4) \\ z &= (\xi + \eta + \zeta)(\xi z_2 + \eta z_3 + \zeta z_4) \\ r &= (\xi + \eta + \zeta) \sqrt{(\xi x_2 + \eta x_3 + \zeta x_4)^2 + (\xi y_2 + \eta y_3 + \zeta y_4)^2} \end{aligned} \quad (9)$$

[Figure 4 about here.]

A ray emanating from node 1 in the plane perpendicular to the crack front ($z = 0, y = \rho x$) is mapped into $\eta = \alpha_1 \xi$ and $\zeta = \alpha_2 \xi$ in natural coordinate system, where α_1 and α_2 are functions of nodal coordinates and ρ (see Appendix A). By substituting these relations into Eq. (9), the distance from the z axis is given by $r = \gamma_1 \xi^2$, and the Jacobian matrix inverse is developed as:

$$\mathbf{J}^{-1} = \frac{\sqrt{\gamma_1}}{c_1 \sqrt{r}} \begin{bmatrix} p_{11} & p_{12} & p_{13} \\ p_{21} & p_{22} & p_{23} \\ p_{31} & p_{32} & p_{33} \end{bmatrix} \quad (10)$$

Here γ_1 , c_1 and p_{ij} are functions of the nodal coordinates and ρ (see Eq. (A.1)). As it is seen, all the components of the Jacobian matrix inverse are square root singular. On the other hand, the components of $\mathbf{C}$ in Eq. (6) are linearly dependent on the natural coordinates. Along a ray emanating from node 1, these components have the form of either a square root function or a combination of constant and square root functions. As a result, from Eq. (5) any component of strain tensor appears as a combination of a singular square root term together with a constant term.

4.2. Edge-based quarter-point tetrahedral (EQPT)

This type of element has straight sides when used near straight crack fronts. However, the edge lying on the crack front becomes curved when this type of element is employed along a curved crack front.

4.2.1. EQPT along straight crack front

Consider a EQPT element shown in Fig. 4b where side 184 lies along the crack front and nodes 5, 7, 9 and 10 are moved to the quarter-point position. Assuming the corner node i is located at (x_i, y_i, z_i) , the mid-side and quarter-point nodes positions are given in terms of the corner nodes coordinates as:

$$\begin{aligned} x_5 &= (3x_1 + x_2)/4, & y_5 &= (3y_1 + y_2)/4, & z_5 &= (3z_1 + z_2)/4 \\ x_6 &= (x_2 + x_3)/2, & y_6 &= (y_2 + y_3)/2, & z_6 &= (z_2 + z_3)/2 \\ x_7 &= (3x_1 + x_3)/4, & y_7 &= (3y_1 + y_3)/4, & z_7 &= (3z_1 + z_3)/4 \\ x_8 &= (x_1 + x_4)/2, & y_8 &= (y_1 + y_4)/2, & z_8 &= (z_1 + z_4)/2 \\ x_9 &= (3x_4 + x_2)/4, & y_9 &= (3y_4 + y_2)/4, & z_9 &= (3z_4 + z_2)/4 \\ x_{10} &= (3x_4 + x_3)/4, & y_{10} &= (3y_4 + y_3)/4, & z_{10} &= (3z_4 + z_3)/4 \end{aligned} \quad (11)$$

Now consider the local Cartesian coordinate system xyz located at node 1 ($x_1 = y_1 = z_1 = 0$) in a way that the straight crack front lies along z axis ($x_4 = y_4 = 0$), as shown in Fig. 4b. The mapping between the natural coordinate $\xi\eta\zeta$ and the local coordinate xyz , and also the polar distance from the z axis, r , are given by:

$$\begin{aligned} x &= (\xi + \eta)(\xi x_2 + \eta x_3) \\ y &= (\xi + \eta)(\xi y_2 + \eta y_3) \\ z &= (\xi + \eta)(\xi z_2 + \eta z_3) + \zeta(1 + \xi + \eta)z_4 \\ r &= (\xi + \eta) \sqrt{(\xi x_2 + \eta x_3)^2 + (\xi y_2 + \eta y_3)^2} \end{aligned} \quad (12)$$

Consider a ray emanating from the point $(x, y, z) = (0, 0, d)$ lying on the plane $z = d$ stretching in the direction of $y = \rho x$. This ray is mapped into $\eta = \beta_1 \xi$ and $\zeta = (d + \beta_2 \xi^2)/(z_2 + \beta_3 \xi)$, in which $\beta_1 = -(y_2 - \rho x_2)/(y_3 - \rho x_3)$, $\beta_2 = -(\beta_1 + 1)z_2 - \beta_1(\beta_1 + 1)z_3$ and $\beta_3 = (\beta_1 + 1)z_4$, in the natural coordinate system. By substituting these relations into Eq. (12), the polar distance from the z axis is given by $r = \gamma_2 \xi^2$, and the inverse of the Jacobian matrix is developed as:

$$\mathbf{J}^{-1} = \frac{\sqrt{\gamma_2}}{c_2 \sqrt{r}} \begin{bmatrix} q_{11} & q_{12} & \frac{f_1 + f_2 \sqrt{r} + f_3 r}{h_1 + h_2 \sqrt{r} + h_3 r} \\ q_{21} & q_{22} & \frac{g_1 + g_2 \sqrt{r} + g_3 r}{h_1 + h_2 \sqrt{r} + h_3 r} \\ 0 & 0 & \frac{c_2 \sqrt{r}}{z_4[\gamma_2 + (1 + \beta_1) \sqrt{r}]} \end{bmatrix} \quad (13)$$

Here γ_2 , c_2 , q_{ij} , f_i , g_i , and h_i are functions of the nodal coordinates and ρ (see Eq. (A.2)). At the region close to the edge 184 ($r \rightarrow 0$) the components of the first two rows of Jacobian matrix inverse are square root singular. In addition, the components of $\mathbf{C}$ in Eq. (6) are linearly dependent of the natural coordinates. Along a ray emanating from the point $(x, y, z) = (0, 0, d)$ and normal to the edge 184, it was shown that $\eta = \beta_1 \xi$ and $\zeta = (d + \beta_2 \xi^2)/(z_2 + \beta_3 \xi)$. Considering a two term Taylor series for ζ about $\xi = 0$ at the region close to the edge 184, the components of $\mathbf{C}$ take the form of either a square root function or a combination of constant and square root functions. As a result, from Eq. (5) any component of strain tensor except ε_{zz} appears as a combination of the dominant terms of a singular square root and a constant. The normal strain along the crack front ε_{zz} , however, appears as a combination of a square root term together with a constant term. It is noteworthy that generally a plane strain condition prevails near the front of an embedded crack, and therefore the strain component ε_{zz} is non-singular.

4.2.2. EQPT along curved crack front

Most 3D embedded cracks have curved crack fronts, and therefore analyzing the performance of quarter-point tetrahedra along curved crack fronts is essential. For simplicity, consider a trirect-angular tetrahedral element of the leg length of L , as shown in Fig. 5. When this element is used as an EQPT along the curved crack front, edge 184 becomes curved and nodes 5, 7, 9 and 10 are placed at the quarter-point position. The curvature of the crack front is controlled by the position of node 8 with respect to nodes 1 and 4. Let us assume that node 8 is located at $(x_8, y_8, z_8) = (\delta_1, \delta_2, L/2)$. The mapping between the natural coordinates $\xi\eta\zeta$ and the local coordinates xyz is given by Eq. (14), which results in the formation of Jacobian matrix determinant, or simply called Jacobian, as in Eq. (15).

[Figure 5 about here.]

$$\begin{aligned} x &= L\xi(\xi + \eta) - 4\zeta\delta_1(\xi + \eta + \zeta - 1) \\ y &= L\eta(\xi + \eta) - 4\zeta\delta_2(\xi + \eta + \zeta - 1) \\ z &= L\zeta(1 + \xi + \eta) \end{aligned} \quad (14)$$

$$|\mathbf{J}| = 2L^2(\xi + \eta)[L(\xi + \eta)(1 + \xi + \eta) + 4\zeta(\zeta - 1)(\delta_1 + \delta_2)] \quad (15)$$

As it is seen in Eq. (15), the Jacobian vanishes both along the crack front ($\xi + \eta = 0$) and on the parabolic cylinder of $\xi + \eta = -1/2 + \sqrt{1/4 - 4\zeta(\zeta - 1)(\delta_1 + \delta_2)/L}$. The Jacobian also becomes negative in the region enclosed by the crack front and this parabolic cylinder (see Fig. 5). If the

Jacobian is found to be negative, the mapping for the element is not bijective, indicating that the region of the parent element enclosed by the edge and the parabolic cylinder has been mapped outside the boundary of the real element. The volume of the overlapped region, and therefore the integration error in the element stiffness matrix, depends on the curvature of the element edge, the element size, and the element aspect ratio. As δ_1 and δ_2 approach zero, the parabolic cylinder becomes narrower, and the numerical error decreases. This parabolic-cylindrical region with negative Jacobian also occurs in the quarter-point twenty-noded brick element (Banks-Sills, 1991), collapsed quarter-point twenty-noded brick element (Manu, 1983), and quarter-point fifteen-noded pentahedral element (Peano and Pasini, 1982), if the surface opposing the crack front remains planar. However, moving the mid-side nodes of that face opposing the crack front defines a parabolic-cylindrical surface, which makes the overlapped region near the crack front vanish. In the case of QPTs, however, there is no element face opposing the crack front elements, and therefore the overlapped region cannot be removed using such a technique. Here it is suggested that the mid-side nodes on the crack front are moved in order to make the EQPTs straight-sided.

4.3. Numerical integration

Despite the singularity of strains at one node in CQPT and along an edge in EQPT, these elements still satisfy the necessary conditions for finite element convergence (Zienkiewicz and Taylor, 1989). These conditions include: (1) Since the elements are isoparametric, inter-element compatibility and continuity are satisfied. (2) The shape functions accommodate the rigid body motion of the element. (3) The element deformation accommodates a constant strain form. (4) The strain energy in these elements is finite. This implies that although the strains are singular at a node or an edge, the components of stiffness matrix in Eq. (7) have finite values. However, in order for the FE convergence to occur, the required order of numerical integration in each element has to be met. In the case of standard quadratic tetrahedral, the lower bound for the number of Gauss points is four (Zienkiewicz and Taylor, 1989).

The lower bound for the number of Gauss points must integrate the volume of quarter-point tetrahedral exactly. This is because as the mesh is indefinitely refined, a constant strain and strain energy is approached throughout each element. In quarter-point tetrahedra, the Jacobian determinant is developed as $|\mathbf{J}| = 12V(\xi + \eta + \zeta)^3$ and $|\mathbf{J}| = 12V(\xi + \eta)^2(1 + \xi + \eta)$ for CQPT and EQPT, respectively, where V is the element volume. It can be shown that a four-point Gauss rule computes the volume of CQPT with 0.43% error, while it determines the exact volume of EQPT. As the CQPTs exist only in a small region near the crack front, this very small error can be neglected. Moreover, although higher-order integrations compute a more accurate stiffness matrix, they add significantly to the computation cost, while the improvement in the accuracy of the finite element solution might be trivial. In fact, the error in the reduced integration scheme may compensate for the overestimation of the structural stiffness, and some of the more complicated displacement modes show less resistance to deformation. Therefore, a reduced integration by a four-point Gauss rule seems to be suitable for the quarter-point tetrahedra. It is noteworthy that a higher order integration may be required for quarter-point tetrahedra when interface/contact elements are used on the crack surface.

Employing quarter-point tetrahedra also introduces quarter-point triangle elements over the crack surfaces (see Fig. 19). To compute the vector of nodal forces produced by surface trac-

tion, a numerical integration is required, for which the minimum order of integration has to be determined. The lower bound of the order of numerical integration must compute the area of quarter-point triangle elements exactly. Considering the Jacobian determinant for straight-sided quarter-point triangles, it can be shown that a three-point quadrature rule computes the area exactly. A higher order numerical integration improves the accuracy of the values of nodal forces produced by surface tractions. In fact, the numerical integration of order four, which requires six integration points, computes the exact values of nodal forces for a uniform surface traction. However, in this case the improvement in the accuracy of the crack tip fields and SIFs when increasing the order is trivial. Hence, a standard three-point Gauss rule, which is already recommended for standard quadratic triangular elements, is also suggested for quarter-point triangles. It is noteworthy that when a non-uniform surface traction is applied on the crack surfaces, or the quarter-point triangles perform as contact elements, a higher order integration may be necessary.

Although a strain singularity occurs at quarter-point tetrahedra, these elements seem to be less accurate than other types of quarter-point elements shown in Fig. 1. Element types collapsed quarter-point hexahedrals and quarter-point pentahedrals are crafted in a fan-shape arrangement around the crack front. Therefore, in addition to reproducing the required strain singularity in their entire domains, they accurately model the angular distributions of crack tip fields. This is not the case for the quarter-point tetrahedra, which are placed randomly around the crack front in arbitrary meshes, and their size and shape are not often controlled. This random arrangement leads to a considerable variation of the size of the QPTs along the crack front. Elements with large angles are also generated that poorly reproduce the angular distribution of the crack tip fields. Therefore, as is shown later in this paper, although QPTs perform significantly better than the standard tetrahedra, there might still be inaccuracies very close to the crack front. Some strategies, which are presented later in this paper, can be used to avoid these inaccuracies influencing the SIF results.

5. Displacement correlation (DC) method to extract SIFs

Techniques for the SIF computation from FE results generally fall into two categories: energy methods and direct approaches. Energy methods are based on the computation of energy released rate $\mathcal{G}$, and the use of the relationships between $\mathcal{G}$ and the SIFs to compute the SIFs indirectly (Irwin, 1956). Three main methods have been proposed to compute $\mathcal{G}$ under LEFM assumption: (i) J -integral, which is equivalent to $\mathcal{G}$ for elastic materials, was originally developed as a contour integral around the crack tip (Rice, 1968), and was later transformed into an equivalent domain integral (DeLorenzi, 1982; Li et al., 1985). (ii) Virtual crack extension (VCE) which was proposed by Parks (1974) and computes the rate of the change in total potential energy for a system for a small virtual extension of the crack. (iii) Virtual crack closure technique which was originally proposed by Rybicki and Kanninen (1977) and uses Irwin's crack closure integral. Direct approaches, on the other hand, are based on the comparison of FE stress or displacement distribution adjacent to the crack with the stress or displacement field expressions. Stress/displacement extrapolation and correlation are the main approaches in this category.

The direct methods based on displacements have been of more interest due to the fact that the FE displacement fields are the most accurate fields obtained from a FE solution. This methodology

was first developed for a general FE solution of a crack problem without using any CTEs or QPEs around the crack tip (Chan et al., 1970). As the FE results for stresses at crack tip are bounded in these solutions, the FE results for displacements are not very accurate close to the crack tip. To avoid these numerical inaccuracies very close the crack tip, Chan et al. (1970) proposed a linear extrapolation scheme. In this approach, the SIFs obtained from displacements at nodes along a ray emanating from the crack tip are extrapolated to the crack tip. The most accurate results were obtained when the extrapolation procedure was based on the displacements on the crack faces. A major drawback of the extrapolation method is that it is based on a relatively arbitrary extrapolation process which can be a source of error in the SIF computation. By the introduction of QPEs, Barsoum (1976) suggested a correlation scheme in which displacements of the quarter-point nodes are fitted to the crack tip displacement expressions. This method, which shall be referred to as displacement correlation (DC), does not require arbitrary extrapolation and computes the SIFs using the displacements of the two quarter-point nodes only, one on the top crack face and the other on the bottom one. Shih et al. (1976) then modified this correlation scheme by correlating the displacement distribution over the entire quarter-point element. This scheme uses the displacements of four nodes of quarter-point elements lying on the crack faces. Ingraffea and Manu (1980) generalized this approach to compute the SIFs for 3D crack configurations using collapsed quarter-point twenty-noded brick elements. The DC method is computationally very cheap and is able to yield very good approximations of the SIFs (Kuna, 2013).

The concept of employing the displacement fields to extract the SIFs has also been widely used in experimental fracture mechanics. The experimental methods like *moiré* and digital image correlation (DIC) provide the experimental displacement fields around the crack front (Dally and Riley, 1991; McNeill et al., 1987). In order to estimate the crack parameters from these fields, correlation methods are generally used to fit the local displacement data points to the established crack tip expressions. Some techniques such as the over-deterministic approach, which was originally developed for experimental estimation of the SIFs (Dally and Riley, 1991), have recently been applied to estimate the 2D crack and sharp notch parameters from the FE displacement solutions (Ayatollahi and Nejati, 2011a,b). This methodology is called the finite element over-deterministic (FEOD) approach, and is based on a least-square scheme to fit the displacements of a large number of points near the crack tip to the crack tip field expressions. This simple and straightforward method is able to compute very accurate results not only for the SIFs but also the higher order parameters of the crack tip asymptotic fields. This literature provides evidence to the applicability and efficiency of the near tip displacement fields for the accurate computation of the SIFs.

▶ The DC approach is conceptually simple and straight-forward, its results can be interpreted easily, and unlike displacement extrapolation, it does not require any arbitrary extrapolation procedure. Unlike energy methods which usually require further integration, which can be a source of error, the DC method directly use the FE nodal values to obtain the SIFs. Therefore, the level of the accuracy of the SIFs values obtained by this method directly indicates the level of the accuracy of the FE solution around the crack tip. However, the applicability and efficiently of the DC method on unstructured meshes has not been investigated so far. This section describes the application of this method on quarter-point tetrahedral elements in an unstructured mesh around the crack front. This is done in order to (i) develop a simple and straightforward method to provide computationally cheap approximations of the SIFs from the unstructured meshes, and (ii) evaluate

the accuracy of the quarter-point tetrahedra in reproducing the square root stress singularity near the crack front. As the DC method directly uses the FE fields to estimate the SIFs, the accuracy of fields obtained by the quarter-point tetrahedra can be assessed by investigating the accuracy of SIFs obtained from the DC method.

Generally, there is no analytical solution for the fields near the crack front of an arbitrary 3D crack configuration. However, it has been shown that asymptotically, as $r \rightarrow 0$, a plane strain condition prevails locally, so that the three-dimensional deformation fields approach the two-dimensional plane strain fields (Nakamura and Parks, 1988, 1989). Therefore, the 2D plane strain fields can be employed to express the stress/displacement fields near any point along the crack front. The so-called Williams series expansions describe the linear elastic stress fields for a 2D cracked plate subjected to an arbitrary load (Williams, 1957). In the region close to the crack tip, the first terms, singular terms, in these expansions are dominant, giving the singular stress fields near the crack tip. The stress field near any point on the crack front of 3D embedded cracks is therefore considered to be in the form of this singular field in the plane strain condition (Anderson, 2005):

$$\begin{pmatrix} \sigma_{xx} \\ \sigma_{yy} \\ \sigma_{xy} \\ \sigma_{zz} \end{pmatrix} = \frac{K_I}{\sqrt{2\pi r}} \begin{pmatrix} \cos \frac{\theta}{2} \left(1 - \sin \frac{\theta}{2} \sin \frac{3\theta}{2} \right) \\ \cos \frac{\theta}{2} \left(1 + \sin \frac{\theta}{2} \sin \frac{3\theta}{2} \right) \\ \cos \frac{\theta}{2} \sin \frac{\theta}{2} \cos \frac{3\theta}{2} \\ 2\nu \cos \frac{\theta}{2} \end{pmatrix} + \frac{K_{II}}{\sqrt{2\pi r}} \begin{pmatrix} \sin \frac{\theta}{2} \left(-2 - \cos \frac{\theta}{2} \cos \frac{3\theta}{2} \right) \\ \sin \frac{\theta}{2} \cos \frac{\theta}{2} \cos \frac{3\theta}{2} \\ \cos \frac{\theta}{2} \left(1 - \sin \frac{\theta}{2} \sin \frac{3\theta}{2} \right) \\ -2\nu \sin \frac{\theta}{2} \end{pmatrix} \quad (16)$$

$$\begin{pmatrix} \sigma_{xz} \\ \sigma_{yz} \end{pmatrix} = \frac{K_{III}}{\sqrt{2\pi r}} \begin{pmatrix} -\sin \frac{\theta}{2} \\ \cos \frac{\theta}{2} \end{pmatrix}$$

Here ν is the Poisson's ratio, and r and θ are the polar coordinates in the local Cartesian coordinate system xyz which is perpendicular to the crack front, as shown in Fig. 6a. At the meeting point of the crack front and free surfaces, where a plane strain condition is no longer valid, the definition of the stress intensity factor loses its meaning, as the order of singularity at these corners is different from the order of singularity at cracks (Nakamura and Parks, 1988, 1989). Therefore, the assumption of plane strain conditions is true anywhere on the crack front at which the definition of the SIFs exists. Using Eq. (16), the displacement fields adjacent to the crack tip are given as (Anderson, 2005):

$$\begin{aligned} \begin{Bmatrix} u \\ v \end{Bmatrix} &= \frac{K_I}{2\mu} \sqrt{\frac{r}{2\pi}} \begin{Bmatrix} \cos \frac{\theta}{2} \left(\kappa - 1 + 2 \sin^2 \frac{\theta}{2} \right) \\ \sin \frac{\theta}{2} \left(\kappa + 1 - 2 \cos^2 \frac{\theta}{2} \right) \end{Bmatrix} + \frac{K_{II}}{2\mu} \sqrt{\frac{r}{2\pi}} \begin{Bmatrix} \sin \frac{\theta}{2} \left(1 + \kappa + 2 \cos^2 \frac{\theta}{2} \right) \\ \cos \frac{\theta}{2} \left(1 - \kappa + 2 \sin^2 \frac{\theta}{2} \right) \end{Bmatrix} \\ w &= \frac{2K_{III}}{\mu} \sqrt{\frac{r}{2\pi}} \sin \frac{\theta}{2} \end{aligned} \quad (17)$$

where $\mu = E/2(1 + \nu)$ is the shear modulus, E and ν are the Young's modulus and Poisson's ratio, and κ is the Kolosov constant which is equal to $\kappa = 3 - 4\nu$ in the plane strain condition. Eq. (17) characterizes the distribution of the displacements in an orthogonal plane to the crack front ($z = 0$) as shown in Fig. 6a). Once the FE analysis is performed, the displacement field over the domain is available and the displacements near crack front can be employed to compute the SIFs by fitting the local FE displacements to the expressions in Eq. (17). The original DC method involves the correlation of the relative FE nodal displacements on the crack faces/surfaces with the crack tip displacement field expressions (Barsoum, 1976; Shih et al., 1976; Ingraffea and Manu, 1980). The displacements are recommended to be taken from the crack faces because there: (i) The displacement fields corresponding to different crack modes are uncoupled; (ii) The displacement corresponding to each mode has a significant value on the crack surfaces compared to other rays emanating from the crack tip, and therefore the relative numerical error in the displacement value is less on the crack surfaces; (iii) Since the relative displacements of the matched nodes lying on top and bottom crack surfaces are used, the rigid body translation and rotation of the crack cancels out (Ayatollahi and Nejati, 2011a). Using Eq. (17), the distribution of relative displacements of the top surface ($\theta = \pi$) with respect to the bottom surface ($\theta = -\pi$) e.g. $\Delta u = u_{\theta=\pi} - u_{\theta=-\pi}$, are given by:

$$\Delta u = K_{II} \left(\frac{\kappa + 1}{\mu} \right) \sqrt{\frac{r}{2\pi}}, \quad \Delta v = K_I \left(\frac{\kappa + 1}{\mu} \right) \sqrt{\frac{r}{2\pi}}, \quad \Delta w = K_{III} \left(\frac{4}{\mu} \right) \sqrt{\frac{r}{2\pi}} \quad (18)$$

[Figure 6 about here.]

When a 3D cracked body is discretized using a structured mesh, one of the three types of quarter-point elements described in Section 2 is often used at the crack front. Due to the special arrangement of these elements, the radial and angular sizes of the elements are fully controlled. Two lateral sides of the quarter-point elements are also constrained to be perpendicular to the crack front (Ingraffea and Manu, 1980; Kuna, 2013). In unstructured meshes, however, no constraint is imposed on the radial and angular sizes of quarter-point tetrahedra. Therefore, despite the reproduction of the singularity over the quarter-point tetrahedra, the displacement fields over these elements may not be as accurate as the fields obtained by the other three types of quarter-point elements. This is because the radial size of the quarter-point elements may vary significantly along the fracture front, and the angular dependence of the displacement fields can only be reproduced poorly due to their arbitrary, and often large, angles. The radial and angular distribution of crack

tip fields may not therefore be captured very accurately, even though the stress singularity has been reproduced. This inaccuracy may not influence the SIF computation when energy methods such as the J -integral are employed. This is because these methods rely on an integration over a domain, which reduces the influence of local numerical inaccuracies on the SIF computation (Nejati et al., 2015). However, the SIF values may be considerably influenced by the local numerical inaccuracies when local displacements are used in a displacement correlation scheme. Therefore, it is expected that a correlation method based on the displacement distribution over the quarter-point tetrahedral elements would be dependent not only on the local mesh size, but also on the quality of mesh near the crack front. In order to demonstrate this mesh dependency, a DC method has been developed in Appendix B, which employs the distribution over the entire CQPTs. The results from this approach, which are presented and discussed in Section 7.2, clearly reveal that the SIF accuracy is influenced significantly by the local mesh size and quality when using a correlation of the displacements over the entire quarter-point element.

In this research it is suggested that the crack tip displacement expressions are correlated with the relative displacements of two matched points located at a fixed distance from the crack front. Assume that two matched points m_+ and m_- located on the top and bottom surfaces of the crack, and the line connecting these matched points to the point s on the crack front is orthogonal to the crack front. These points have the coordinates (r_m, π) and $(r_m, -\pi)$ in the local coordinate system xyz located at the point s (see Fig. 6b). Since these points are located at a fixed distance r_m from the point s , they do not necessarily belong to the quarter-point tetrahedral elements. A search algorithm can find the tetrahedral and triangular elements that contain these points (see Appendix C). The natural coordinates of these points in their corresponding elements can also be determined by using the relations given in Appendix C. Once the natural coordinates are obtained, the displacements are readily computed using the shape functions. The relative displacement in the local coordinate system xyz are then given by $\Delta u = u_{m_+} - u_{m_-}$, $\Delta v = v_{m_+} - v_{m_-}$, and $\Delta w = w_{m_+} - w_{m_-}$. Due to the presence of symmetry in the geometry and symmetry/antisymmetry in the loading conditions, only one of the crack faces may be modeled. In these cases the crack is deformed under only one of the deformation modes, and the following relations hold: $v_{m_+} = -v_{m_-}$ for pure mode I, $u_{m_+} = -u_{m_-}$ for pure mode II, and $w_{m_+} = -w_{m_-}$ for pure mode III. Therefore, the relative displacement for half-crack models can be obtained by $\Delta u = 2u_{m_+} = -2u_{m_-}$, $\Delta v = 2v_{m_+} = -2v_{m_-}$, and $\Delta w = 2w_{m_+} = -2w_{m_-}$. By correlating the numerical values of the relative displacements with the expressions in Eq. (18), the pointwise SIFs at the point s are then computed from:

$$K_I = \sqrt{\frac{2\pi}{r_m}} \left(\frac{\mu}{\kappa + 1} \right) \Delta v, \quad K_{II} = \sqrt{\frac{2\pi}{r_m}} \left(\frac{\mu}{\kappa + 1} \right) \Delta u, \quad K_{III} = \sqrt{\frac{2\pi}{r_m}} \left(\frac{\mu}{4} \right) \Delta w \quad (19)$$

6. Numerical examples

In order to demonstrate the efficiency and the accuracy of the proposed displacement correlation approach, the SIFs were computed for the following three crack configurations: (i) through-the-thickness crack in a large thin plate with lateral constraint (plane strain condition); (ii) penny-shaped crack embedded in a large cube; and (iii) elliptical crack embedded in a large cube (see Fig. 7).

[Figure 7 about here.]

6.1. Experimental setup

All the cracked bodies are subjected to a uniform uniaxial tension in X_2 direction over the top and bottom surfaces. The cracks lie in the plane $X_2 = X_1 \cot \beta$ which makes an angle of β with the direction of applied load. A horizontal crack configuration ($\beta = 90^\circ$) produces pure mode I crack deformation, while the inclined one ($0^\circ < \beta < 90^\circ$) creates a mixed-mode condition. In these configurations a denotes half of the crack length for the through crack, crack radius for the penny-shaped crack, and semi-major axis for the elliptical crack. The semi-minor axis b of the elliptical crack is perpendicular to the X_1X_2 plane. A crack length to body width ratio of $a/w = 0.1$ was considered for all the cracked bodies. Crack length to plate thickness ratio of $a/t = 1$ was also considered for the through-the-thickness crack configuration. As the fracture parameters of these crack configurations are independent of the value of Young's modulus, the arbitrary value of $E = 1$ was used in all models. This is not the case for Poisson's ratio since the modes II and III SIFs of embedded cracks depend strongly on the value of this material property (see analytical solutions in Appendix D). In this research, a Poisson's ratio of $\nu = 0.3$ was used for all the crack simulations except the ones in Section 7.4.

6.1.1. Boundary conditions

Due to the symmetry in geometry and loading conditions, only one-eighth ($X_1 > 0, X_2 > 0, X_3 < 0$) and one-half ($X_3 < 0$) of the cracked bodies were modeled for pure mode I ($\beta = 90^\circ$) and mixed-mode ($\beta = 45^\circ$) conditions, respectively. The following boundary conditions were applied for mode I models: $U_1 = 0$ over the plane $X_1 = 0$, $U_2 = 0$ over the plane $X_2 = 0$ except over the crack surface, $U_3 = 0$ over the plane $X_3 = 0$, and $\sigma = 1$ over the plane $X_2 = W$. The applied boundary conditions for the mixed-mode models are also as follows: $U_1 = 0$ at the point $X_1 = X_2 = -W, X_3 = 0$, $U_2 = 0$ over the plane $X_2 = -W$, $U_3 = 0$ over the plane $X_3 = 0$, and $\sigma = 1$ over the plane $X_2 = W$. For the through-the-thickness crack, the following additional boundary condition was also applied, to ensure zero lateral displacement: $U_3 = 0$ over the plane $X_3 = -t$. This boundary condition imposes a plane strain condition over the cracked plate, where the pointwise SIFs at any point on the crack front follows the solution of the equivalent 2D problem of an inclined central crack in a large plane. This solution gives the SIFs as follows: $K_I = \sigma \sqrt{\pi a} \sin^2 \beta$, $K_{II} = \sigma \sqrt{\pi a} \sin \beta \cos \beta$, and $K_{III} = 0$. These formulas along with the analytical solutions for the SIFs of embedded inclined penny-shaped and elliptical cracks in infinite solids given in Appendix D will be used to validate the numerical results.

6.1.2. Mesh

An octree-based mesh generation software was employed to generate arbitrary meshes for all specimens by using 10-noded isoparametric tetrahedral elements. For the elements attached to the crack front, the nodes near the front are moved from the mid-side point to the quarter-point position to produce quarter-point tetrahedral elements. The curved edges on the curved crack fronts were straightened by moving the mid-side nodes of the curved segments. This avoids the Jacobian becoming negative near the crack front (see Section 4.2.2). The refinement of the mesh near the crack front was controlled by assigning the number of segments along the crack front. Consider

the crack front of length L_f is discretized by N_f segments. A parameter called the nominal length (size) of the elements in the crack front region can be defined as $L_n = L_f/N_f$. The nominal element length L_n represents the approximate length of the elements sides near the crack front, and therefore gives an approximation for the average size of the quarter-point elements in the crack front region. In all models, the degree of mesh refinement in the crack front region was controlled by keeping the nominal crack front element size about 0.03 of the crack length ($L_n \approx a/33$). Fig. 8 shows the finite element mesh of the mixed-mode penny-shaped crack problem together with the local mesh refinements near the crack front in different mixed-mode crack configurations. Four-point and three-point Gaussian quadrature rules were employed for the numerical integration over tetrahedral and triangular elements, respectively.

[Figure 8 about here.]

6.2. Numerical results

The pointwise SIF values were computed at the location of existing crack front nodes using Eq. (19) when considering $r_m = 2L_n$. The reason for this choice is discussed in Section 7.3. The average numerical error of SIF computation for individual modes e_i ($i = \text{I, II, III}$) and average total error e_t were then evaluated by using Eq. (20). In these expressions K_i^A and K_i^N are the pointwise analytical and numerical mode i SIFs, respectively, and L_f is the crack front length. Wherever closed-form integration was not possible, the trapezoidal rule has been employed to evaluate the integrals numerically.

$$e_i = \frac{\int_{L_f} |K_i^A - K_i^N| dl}{\int_{L_f} |K_i^A| dl} \quad i = \text{I, II, III} \quad e_t = \frac{\sum_{i=\text{I}}^{\text{III}} \int_{L_f} |K_i^A - K_i^N| dl}{\sum_{i=\text{I}}^{\text{III}} \int_{L_f} |K_i^A| dl} \quad (20)$$

[Figure 9 about here.]

Fig. 9 shows the variation of pointwise mode I stress intensity factor along the crack front of different crack configurations when the cracks are subjected to pure mode I loading condition ($\beta = 90^\circ$). Analytical solutions for a 2D plane strain central crack problem, and 3D penny-shaped and elliptical cracks embedded in infinite solids (Appendix D) are also plotted. The average error e_t for these four sets varies from $e_t = 0.009$ in through-the-thickness crack to $e_t = 0.037$ in the elliptical crack with $b/a = 0.4$. Fig. 10 also shows the variation of pointwise mixed-mode SIFs along the crack front of four different crack configurations when $\beta = 45^\circ$. The average total error e_t varies from $e_t = 0.014$ in through-the-thickness crack to $e_t = 0.039$ in the elliptical crack with $b/a = 0.4$. These results are obtained from the meshes shown in Fig. 8, and the use of finer meshes will result in the computation of more accurate SIFs. These results demonstrate the efficiency of the displacement correlation method for computing very good approximations of the SIFs from arbitrary meshes. Section 7 discusses the effects of different parameters involved in the DC method on these results.

[Figure 10 about here.]

7. Discussion

It was mathematically proved in Section 4 that a square root strain singularity is reproduced near the crack front in the quarter-point tetrahedral elements. A displacement correlation scheme was also suggested in Section 5 for the fast approximation of the SIFs from unstructured meshes. Several numerical tests were then performed using the quarter-point tetrahedra, and the SIFs were computed using the DC approach. This section aims to discuss these numerical results. To this end, first the performance of the quarter-point tetrahedra in reproducing the square root singularity is addressed. Then, the reason for correlating the displacements at points located at a fixed distance from the crack front is explained. The influence of r_m as the main input parameter in the proposed DC method on the accuracy of the SIFs is discussed afterwards. Finally, the influence of Poisson's ratio on the accuracy of DC method and the applicability of the DC method to non-matched crack surface meshes are addressed.

7.1. The performance of quarter-point tetrahedra

This section evaluates the performance of quarter-point tetrahedra in reproducing singularity, and compares them with the standard tetrahedra. Consider the penny-shaped crack configuration shown in Fig. 7b in a mixed-mode loading condition ($\beta = 45^\circ$), with a crack surface mesh structure shown in Fig. 11a. Two points on the crack front are selected, and the normal rays emanating from these points, which also lie on the crack surfaces, are shown in Fig. 11a. The relative displacements of the top surface with respect to the bottom surface, i.e. $\Delta u, \Delta v, \Delta w$ shown in Fig. 6b, are computed for the points along these rays. These values are then normalized using the analytical values of relative displacements at the points $r = 3L_n$ on each ray ($\Delta u^*, \Delta v^*$, and Δw^*). Figs. 11b-d compare the numerical values of these normalized relative displacements along the two rays with the analytical results obtained from Eq. (18). The numerical values are reported for two cases: (i) when quarter-point tetrahedra are used at the crack front, where ray 1 and ray 2 pass through a CQPT and an EQPT, respectively, and (ii) when standard tetrahedra are employed at the crack front.

[Figure 11 about here.]

The main features of these plots are as follows: (1) The quarter-point tetrahedra significantly improve the FE displacements near the crack front by reproducing the square root singularity at the crack front. The standard tetrahedra, however, capture poorly the high displacement gradients near the crack front, which results in considerable numerical error near the crack front. These plots clearly depict the difference between a polynomial interpolation of displacement in standard tetrahedra and a square root one in quarter-points tetrahedra. (2) For either of these element types, the displacement variation near the crack front ($r/L_n < 1.5$) differs slightly from one ray to another. This suggests that the FE results are sensitive to the quality of the elements near the crack front. This mesh sensitivity, however, decays at further points from the crack front, and the displacement variations along all rays match very well. (3) For $r/L_n > 1.5$ an offset is observed between the relative displacements from quarter-point and standard tetrahedra, with the result from quarter-point tetrahedra being more accurate. This suggests that the use of the quarter-point tetrahedra improves not only the near-front fields, but also the displacements far from the crack front. (4) It is

seen that the FE results, when using either of the quarter-point element types, start deviating from the analytical values at $r/L_n = 2$. The reason is that the analytical formula in Eq. (18) ignores the higher-order terms of the crack tip field expressions, and only considers the displacements generated by the singular stress terms. The FE results, however, capture the effects of higher order terms. Therefore, the points far from the crack front should not be used in a correlation scheme for the SIF computation. The displacement variation along any other ray follows the same behavior. Overall, quarter-point tetrahedra provide much more accurate results compared with standard tetrahedra, and thus, should generally be favoured.

7.2. The method of correlation

A similar correlation scheme to the one proposed for collapsed quarter-point hexahedra (Ingraffea and Manu, 1980) is developed for the quarter-point tetrahedra in Appendix B. This scheme uses the displacement distribution over the entire corner-based quarter-point elements. From Eqs. (B.4) and (B.5), it is clear that the correlation is carried out using the displacements at two points: point p located at the intersection of the normal to the crack front and the element edge opposing the crack front, and point q located at the quarter-point position of point p . It is also seen that the displacement of the mid-side node on the edge opposing to the crack front, node 6, cancels out in this formulation. The penny-shaped crack under pure mode I condition ($\beta = 90^\circ$) is now used to compare the SIF results from the two-point correlation scheme with the values obtained from the proposed scheme in Section 5. Fig. 12a shows the mesh over the crack surface, where the normals to the crack front at two nodes are drawn, and the points p , q and m on the normal line are marked. The points m are located at fixed distances from the crack front, with $r_m = L_n$ or $r_m = 2L_n$. Fig. 12b compares the normalized mode I analytical SIF with the numerical ones obtained from different correlation schemes. Two-point correlation scheme uses Eq. (B.5) in which the displacements at both points p and q are used in the correlation process. Correlations at p and q employ the displacements at those points, and correlation at m uses the displacements at fixed distances from the crack front.

[Figure 12 about here.]

The following features in this plot are highlighted: (i) The two-point correlation computes the least accurate and the most mesh sensitive SIFs. Although this scheme gives accurate values at some points on the crack front, considerable fluctuations in the SIFs are seen, especially at the places where the radial size of the quarter-point elements varies significantly (see Fig. 12a). The main reason for these fluctuations seems to be the significant variation of the size of quarter-point elements, which influences the accuracy of the displacement fields over these elements. Moreover, the absence of the displacement at node 6 in the formulation of two-point correlation may also influence the accuracy of the results (see Fig. 17 and Eq. (B.5)). (ii) The results for the correlation at only one point p or q are more accurate than the two-point correlation scheme, with the results for point p being considerably more accurate than the ones for the point q . This is mainly because the relative numerical error is usually higher for the point closer to the crack front. However, slight fluctuations are still visible in the variation of the SIFs even when using correlation at the point p . (iii) The fluctuations decay considerably when correlating the displacement at point m

($r_m = L_n$), giving more accurate results for the SIFs throughout the entire crack front. When further points from the crack front are used ($r_m = 2L_n$), the fluctuations disappear completely, and the SIFs are no longer sensitive to mesh quality at the crack front elements. The same behavior is seen in other crack configurations and loading conditions. Overall, these results suggest that the two-point correlation scheme based the displacement distribution over the entire quarter-point tetrahedral element exhibits sensitivity to the quality of mesh near crack front, whereas a simple one-point correlation at a fixed distance from the crack front is able to provide accurate SIFs, exhibiting no sensitivity to the quality of quarter-point tetrahedra as long as the correlation points are far enough from the crack front.

7.3. The distance of the point of correlation from the crack front (r_m)

The main parameter in the proposed DC method is the distance of the correlation point from the crack front (r_m). On the one hand, r_m must be small enough compared to the crack size so that the point of correlation remains in the singular dominant region, where a plane strain condition prevails. Moreover, higher-order terms influence the crack tip displacement fields significantly at the region far from the crack front, which is another reason why one should avoid using points at that region. On the other hand, r_m must be large enough to avoid high numerical errors and displacement inaccuracies in the region very close to the crack front due to the complex singular stress state there. The relative numerical error is also much higher as the displacements assign smaller magnitudes there. Therefore, the use of the points very close to the crack tip is also problematic. The accuracy of the near front FE fields depends considerably on the mesh refinement in that region. Therefore, for each mesh resolution, there must be an optimum value for the r_m at which the computed fracture parameters are most accurate. As the degree of the accuracy of the fields near the crack depends on the type and refinement of the elements in that region, it is expected that the optimum r_m depends mainly on the type and size of the elements in the crack front region. In an arbitrary mesh around the crack front, the size of the elements may vary significantly, and therefore an approximate (nominal) value shall be used to represent the average size of the elements. The nominal crack front element size can be defined as $L_n = L_f/N_f$ where L_f and N_f are the length of the crack front and number of segments used to discretize it, respectively.

[Figure 13 about here.]

In order to evaluate the idea of the presence of an optimum r_m , an extensive parametric study was carried out to relate the SIF computation error to r_m in different mesh refinements. The SIFs of the different crack configurations were computed while the points of correlation moved further away from crack front in different mesh densities. Fig. 12 shows the variation of the total SIF computation error e_t , computed from Eq. (20), versus the normalized distance of the correlation point from the crack front, r_m/L_n , for different mesh refinements expanding from coarse meshes $a/L_n \approx 10$ to fine meshes $a/L_n \approx 45$. The main feature of the results in these plots is that for all crack configurations except very coarse meshes, e_t slightly drops by increasing r_m , reaching its minimum between $r_m = L_n$ and $r_m = 2L_n$, and then increases gradually for points further from the crack front. The decreasing trend in the beginning is explained by the fact that high numerical errors and displacement inaccuracies exist near the crack front, generating large relative numerical

error due to the small magnitude of the displacements there. By correlating at points further away, this relative numerical error drops, and more accurate SIFs are computed. The growth trend is because the displacements at point far from the crack front is more likely to include the influence of higher order terms, and also due to the fact that the plane strain condition no longer prevails at those points. The plots clearly show that there exists an optimum r_m in the range of $L_n \leq r_m \leq 2L_n$ where the SIF computation error hits its minimum. The optimum distance approaches $r_m = L_n$ and $r_m = 2L_n$ for coarse and fine meshes, respectively. A distance of $r_m = 1.5L_n$ can be chosen as the best choice that works for both fine and coarse meshes.

The authors have also recently developed a domain integral approach which computes SIFs with an average error of about 1% (Nejati et al., 2015). A comparison of the SIF values from DC and domain integral methods indicates that their dependency on the size of quarter-point elements is analogous. Similar to the concept of optimum sampling distance for the DC method, there is an optimum mesh size-dependent domain size for the domain integral method (see (Nejati et al., 2015)). The only difference is that results from the domain integral method for the through-the-thickness crack show that the error drops slightly from $R_d = 0.5L_n$ to $R_d = 1.5L_n$, at which point it stabilizes (see Fig. 12 in (Nejati et al., 2015)). In contrast, when using the DC method, as seen in Fig. 13, the error starts increasing at $r_m = L_n$. The reason for this behavior lies in the main difference between these methods. In the through-the-thickness crack the whole plate is under plane strain, and the 3D solution fields approach the fields obtained from a 2D plane strain crack problem. It is well known that the J -integral exhibits path-independence for a 2D crack problem (Rice, 1968). Therefore, higher-order terms cannot influence the SIFs obtained from the domain integral method, even when very large domains are employed. This is not the case for the DC method, where the effect of higher-order terms are assumed to be negligible (see Eq. (17)) while the higher-order terms may have a significant influence on the FE displacements far from the crack front. Therefore, there is an increasing trend of the SIF error with r_m due to the higher order terms which influence FE displacements far from the crack front. It is noteworthy that, as compared to the DC method, the SIFs obtained using the domain integral approach require less dense meshes.

Fig. 14 demonstrates the variation of the total SIF computation error e_t versus the normalized distance of the correlation point from the crack front r_m/L_n , when standard tetrahedral elements are employed at the crack front region instead of quarter-point elements. The following are the main features in these plots: (i) The SIF computation error is significantly higher in these plots compared to the ones in Fig. 13, especially at small values of r_m . The errors in these plots are approximately 2 to 3 times larger than the errors in Fig. 13. This highlights the efficiency of the quarter-point elements in improving the numerical solution of the crack tip fields. It is noteworthy that the results of the domain integral approach also demonstrate the significant improvement of the accuracy of the SIFs by quarter-point tetrahedra, reducing the error 2-3 times as opposed to standard tetrahedra (Nejati et al., 2015). (ii) Similar trends are observed in these plots as those shown in Fig. 13. One important difference is that the errors for points close to crack front are significantly higher than those in Fig. 13. This indicates that when standard tetrahedral elements are used, a larger r_m should be preferred to compute accurate SIF values.

[Figure 14 about here.]

7.4. Poisson's ratio value

The SIFs obtained from the DC method proposed by Ingraffea and Manu (1980) exhibited dependency on the value of Poisson's ratio. This dependency is justifiable when analyzing the SIFs near a corner point, i.e., the meeting point of a crack front and a free surface. This is because at these points a corner singularity occurs, where the order of singularity, which depends on Poisson's ratio as well as loading conditions, is different from the crack singularity (Bentham, 1977; Bažant and Estenssoro, 1979). Therefore, the SIFs near the corner points differs from one value of the Poisson's ratio to another one. However, the analytical mode I stress intensity factor of an embedded penny-shaped crack does not depend on the value of Poisson's ratio, whereas the numerical results in Ingraffea and Manu (1980) show significant dependency of the SIFs on this material property. The reason for this dependency is not explained in that paper.

All the previous SIF results in this paper are obtained by considering $\nu = 0.3$. In order to evaluate the influence of Poisson's ratio value, two other values, $\nu = 0.15$ and $\nu = 0.45$, were considered to compute the SIFs of the penny-shaped crack under mixed-mode loading. Fig. 15 shows the variation of the total SIF computation error e_t versus the normalized distance of the correlation point from the crack front r_m/L_n for different mesh refinements and Poisson's ratios. A comparison of these two plots and Fig. 13b, in which the results for $\nu = 0.3$ are reported, demonstrates that the error of the SIF values obtained by the proposed DC method in this paper are barely influenced by Poisson's ratio value. For example, at the distance $r_m = 2L_n$, $e_t = 0.024$, $e_t = 0.025$, and $e_t = 0.033$, are corresponding errors for Poisson's ratio values of $\nu = 0.15$, $\nu = 0.3$, $\nu = 0.45$, respectively. It is also seen in these plots that the optimum distance from the crack front is not influenced by the value of Poisson's ratio. In fact, unlike the results in Ingraffea and Manu (1980), which suggest an optimum Poisson's ratio dependent element size, the results from the proposed DC method here suggest that the optimum distance from the crack front is independent of Poisson's ratio, and only depends on the mesh refinement near the crack front.

[Figure 15 about here.]

7.5. The method for non-matched meshes

All the previous proposed DC schemes rely on the generation of matched elements over the crack surfaces as they use the displacements of matched nodes to compute the relative displacements between the two surfaces. The proposed DC approach in this research, however, does not require the crack surface elements to be matched. This is of great importance, as a considerable constraint is removed from meshing procedures by allowing non-matched meshes over the crack surfaces. The penny-shaped crack in a mixed-mode loading condition ($\beta = 45^\circ$), as shown in Fig. 7b, was considered in order to evaluate the results of the DC method for non-matched meshes. The crack surface mesh structure is shown in Fig. 16a. Fig. 16b presents the variation of point-wise mixed-mode SIFs along the crack front. The average total error e_t is about $e_t = 0.02$. These results demonstrate the efficiency of the proposed DC approach for computing accurate SIFs from arbitrary meshes with non-matched crack surface elements.

[Figure 16 about here.]

8. Conclusion

It has been demonstrated that both types of the quarter-point tetrahedral elements generated at the crack front can reproduce a square root stress singularity near the crack front. It is also shown that the Jacobian becomes negative in a small region near the curved side of the quarter-point tetrahedra attached to the curved crack fronts. It is therefore suggested to make these curve sides straight when using the quarter-point tetrahedra along the curved crack fronts. The numerical results on the relative displacements over the crack surfaces clearly demonstrate very good performance of the quarter-point tetrahedra in reproducing a square root displacement variation near the crack front. An efficient displacement correlation (DC) method is also proposed for computing good approximations of the SIFs. This DC method is computationally very cheap, can be readily implemented in any FE code, and can be applied on unstructured meshes even when the elements on the crack surfaces are non-matched. The results of this method have been validated for a number of crack configurations in mode I and mixed-mode loadings, where the average SIF computation error varies from 1% for through-the thickness crack, to about 4% for elongated elliptical ones. A comparison of the results from the DC method for standard and quarter-point elements also reveals that the average SIF computation error more than doubles when using standard tetrahedra instead of quarter-point ones at the crack front region. The results from an extensive parametric study suggest that there is an optimum mesh-dependent distance from the crack front at which the average SIF computation error by the DC method hits its minimum. This distance is about once to twice the average (nominal) size of the elements at the crack front region. This research provides further evidence to the applicability, efficiency and accuracy of unstructured meshes to analyze cracked bodies.

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Appendix A. Components of Jacobian matrix inverse for CQPT and EQPT elements

$$\begin{aligned}
 \alpha_1 &= \frac{(\rho x_4 - y_4)z_2 + (y_2 - \rho x_2)z_4}{(y_4 - \rho x_4)z_3 + (\rho x_3 - y_3)z_4} \\
 \alpha_2 &= \frac{(y_3 - \rho x_3)z_2 + (\rho x_2 - y_2)z_3}{(y_4 - \rho x_4)z_3 + (\rho x_3 - y_3)z_4} \\
 \gamma_1 &= \frac{|z_2[y_4 - y_3 - \rho(x_4 - x_3)] + z_3[y_2 - y_4 - \rho(x_2 - x_4)] + z_4[y_3 - y_2 - \rho(x_3 - x_2)]|}{[(\rho x_4 - y_4)z_3 + (y_3 - \rho x_3)z_4]^2} \\
 &\quad |x_2(y_3z_4 - y_4z_3) + x_3(y_4z_2 - y_2z_4) + x_4(y_2z_3 - y_3z_2)| \sqrt{1 + \rho^2} \\
 c_1 &= 2(1 + \alpha_1 + \alpha_2)^2 [x_4(y_3z_2 - y_2z_3) + x_3(y_2z_4 - y_4z_2) + x_2(y_4z_3 - y_3z_4)] \\
 p_{11} &= y_2(z_3 - z_4) + z_2(y_4 - y_3) + (1 + 2\alpha_1 + 2\alpha_2)(y_4z_3 - y_3z_4) \\
 p_{21} &= x_2(z_4 - z_3) + z_2(x_3 - x_4) + (1 + 2\alpha_1 + 2\alpha_2)(x_3z_4 - x_4z_3) \\
 p_{31} &= x_2(y_3 - y_4) + y_2(x_4 - x_3) + (1 + 2\alpha_1 + 2\alpha_2)(x_4y_3 - x_3y_4) \\
 p_{12} &= \alpha_1 y_3(z_4 - z_2) + \alpha_1 z_3(y_2 - y_4) + (2 + \alpha_1 + 2\alpha_2)(y_2z_4 - y_4z_2) \\
 p_{22} &= \alpha_1 x_3(z_2 - z_4) + \alpha_1 z_3(x_4 - x_2) + (2 + \alpha_1 + 2\alpha_2)(x_4z_2 - x_2z_4) \\
 p_{32} &= \alpha_1 x_3(y_4 - y_2) + \alpha_1 y_3(x_2 - x_4) + (2 + \alpha_1 + 2\alpha_2)(x_2y_4 - x_4y_2) \\
 p_{13} &= \alpha_2 y_4(z_2 - z_3) + \alpha_2 z_4(y_3 - y_2) + (2 + 2\alpha_1 + \alpha_2)(y_3z_2 - y_2z_3) \\
 p_{23} &= \alpha_2 x_4(z_3 - z_2) + \alpha_2 z_4(x_2 - x_3) + (2 + 2\alpha_1 + \alpha_2)(x_2z_3 - x_3z_2) \\
 p_{33} &= \alpha_2 x_4(y_2 - y_3) + \alpha_2 y_4(x_3 - x_2) + (2 + 2\alpha_1 + \alpha_2)(x_3y_2 - x_2y_3)
 \end{aligned} \tag{A.1}$$

$$\begin{aligned}
 \beta_1 &= -\frac{(y_2 - \rho x_2)}{(y_3 - \rho x_3)} \\
 \beta_2 &= -(\beta_1 + 1)z_2 - \beta_1(\beta_1 + 1)z_3 \\
 \beta_3 &= (\beta_1 + 1)z_4 \\
 \gamma_2 &= \frac{|(\rho x_2 - y_2 - \rho x_3 + y_3)(x_3 y_2 - x_2 y_3)|}{(\rho x_3 - y_3)^2} \sqrt{1 + \rho^2} \\
 c_2 &= 2(x_3 y_2 - x_2 y_3)(1 + \beta_1)^2 \\
 q_{11} &= -y_2 - y_3(1 + 2\beta_1) \\
 q_{21} &= x_2 + x_3(1 + 2\beta_1) \\
 q_{12} &= y_3\beta_1 + y_2(2 + \beta_1) \\
 q_{22} &= -x_3\beta_1 - x_2(2 + \beta_1) \\
 f_1 &= d\gamma_2 z_4 (y_3 - y_2)(1 + \beta_1) \\
 f_2 &= 2\sqrt{\gamma_2} z_4 (y_3 z_2 - y_2 z_3)(1 + \beta_1)^2 \\
 f_3 &= z_4(1 + \beta_1)\beta_2(y_3 - y_2) + 2(y_3 z_2 - y_2 z_3)(1 + \beta_1)^2 \beta_3 \\
 g_1 &= d\gamma_2 z_4 (x_2 - x_3)(1 + \beta_1) \\
 g_2 &= -2\sqrt{\gamma_2} z_4 (x_3 z_2 - x_2 z_3)(1 + \beta_1)^2 \\
 g_3 &= z_4 \beta_2(1 + \beta_1)(x_2 - x_3) - 2(x_3 z_2 - x_2 z_3)(1 + \beta_1)^2 \beta_3 \\
 h_1 &= \gamma_2 z_4^2 \\
 h_2 &= \sqrt{\gamma_2} z_4 (z_4(1 + \beta_1) + \beta_3) \\
 h_3 &= z_4(1 + \beta_1)\beta_3
 \end{aligned} \tag{A.2}$$

Appendix B. A displacement correlation scheme for corner-based quarter-point tetrahedral elements

Quarter-point tetrahedral elements generate two types of triangular elements over the crack surfaces: (i) when a CQPT shares a face with the crack surface, a corner-based quarter-point triangular (CQPTr) element is generated which shares only one node with the crack front; (ii) when a EQPT shares a face with the crack surface, an edge-based quarter-point triangle (EQPTr) is developed, which shares three nodes with the crack front. Since the square root singularity occurs in the entire domain of the CQPTs, the displacement representation of these elements is employed here for the SIF computation. However, the same approach can be applied to approximate the SIFs from the displacement field in the EQPTs. Assume that the element face $\zeta = 0$ of a CQPT is one of the corner-based quarter-point triangles shown in Fig. 17. By using Eq. (1), the distribution of displacement component u , which is along the x axis in the local coordinate system xyz , is given by $u = N_1 u_1 + N_2 u_2 + N_3 u_3 + N_5 u_5 + N_6 u_6 + N_7 u_7$. Assume that the ray normal to the crack front, OP in Fig. 17, is defined by the natural coordinate $0 \leq \psi \leq 1$ in such a way that $\psi = 0$ and $\psi = 1$ represents points O and P , respectively. Along this line, the natural coordinates ξ and η are $\xi = \xi_P \psi$ and $\eta = \eta_P \psi$ where $(\xi_P, \eta_P, 0)$ represents the coordinate of the point P in the natural coordinate system $\xi\eta\zeta$. Using Eq. (2), the relative displacement along the ray OP with respect to crack tip displacement is written as:

$$u = (\xi_P(4u_5 - u_2) + \eta_P(4u_7 - u_3))\psi + 2(\xi_P(u_2 - 2u_5) + \eta_P(u_3 - 2u_7) + 2\xi_P\eta_P(u_6 - u_5 - u_7))\psi^2 \quad (\text{B.1})$$

[Figure 17 about here.]

Employing Eqs. (1) and (2), the distance of any point lying on OP from the crack tip is obtained from $r = L_P\psi^2$, where $L_P = \sqrt{(\xi_P x_2 + \eta_P x_3)^2 + (\xi_P y_2 + \eta_P y_3)^2 + (\xi_P z_2 + \eta_P z_3)^2}$ is the length of the line OP . The displacement along the ray OP is therefore given by:

$$u = (\xi_P(4u_5 - u_2) + \eta_P(4u_7 - u_3))\sqrt{\frac{r}{L_P}} + 2(\xi_P(u_2 - 2u_5) + \eta_P(u_3 - 2u_7) + 2\xi_P\eta_P(u_6 - u_5 - u_7))\frac{r}{L_P} \quad (\text{B.2})$$

In a special case when $\xi_P = 1$ or $\eta_P = 1$, one of the sides of triangle is normal to the crack front. The displacement is then given by $u = (4u_5 - u_2)\sqrt{r/L_2} + (2u_2 - 4u_5)r/L_2$ and $u = (4u_7 - u_3)\sqrt{r/L_3} + (2u_3 - 4u_7)r/L_3$ for $\xi_P = 1$ and $\eta_P = 1$, respectively. Here $L_2 = \sqrt{x_2^2 + y_2^2 + z_2^2}$ and $L_3 = \sqrt{x_3^2 + y_3^2 + z_3^2}$ are the lengths of the element sides on ξ and η axes, respectively. The equation for this special case is similar to the ones reported in Shih et al. (1976); Ingraffea and Manu (1980). The first term in Eq. (B.2) reproduces the displacement field due to the singular stress field, while the second term represents the displacement due to the constant stress. To compute the coefficients of singular stress terms, only the first term need to be considered. One can now write these expressions in terms of the relative displacement of the top surface element with respect to the bottom surface element, and extend these equations to include the displacement variation in y and z directions (v and w) as Eq. (B.3). Equating Eqs. (B.3) and (18) gives the SIFs as Eq. (B.4).

$$\begin{aligned} \Delta u &= \left[\xi_P(4(u_5 - u_{5^*}) - (u_2 - u_{2^*})) + \eta_P(4(u_7 - u_{7^*}) - (u_3 - u_{3^*})) \right] \sqrt{\frac{r}{L_P}} \\ \Delta v &= \left[\xi_P(4(v_5 - v_{5^*}) - (v_2 - v_{2^*})) + \eta_P(4(v_7 - v_{7^*}) - (v_3 - v_{3^*})) \right] \sqrt{\frac{r}{L_P}} \\ \Delta w &= \left[\xi_P(4(w_5 - w_{5^*}) - (w_2 - w_{2^*})) + \eta_P(4(w_7 - w_{7^*}) - (w_3 - w_{3^*})) \right] \sqrt{\frac{r}{L_P}} \end{aligned} \quad (\text{B.3})$$

$$\begin{aligned} K_{\text{I}} &= \sqrt{\frac{2\pi}{L}} \left(\frac{\mu}{\kappa + 1} \right) \left[\xi_P(4(v_5 - v_{5^*}) - (v_2 - v_{2^*})) + \eta_P(4(v_7 - v_{7^*}) - (v_3 - v_{3^*})) \right] \\ K_{\text{II}} &= \sqrt{\frac{2\pi}{L}} \left(\frac{\mu}{\kappa + 1} \right) \left[\xi_P(4(u_5 - u_{5^*}) - (u_2 - u_{2^*})) + \eta_P(4(u_7 - u_{7^*}) - (u_3 - u_{3^*})) \right] \\ K_{\text{III}} &= \sqrt{\frac{2\pi}{L}} \left(\frac{\mu}{4} \right) \left[\xi_P(4(w_5 - w_{5^*}) - (w_2 - w_{2^*})) + \eta_P(4(w_7 - w_{7^*}) - (w_3 - w_{3^*})) \right] \end{aligned} \quad (\text{B.4})$$

With the presence of symmetry in the geometry and symmetry/antisymmetry in the loading conditions, only one of the crack faces needs to be modeled. In this case $u_{\theta=-\pi} = -u_{\theta=\pi}$, $v_{\theta=-\pi} =$

$-v_{\theta=\pi}$ and $w_{\theta=-\pi} = -w_{\theta=\pi}$, and therefore the SIFs are computed using the displacements of the nodes on the top crack surface as:

$$\begin{aligned} K_I &= \sqrt{\frac{2\pi}{L}} \left(\frac{2\mu}{\kappa+1} \right) \left(\xi_P(4v_5 - v_2) + \eta_P(4v_7 - v_3) \right) \\ K_{II} &= \sqrt{\frac{2\pi}{L}} \left(\frac{2\mu}{\kappa+1} \right) \left(\xi_P(4u_5 - u_2) + \eta_P(4u_7 - u_3) \right) \\ K_{III} &= \sqrt{\frac{2\pi}{L}} \left(\frac{\mu}{2} \right) \left(\xi_P(4w_5 - w_2) + \eta_P(4w_7 - w_3) \right) \end{aligned} \quad (B.5)$$

Appendix C. Obtaining field values at a given point in tetrahedral/triangle elements

The computation of the SIFs from the proposed DC method requires the computation of the displacement values at a given point inside tetrahedra or triangles. In order to obtain the field values at the given point p first the tetrahedral or triangular element containing it must be identified through a search algorithm. Then, the natural coordinates of that given point inside the element must be determined. The fields can then be readily obtained through the shape functions.

Appendix C.1. Tetrahedral element

Consider a tetrahedral element of any type with straight edges as shown in Fig. 18a-c. The corner node i of these elements has the coordinates (x_i, y_i, z_i) , and the point p is located at (x_p, y_p, z_p) in the coordinate system xyz . The volume of the tetrahedral element V is computed by the determinant given in Eq. (C.1). The volumes of smaller internal tetrahedra which are generated with one face of the main tetrahedral and the point p are also computed from the determinants in Eq. (C.2). The point p is inside the tetrahedral element if all the determinants, or volumes, in Eq. (C.2) are non-negative ($V_i \geq 0$).

[Figure 18 about here.]

$$V = \frac{1}{6} \begin{vmatrix} x_2 & y_2 & z_2 & 1 \\ x_3 & y_3 & z_3 & 1 \\ x_4 & y_4 & z_4 & 1 \\ x_1 & y_1 & z_1 & 1 \end{vmatrix} \quad (C.1)$$

$$V_1 = \frac{1}{6} \begin{vmatrix} x_2 & y_2 & z_2 & 1 \\ x_3 & y_3 & z_3 & 1 \\ x_4 & y_4 & z_4 & 1 \\ x_p & y_p & z_p & 1 \end{vmatrix}, \quad V_2 = \frac{1}{6} \begin{vmatrix} x_p & y_p & z_p & 1 \\ x_3 & y_3 & z_3 & 1 \\ x_4 & y_4 & z_4 & 1 \\ x_1 & y_1 & z_1 & 1 \end{vmatrix}, \quad V_3 = \frac{1}{6} \begin{vmatrix} x_2 & y_2 & z_2 & 1 \\ x_p & y_p & z_p & 1 \\ x_4 & y_4 & z_4 & 1 \\ x_1 & y_1 & z_1 & 1 \end{vmatrix}, \quad V_4 = \frac{1}{6} \begin{vmatrix} x_2 & y_2 & z_2 & 1 \\ x_3 & y_3 & z_3 & 1 \\ x_p & y_p & z_p & 1 \\ x_1 & y_1 & z_1 & 1 \end{vmatrix} \quad (C.2)$$

The point p inside any type of tetrahedral element in Fig. 18a-c is mapped to the point p' inside the parent tetrahedral element shown in Fig. 18d. In the case of standard tetrahedral element in

Fig. 18a, the global coordinates are mapped linearly into the natural ones through Eq. (C.3). Solving these equations for the natural coordinates gives the coordinates of p' as volume fractions in Eq. (C.4):

$$\begin{aligned} x &= x_1 + (x_2 - x_1)\xi + (x_3 - x_1)\eta + (x_4 - x_1)\zeta \\ y &= y_1 + (y_2 - y_1)\xi + (y_3 - y_1)\eta + (y_4 - y_1)\zeta \\ z &= z_1 + (z_2 - z_1)\xi + (z_3 - z_1)\eta + (z_4 - z_1)\zeta \end{aligned} \quad (C.3)$$

$$\xi_{p'} = \frac{V_2}{V}, \quad \eta_{p'} = \frac{V_3}{V}, \quad \zeta_{p'} = \frac{V_4}{V} \quad (C.4)$$

In the case of quarter-point tetrahedra, however, careful attention is required, as the mapping is not linear, and the volume fractions in Eq. (C.4) are no longer valid for the computation of the natural coordinates. In addition, these types of elements have specific orientations, which need to be taken into account. Assume the orientations shown in Fig. 18b,c, which renders the midside nodes 5, 7, and 8 for the CQPT moved to the quarter-point position from node 1, and the nodes and 5, 7, 9, and 10 for the EQPT moved to the quarter-point position from nodes 1 and 4. The mapping functions are developed as Eqs. (C.5) and (C.6) for the CQPT and EQPT, respectively. Solving these equations for non-negative natural coordinates, and simplifying the resulting algebraic equations give the natural coordinates of p' for CQPT and EQPT through Eqs. (C.7) and (C.8), respectively.

$$\begin{aligned} x &= x_1 + (\xi + \eta + \zeta)[(x_2 - x_1)\xi + (x_3 - x_1)\eta + (x_4 - x_1)\zeta] \\ y &= y_1 + (\xi + \eta + \zeta)[(y_2 - y_1)\xi + (y_3 - y_1)\eta + (y_4 - y_1)\zeta] \\ z &= z_1 + (\xi + \eta + \zeta)[(z_2 - z_1)\xi + (z_3 - z_1)\eta + (z_4 - z_1)\zeta] \end{aligned} \quad (C.5)$$

$$\begin{aligned} x &= x_1 + (\xi + \eta)[(x_2 - x_1)\xi + (x_3 - x_1)\eta] + (x_4 - x_1)(1 + \xi + \eta)\zeta \\ y &= y_1 + (\xi + \eta)[(y_2 - y_1)\xi + (y_3 - y_1)\eta] + (y_4 - y_1)(1 + \xi + \eta)\zeta \\ z &= z_1 + (\xi + \eta)[(z_2 - z_1)\xi + (z_3 - z_1)\eta] + (z_4 - z_1)(1 + \xi + \eta)\zeta \end{aligned} \quad (C.6)$$

$$\xi_{p'} = \frac{V_2}{\sqrt{V(V - V_1)}}, \quad \eta_{p'} = \frac{V_3}{\sqrt{V(V - V_1)}}, \quad \zeta_{p'} = \frac{V_4}{\sqrt{V(V - V_1)}} \quad (C.7)$$

$$\xi_{p'} = \frac{V_2}{\sqrt{V(V_2 + V_3)}}, \quad \eta_{p'} = \frac{V_3}{\sqrt{V(V_2 + V_3)}}, \quad \zeta_{p'} = \frac{V_4}{V + \sqrt{V(V_2 + V_3)}} \quad (C.8)$$

Once the local coordinates are known, the displacements of the point p are obtained by interpolating the values of nodal displacements. The displacement gradients and strains are also determined by substituting the natural coordinates in the so-called B matrix. The stress tensor is then computed from the strains using $\sigma = \mathbf{D}\varepsilon$, where $\mathbf{D}$ is the elasticity matrix containing the material properties.

Appendix C.2. Triangular element

Due to moving of the mid-side nodes to the quarter-point position at the crack front region, two types of quarter-points triangles are also developed at the crack surfaces: corner-based quarter-point triangles (CQPTr) which share one node with the crack front, and edge-based quarter-point

triangles (EQPTr) which share one edge with the crack front. Consider a planar triangular element of any type with straight edges on the crack surfaces as shown in Fig. 19a-c. The corner node i of these elements has the coordinates (x_i, y_i, z_i) , and the point p lies on the crack surface, locating at (x_p, y_p, z_p) in the global coordinate system xyz . The normal vector to these elements ($n = (n_x, n_y, n_z)$) is computed from Eq. (C.9), and the area of the triangular element A is determined by the determinant given in Eq. (C.10). The area of smaller internal triangles which are generated with one edge of the main triangle and the point p are also computed from the determinants in Eq. (C.11). The point p is inside the triangle element if all the determinants in Eq. (C.11) are non-negative ($A_i \geq 0$).

[Figure 19 about here.]

$$n_x = \begin{vmatrix} 1 & 0 & 0 & 0 \\ x_2 & y_2 & z_2 & 1 \\ x_3 & y_3 & z_3 & 1 \\ x_1 & y_1 & z_1 & 1 \end{vmatrix}, \quad n_y = \begin{vmatrix} 0 & 1 & 0 & 0 \\ x_2 & y_2 & z_2 & 1 \\ x_3 & y_3 & z_3 & 1 \\ x_1 & y_1 & z_1 & 1 \end{vmatrix}, \quad n_z = \begin{vmatrix} 0 & 0 & 1 & 0 \\ x_2 & y_2 & z_2 & 1 \\ x_3 & y_3 & z_3 & 1 \\ x_1 & y_1 & z_1 & 1 \end{vmatrix} \quad (C.9)$$

$$A = \frac{1}{2|n|} \begin{vmatrix} n_x & n_y & n_z & 0 \\ x_2 & y_2 & z_2 & 1 \\ x_3 & y_3 & z_3 & 1 \\ x_1 & y_1 & z_1 & 1 \end{vmatrix} \quad (C.10)$$

$$A_1 = \frac{1}{2|n|} \begin{vmatrix} n_x & n_y & n_z & 0 \\ x_2 & y_2 & z_2 & 1 \\ x_3 & y_3 & z_3 & 1 \\ x_p & y_p & z_p & 1 \end{vmatrix}, \quad A_2 = \frac{1}{2|n|} \begin{vmatrix} n_x & n_y & n_z & 0 \\ x_p & y_p & z_p & 1 \\ x_3 & y_3 & z_3 & 1 \\ x_1 & y_1 & z_1 & 1 \end{vmatrix}, \quad A_3 = \frac{1}{2|n|} \begin{vmatrix} n_x & n_y & n_z & 0 \\ x_2 & y_2 & z_2 & 1 \\ x_p & y_p & z_p & 1 \\ x_1 & y_1 & z_1 & 1 \end{vmatrix} \quad (C.11)$$

Using the shape functions of a quadratic triangular element in Eq. (C.12), the point p inside any type of triangular elements in Fig. 19a-c is mapped to the point p' inside the parent triangle element shown in Fig. 19d ($\lambda = 1 - \xi - \eta$). Consider two arbitrary unit vectors t_1 and t_2 which lie on the plane passing through element face in a way that three vector t_1 , t_2 , and n build a right-handed Cartesian coordinate system $x'y'z'$ ($n = t_1 \times t_2$). Also consider the vectors $r_p = (x_p, y_p, z_p)$, and $r_i = (x_i, y_i, z_i)$, $i = 1, 2, 3$. The mapping function of a standard triangular element in Fig. 19a from $x'y'z'$ space to $\xi\eta$ space is therefore obtained as Eq. (C.13). Solving these equations for the natural coordinates and simplifying the resulting equations using $t_1 \times t_2 = n/|n|$ give the coordinates of p' as the area fractions in Eq. (C.14):

$$N_1 = \lambda(2\lambda - 1), \quad N_2 = \xi(2\xi - 1), \quad N_3 = \eta(2\eta - 1), \quad N_4 = 4\lambda\xi, \quad N_5 = 4\xi\eta, \quad N_6 = 4\lambda\eta \quad (C.12)$$

$$\begin{aligned} x' &= t_1 \cdot r_p = t_1 \cdot r_1 + t_1 \cdot (r_2 - r_1)\xi + t_1 \cdot (r_3 - r_1)\eta \\ y' &= t_2 \cdot r_p = t_2 \cdot r_1 + t_2 \cdot (r_2 - r_1)\xi + t_2 \cdot (r_3 - r_1)\eta \\ z' &= n \cdot r_p = n \cdot r_1 \end{aligned} \quad (C.13)$$

$$\xi_p = \frac{A_2}{A}, \quad \eta_p = \frac{A_3}{A} \quad (\text{C.14})$$

In the case of quarter-point triangles, special attention is required as the mapping is no longer linear and these elements have specific orientations. Assume the orientations shown in Fig. 19b,c, which renders the midside nodes 4 and 6 in the CQPTr are moved to the quarter-point position from node 1, and the nodes 4 and 5 for the EQPTr are moved to the quarter-point positions from nodes 1 and 3, respectively.. Using the shape functions in Eq. (C.12), the mapping functions are developed as Eqs. (C.15) and (C.16) for the CQPTr and EQPTr elements, respectively. Solving these equations for non-negative natural coordinates and simplifying the resulting algebraic equations give the natural coordinates of p' for CQPTr and EQPTr through Eqs. (C.17) and (C.18), respectively.

$$\begin{aligned} x' &= t_1.r_p = t_1.r_1 + [t_1.(r_2 - r_1)\xi + t_1.(r_3 - r_1)\eta](\xi + \eta) \\ y' &= t_2.r_p = t_2.r_1 + [t_2.(r_2 - r_1)\xi + t_2.(r_3 - r_1)\eta](\xi + \eta) \\ z' &= n.r_p = n.r_1 \end{aligned} \quad (\text{C.15})$$

$$\begin{aligned} x' &= t_1.r_p = t_1.r_1 + t_1.(r_2 - r_1)\xi^2 + t_1.(r_3 - r_1)(\xi + 1)\eta \\ y' &= t_2.r_p = t_2.r_1 + t_2.(r_2 - r_1)\xi^2 + t_2.(r_3 - r_1)(\xi + 1)\eta \\ z' &= n.r_p = n.r_1 \end{aligned} \quad (\text{C.16})$$

$$\xi_{p'} = \frac{A_2}{\sqrt{A(A_2 + A_3)}}, \quad \eta_{p'} = \frac{A_3}{\sqrt{A(A_2 + A_3)}} \quad (\text{C.17})$$

$$\xi_{p'} = \sqrt{\frac{A_2}{A}}, \quad \eta_{p'} = \frac{A_3}{A + \sqrt{AA_2}} \quad (\text{C.18})$$

Once the local coordinates are known, the displacements of the point p are obtained by interpolating the values of nodal displacements using triangle shape functions in Eq. (C.12) and $u = \sum_{i=1}^6 N_i u_i$, $v = \sum_{i=1}^6 N_i v_i$, $w = \sum_{i=1}^6 N_i w_i$. The surface tractions are also computed in the same way using the values of tractions at the nodes. The nodal tractions may be known through predefined boundary conditions, or the FE results of a contact treatment on the crack surfaces.

Appendix D. Stress intensity factors of an embedded penny-shaped/elliptical crack in an infinite body under uniaxial tension

Analytical solutions for the SIFs of penny-shaped and elliptical cracks embedded in infinite solids subjected to uniform tension or shear have been derived in Kassir and Sih (1975). Consider an inclined penny-shaped/elliptical crack embedded in a solid under uniaxial tension σ , as shown in Fig. 7b. The crack plane is perpendicular to the $X_1 X_2$ plane, and makes an angle β with the applied load direction which is oriented along the X_2 axis. The normal and shear stress components on the crack face are $\sigma_{zz} = \sigma \sin^2 \beta$ and $\sigma_{zx} = \sigma \sin \beta \cos \beta$. The SIFs of the penny-shaped crack are therefore given by

$$\begin{aligned}
 K_I &= 2\sigma \sqrt{a/\pi} \sin^2 \beta \\
 K_{II} &= \frac{2\sigma \sqrt{a/\pi}}{2-\nu} \sin 2\beta \cos \phi \\
 K_{III} &= \frac{2(1-\nu)\sigma \sqrt{a/\pi}}{2-\nu} \sin 2\beta \sin \phi
 \end{aligned} \tag{D.1}$$

where a and ν are the crack radius and Poisson's ratio, respectively, and ϕ is the polar angle, as shown in Fig. 20a. It should be noted that incorrect solutions for the SIFs of penny-shaped cracks were reported by Cherepanov (1979). These solutions, which do not contain Poisson's ratio, were incorrectly employed to validate the numerical results by Nikishkov and Atluri (1987). The SIFs of the elliptical crack are given by

$$\begin{aligned}
 K_I(\omega) &= \frac{\sigma \sqrt{\pi a}}{E(k)} \sin^2 \beta \Pi(\omega) \\
 K_{II}(\omega) &= \frac{\Psi k' \sigma \sqrt{\pi a}}{2\Pi(\omega)} \sin 2\beta \cos \omega \\
 K_{III}(\omega) &= \frac{\Psi(1-\nu)\sigma \sqrt{\pi a}}{2\Pi(\omega)} \sin 2\beta \sin \omega
 \end{aligned} \tag{D.2}$$

where

$$\begin{aligned}
 \Psi &= \frac{k^2 k'}{(k^2 - \nu)E(k) + \nu k'^2 K(k)} \\
 \Pi(\omega) &= \left(k'^2 \sin^2 \omega + k'^4 \cos^2 \omega \right)^{1/4}
 \end{aligned} \tag{D.3}$$

[Figure 20 about here.]

In these formulas, $k' = b/a$, $k^2 = 1 - k'^2$, a and b are the lengths of semi-major and semi-minor axes of the ellipse ($a > b$), and $K(k)$ and $E(k)$ are the complete first and second elliptic integrals, given by

$$\begin{aligned}
 K(k) &= \int_0^{\pi/2} \frac{1}{\sqrt{1 - k^2 \sin^2 t}} dt \\
 E(k) &= \int_0^{\pi/2} \sqrt{1 - k^2 \sin^2 t} dt
 \end{aligned} \tag{D.4}$$

These integrals cannot be expressed in terms of elementary functions, and have to be evaluated numerically. The approximated values are tabulated in handbooks (see for example Abramowitz and Stegun (1968)), or can be obtained from commercial mathematical tools. Some approximate formulas such as $E(k) \approx 1 + 464(1 - k^2)^{1.65}$ have also been widely used to compute the SIFs of

elliptical cracks. Angle ω parameterizes the points of the ellipse by the equations $x = a \cos \omega$, $y = b \sin \omega$, and is related to the polar angle ϕ by $k' \tan \omega = \tan \phi$ (see Fig. 20b). Rewriting Eq. (D.4) in terms of the polar angle ϕ gives (Kachanov et al., 2003):

$$\begin{aligned} K_I(\phi) &= \frac{k' \sigma \sqrt{\pi a}}{E(k)} \frac{\Pi_1(\phi)}{\Pi_2(\phi)} \sin^2 \beta \\ K_{II}(\phi) &= \frac{\Psi k'^2 \sigma \sqrt{\pi a}}{2 \Pi_1(\phi) \Pi_2(\phi)} \sin 2\beta \cos \phi \\ K_{III}(\phi) &= \frac{\Psi(1 - \nu) \sigma \sqrt{\pi a}}{2 \Pi_1(\phi) \Pi_2(\phi)} \sin 2\beta \sin \phi \end{aligned} \quad (D.5)$$

where

$$\begin{aligned} \Pi_1(\phi) &= \left(\sin^2 \phi + k'^4 \cos^2 \phi \right)^{1/4} \\ \Pi_2(\phi) &= \left(k'^2 \sin^2 \phi + k'^4 \cos^2 \phi \right)^{1/4} \end{aligned} \quad (D.6)$$

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Figure 1: (a) Quarter-point eight-noded quadrilateral element, (b) Collapsed quarter-point eight-noded quadrilateral element, (c) Quarter-point six-noded triangular elements (d) Quarter-point twenty-noded brick element (e) Collapsed quarter-point twenty-noded brick element, (f) Quarter-point fifteen-noded pentahedral element.

Figure 2: Tetrahedral finite element in (a) local and (b) natural coordinate systems.

Figure 3: Three types of tetrahedral elements generated along the crack front.

Figure 4: Different types of quarter-point tetrahedral finite elements: (a) Corner-based quarter-point tetrahedral (CQPT), (b) Edge-based quarter-point tetrahedral (EQPT).

Figure 5: Trirectangular EQPT attached to a curved crack front in (a) local and (b) natural coordinate systems.

Figure 6: (a) Local Cartesian coordinate system at a point along a curved crack front and crack tip stresses, (b) The relative displacements of two matched points lie on top $m_+(r_m, \pi)$ and bottom $m_-(r_m, -\pi)$ surfaces.

Figure 7: Schematics of (a) Through-the-thickness crack in a large thin plate under uniaxial tension; (b) Penny-shaped/elliptical crack embedded in a large cube under uniaxial tension.

Figure 8: (a) Finite element mesh discretizing one-half of an embedded penny-shaped crack (Total number of nodes: 43141, Total number of elements: 32892). Details of mesh in crack-front region for (b) through-the thickness ($L_n/a \approx 0.032$), (c) penny-shaped ($L_n/a \approx 0.030$), (d) elliptical ($b/a = 0.7, L_n/a \approx 0.029$), (e) elliptical ($b/a = 0.4, L_n/a \approx 0.026$) cracks.

Figure 9: The variation of normalized mode I ($\beta = 90^\circ$) analytical and numerical SIFs along the fronts of (a) through-the-thickness ($L_n/a \approx 0.032$), (b) penny-shaped ($L_n/a \approx 0.03$), (c) elliptical ($b/a = 0.7, L_n/a \approx 0.029$), (d) elliptical ($b/a = 0.4, L_n/a \approx 0.024$) cracks. For all cases $r_m = 2L_n$. The mode I average error is as follows: (a) $e_1 = 0.009$, (b) $e_1 = 0.023$, (c) $e_1 = 0.024$, (d) $e_1 = 0.037$.

Figure 10: The variation of normalized mixed-mode ($\beta = 45^\circ$) analytical and numerical SIFs along the fronts of (a) through-the-thickness, (b) penny-shaped, (c) elliptical ($b/a = 0.7$), (d) elliptical ($b/a = 0.4$) cracks. The meshes are shown in Fig. 8. For all cases $r_m = 2L_n$. The average total SIF computation error is as follows: (a) $e_t = 0.014$, (b) $e_t = 0.025$, (c) $e_t = 0.028$, (d) $e_t = 0.039$.

Figure 11: (a) The mesh structure on the crack surfaces of a penny-shaped crack under mixed-mode loading condition ($\beta = 45^\circ$, $L_n/a \approx 0.030$). It also shows two normal rays to the crack front which lie on the crack surface and emanate from two arbitrary points. (b,c,d) The variation of normalized relative displacements of the crack surfaces along the two rays against the normalized distance from the crack front. The results are reported for two cases: (QPT) when quarter-point tetrahedra are used at the crack front; and (ST) when standard tetrahedra are employed at the crack front. $\Delta u^* = K_{II}(\kappa + 1) \sqrt{3L_n/2\pi}/\mu$, $\Delta v^* = K_I(\kappa + 1) \sqrt{3L_n/2\pi}/\mu$, $\Delta w^* = 4K_{III} \sqrt{3L_n/2\pi}/\mu$ where K_I , K_{II} , and K_{III} are the analytical values of the SIFs at the corresponding points (see Appendix D).

Figure 12: (a) Mesh structure on the crack surfaces of the penny-shaped crack ($L_n/a \approx 0.03$), and the points used in the correlation method, (b) The variation of normalized mode I ($\beta = 90^\circ$) analytical and numerical SIFs along the crack front when different correlation schemes are used.

Figure 13: The variation of the total numerical error e_t against the normalized distance from the crack front r_m/L_n for (a) through-the-thickness, (b) penny-shaped, (c) elliptical ($b/a = 0.7$), (d) elliptical ($b/a = 0.4$) cracks in different mesh refinements when using quarter-point tetrahedral elements ($\beta = 45^\circ$).

Figure 14: The variation of the total numerical error e_t against the normalized distance from the crack front r_m/L_n for (a) through-the-thickness, (b) penny-shaped, (c) elliptical ($b/a = 0.7$), (d) elliptical ($b/a = 0.4$) cracks in different mesh refinements and in the absence of quarter-point tetrahedral elements.

(a)

(b)

Figure 15: The effect of Poisson's ratio value on the variation of the total numerical error e_t against the normalized distance from the crack front r_m/L_n for penny-shaped under mixed-mode loading ($\beta = 45^\circ$): (a) $\nu = 0.15$, (b) $\nu = 0.45$.

(a)

(b)

Figure 16: (a) Non-matched mesh over the crack surfaces, (b) The variation of normalized mixed-mode ($\beta = 45^\circ$) analytical and numerical SIFs along the fronts of penny-shaped crack with non-matched elements over the crack surfaces. $a/L_n = 30.2$, $r_m = 2L_n$, $e_I = 0.02$, $e_{II} = 0.021$, $e_{III} = 0.0177$, $e_t = 0.02$.

Figure 17: Matching triangular elements used for extracting the SIFs from CQPTs.

Figure 18: Mapping of the point p inside (a) standard quadratic tetrahedron, (b) corner-based quarter-point tetrahedron (CQPT), and (c) edge-based quarter-point tetrahedron (EQPT) from global coordinate system xyz to point p' inside (d) parent tetrahedral element in natural system $\xi\eta\zeta$.

Figure 19: Mapping of point p inside (a) standard quadratic triangle, (b) corner-based quarter-point triangle (CQPTr), and (c) edge-based quarter-point triangle (EQPTr) from global coordinate system xyz to point p' inside (d) parent triangle element in natural coordinate system $\xi\eta$ ($\bar{n} = n/|n|$).

Figure 20: Configurations of (a) penny-shaped and (b) elliptical cracks.

Nomenclature

a	semi-crack length, crack radius, and semi-major axis at through, penny-shaped, and elliptical cracks
b	semi-minor axis at elliptical crack
$\mathbf{B}$	matrix containing shape function derivatives with respect to local coordinates
$\mathbf{C}$	matrix containing the derivatives of shape functions with respect to natural coordinates
$\mathbf{D}$	elasticity matrix
E	Young's modulus
e_i	individual mode $i = \text{I, II, III}$ stress intensity factor computation error
e_t	average total stress intensity factor computation error
$\mathbf{J}$	Jacobian matrix
$\hat{\mathbf{J}}$	extended Jacobian matrix inverse
$\mathbf{K}^e$	element stiffness matrix
L_f	crack front length
L_m	nominal (average) edge length of tetrahedral elements attached to the crack front
$\mathbf{N}$	vector containing element shape functions N_i
K_I, K_{II}, K_{III}	modes I, II and III stress intensity factors
r, θ	polar coordinate components
r_m	normal distance of correlation point m from the crack front
t	semi-thickness of the cracked plate
U_1, U_2, U_3	displacement components in Cartesian coordinate system $X_1X_2X_3$
u, v, w	displacement components in Cartesian coordinate system xyz
W	semi-length of cube, and semi-width and semi-height of cracked plate
$xyz, X_1X_2X_3$	local and global Cartesian coordinate systems
β	crack inclination angle
ε_{ij}	crack tip strain components in local Cartesian coordinate
κ	Kolosov constant
μ	shear modulus
ν	Poisson's ratio
$\xi, \eta, \zeta, \lambda$	element's natural coordinate components
σ	far field tensile load
σ_{ij}	crack tip stress components in local Cartesian coordinate
ϕ	polar angle of penny-shaped and elliptical cracks
ω	parametric angle of elliptical crack

Abbreviations

2D	two-dimensional
3D	three dimensional
CTE	crack tip element
CQPT	corner-based quarter-point tetrahedral
CQPTr	corner-based quarter-point triangle
DC	displacement correlation
EQPT	edge-based quarter-point tetrahedral
EQPTr	edge-based quarter-point triangle
FE	finite element
LEFM	linear elastic fracture mechanics
QPE	quarter-point element
QPT	quarter-point tetrahedral
SIF	stress intensity factor