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Finite element simulation of articular contact mechanics with quadratic tetrahedral elements

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ABSTRACT

Although it is easier to generate finite element discretizations with tetrahedral elements, trilinear hexahedral (HEX8) elements are more often used in simulations of articular contact mechanics. This is due to numerical shortcomings of linear tetrahedral (TET4) elements, limited availability of quadratic tetrahedron elements in combination with effective contact algorithms, and the perceived increased computational expense of quadratic finite elements. In this study we implemented both ten-node (TET10) and fifteen-node (TET15) quadratic tetrahedral elements in FEBio (www.febio.org) and compared their accuracy, robustness in terms of convergence behavior and computational cost for simulations relevant to articular contact mechanics. Suitable volume integration and surface integration rules were determined by comparing the results of several benchmark contact problems. The results demonstrated that the surface integration rule used to evaluate the contact integrals for quadratic elements affected both convergence behavior and accuracy of predicted stresses. The computational expense and robustness of both quadratic tetrahedral formulations compared favorably to the HEX8 models. Of note, the TET15 element demonstrated superior convergence behavior and lower computational cost than both the TET10 and HEX8 elements for meshes with similar numbers of degrees of freedom in the contact problems that we examined. Finally, the excellent accuracy and relative efficiency of these quadratic tetrahedral elements was illustrated by comparing their predictions with those for a HEX8 mesh for simulation of articular contact in a fully validated model of the hip. These results demonstrate that TET10 and TET15 elements provide viable alternatives to HEX8 elements for simulation of articular contact mechanics.

1. Introduction

Advances in imaging and computational methods make it possible to create and analyze detailed subject-specific models of biomechanical structures from high resolution image data. In this paper we focus on subject-specific finite element (FE) analysis of articular joint contact mechanics. Both generic and subject-specific models of articular contact have been developed and validated to gain insight into load transfer, cartilage mechanics and the etiology of osteoarthritis in the knee (Khoshgoftar et al., 2015; Luczkiewicz et al., 2015), hip (Harris et al., 2012; Henak et al., 2014) ankle (Anderson et al., 2007; Kern and Anderson, 2015) and spine (Dreischarf et al., 2014; Von Forell et al., 2015), among other joints. Despite the progress that has been made in modeling subject-specific joint contact mechanics, many challenges still remain. The articular cartilage of most joints in the human body has complex geometry, undergoes large deformations, is subjected to large compressive loads, and is often thin compared to the surrounding anatomical support. These challenges make it difficult to obtain accurate, validated computational models of articular contact mechanics.

The element type used to discretize the articular geometry is one of the most important choices that affects accuracy and robustness in simulations of articular contact. Linear tetrahedral (TET4) elements are often used due to the ease and robustness of performing automatic meshing, and local and adaptive refinement with tetrahedral elements (Hubsch et al., 1995; Johnson and MacLeod, 1998; Prakash and Ethier, 2001; Spilker et al., 1992) (Delaunay, 1934; Lo, 1991a, 1991b; Lohner, 1996; McErlain et al., 2011; Shephard and Georges, 1991; Wrazidlo et al., 1991). There are several examples in the recent literature that have used TET4 elements to discretize articular cartilage (Das Neves Borges et al.,

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2014; Johnson et al., 2014; McErlain et al., 2011). However, the TET4 element has several well-known numerical issues. First, TET4 elements can only represent a constant strain state, which necessitates a very fine discretization, often requiring long solution times. Second, TET4 elements lock for nearly incompressible materials as well as under bending deformations (Hughes, 2000), which further reduces their accuracy. Because of these issues, trilinear hexahedral elements (HEX8) have seen much wider use in joint contact analyses, despite the fact that creating hexahedral meshes for complex geometries can be challenging and time consuming. Alternative formulations for TET4 elements have been designed to circumvent their problems (e.g., (Gee et al., 2009; Puso and Solberg, 2006) based on nodal averaging of the deformation gradient). Although they reduce locking, they have other problems such us spurious deformation modes (Maas, 2011), which make them inaccurate for contact analysis.

Quadratic tetrahedral elements are an attractive alternative to TET4 elements. They maintain the advantages of tetrahedral mesh generation and they can represent curved boundaries more accurately than HEX8 elements since their edges and faces can deform. Although quadratic tetrahedral elements have been investigated as alternatives to HEX8 elements (e.g., (Cifuentes and Kalbag, 1992; Tadepalli et al., 2011; Weingarten, 1994)), none of these studies investigated their application for simulation of articular contact analyses. The 10-node tetrahedron (TET10) has seen some limited use for contact mechanics (Bunbar et al., 2001; Hao et al., 2011; Tadepalli et al., 2011; Wan et al., 2013; Yang and Spilker, 2006). To our knowledge the 15-node tetrahedron (TET15) has never been used in computational biomechanics and it has seen very limited use in nonlinear computational solid mechanics at all (Danielson, 2014), although it has been used in the fluid mechanics community (Bertrand et al., 1992).

The objectives of this study were to determine the efficacy in terms of accuracy of the recovered stresses, robustness in terms of the convergence behavior, and computational expense of the TET10 and TET15 elements compared to the HEX8 element in the context of articular contact mechanics. First, the effects of different integration rules on the stress predictions and computational cost were investigated and used to determine suitable integration rules for both the TET10 and TET15 elements. Then using these integration rules, the accuracy and computational cost of both elements were compared to the HEX8 element for several benchmark contact problems. For one of these problems, we examined the results obtained using TET4 elements to contrast their performance with the quadratic elements. Finally, we compared predictions of contact stresses using HEX8, TET10, and TET15 elements for a validated model of hip contact mechanics (Henak et al., 2014).

2. Methods

2.1. Element formulation and numerical integration

All element formulations in this research were implemented in the FEBio software suite (www.febio.org), which uses an implicit, Newton-based method to solve the nonlinear FE equations of solid mechanics (Maas et al., 2012a). The TET10 element has 10 nodes: 4 corner nodes and 6 nodes located at the midpoint of the edges (Fig. 1). Due to the quadratic shape functions, the facets and edges of this element can distort and therefore the element behavior is "softer" than the TET4 element. The TET15 element adds one more node at the center of each facet, and one in the center of the tetrahedron (Fig. 1). Although the TET15 element has more nodes than the TET10, it is still a quadratic element since the highest order of complete polynomial that can be represented by the shape functions is second order. The TET15 element can represent some forms of quadratic strains, whereas the TET10 element can only represent linear strains.

In a FE formulation, the discretized form of the equilibrium equations requires the use of appropriate numerical integration schemes. For second-order elements, the integration rule should have at least second-order accuracy, at least for linear analyses. The ideal integration rule is less clear for large deformation nonlinear analyses. For this reason, we implemented and compared several volumetric integration rules. We denote volume integration rules as V(n) where (n) indicates the number of integration points. Similarly, the notation S(n) is used to denote surface integration rules. For the TET10 element, both 4-point (V4) and 8-point (V8) Gauss integration rules were implemented (Abramowitz and Stegun, 1964). For the TET15 element, 11-point (V11) and 15-point (V15) Gauss integration rules were implemented (Keast, 1986). All of these rules are at least second-order accurate (for linear analyses) and are symmetric, i.e. the integration points are distributed in a symmetrical spatial pattern.

For contact enforcement, a surface integration rule is required to integrate the traction forces over the discrete surface, represented by facets of the finite elements. The facets of the TET10 element are 6-node quadratic triangles. Two surface integration rules were implemented and compared: 3-point Gauss (S3), and 7-point Gauss (S7) (Fig. 2). For the TET15 element, a 7-node quadratic facet, and the same S3 and S7 integration rules were implemented. Again, these rules have at least second-order accuracy and are symmetric (Abramowitz and Stegun, 1964).

The mean dilatation formulation was used for the HEX8 models (Simo and Taylor, 1991). This formulation is known to perform well for nearly-incompressible materials for which the standard displacement-based formulation, using full integration, has a tendency to lock.

All analyses were performed using the quasi-Newton solver in FEBio (Maas et al., 2012b), which is based on the Broyden–Fletcher–Goldfarb–Shanno (BFGS) method (Matthies and Strang, 1979). This nonlinear solver begins with a full formation and factorization of the stiffness matrix and then proceeds with a user-defined number of BFGS updates, which involve computation of the right-hand-side (RHS) vector. For two of the problems below, we report both the number of stiffness matrix reformations and RHS evaluations as metrics of nonlinear convergence and computational effort. All contact analyses used the "sliding-tension-compression" contact algorithm in FEBio (Maas et al., 2012b). This algorithm implements a facet-on-facet, frictionless sliding contact where the contacting surfaces can separate but not penetrate (Laursen, 2002). The augmented Lagrangian method was used to enforce the contact constraint to a user-defined tolerance (Laursen and Maker, 1995).

2.2. Stress recovery

During the FE solution process, stresses are typically evaluated at the integration points. Since stresses are calculated using the shape function derivatives, they are usually discontinuous across element boundaries. For visualization and for further post-processing analysis (e.g. a-posteriori stress error estimates (Zienkiewicz and Zhu,

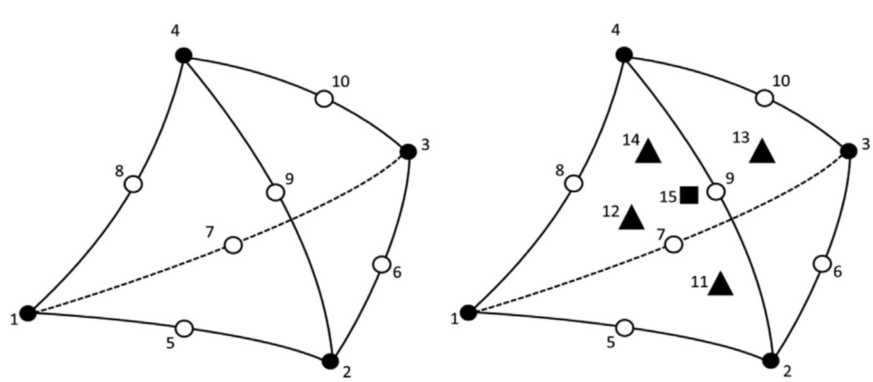

Fig. 1. Schematic of the node topology for two quadratic tetrahedral elements that were examined in this study. Left, 10-node quadratic tetrahedron (TET10). Right, 15-node quadratic tetrahedron (TET15). Closed circles represent corner nodes, open circles represent edge nodes, triangles represent facet center nodes, and the square in the right image represents the center node of the TET15 element.