Facet Elements and the Application of Traction Boundary Conditions in the Context of Finite Deformations

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1 Abstract

Summary of issues, brief description of approach.

2 Introduction

Description of "facet elements," and their intended purpose.

Summary of finite deformations, and the necessary computed quantities for traction boundary conditions (α, $\frac{\partial \alpha}{\partial \hat{u}_{kb}}$, $\mathbf{n}$, and $\frac{\partial \mathbf{n}}{\partial \hat{u}_{kb}}$).

Issues related to constructing in-plane shape function gradients $\varphi_{a,j}$.

Deficiencies of the deformation gradient $\mathbf{F}$ for facet elements.

Approaches for constructing in-plane gradients, and computing desired quantities.

3 Finite Deformations

Overview of equations and quantities:

$$R_{ia} = \int_{\kappa_0} P_{ij} \varphi_{a,j} dv - \int_{\kappa_0} \rho_0 b_i dv - \int_{\partial_t \kappa_0} \bar{p}_i \varphi_a da = 0 \tag{1}$$

$$\frac{\partial R_{ia}}{\partial \hat{u}_{kb}} = \int_{\kappa_0} \frac{\partial P_{ij}}{\partial \hat{u}_{kb}} \varphi_{a,j} dv - \int_{\partial_t \kappa_0} \frac{\partial \bar{p}_i}{\partial \hat{u}_{kb}} \varphi_a da \tag{2}$$

For traction boundary conditions, we will need $\bar{p}_i$ (the Piola traction vector) and $\frac{\partial \bar{p}_i}{\partial \hat{u}_{kb}}$ (derivatives with respect to incremental nodal displacements).

The Piola traction vector can take on several different representations, depending on the type of traction being applied:

(a) Piola traction

$$\bar{p}_i \text{ (specified directly)} \tag{3}$$

(b) Cauchy traction

$$\bar{p}_i = \alpha \bar{t}_i \quad (\bar{t}_i \text{ specified}) \tag{4}$$

Computed quantities: α, and $\frac{\partial \alpha}{\partial \hat{u}_{kb}}$.

(c) Piola pressure

$$\bar{p}_i = \bar{p}^p n_i \quad (\bar{p}^p \text{ specified}) \tag{5}$$

Computed quantities: n_i, and $\frac{\partial n_i}{\partial \hat{u}_{kb}}$.

(d) Cauchy pressure

$$\bar{p}_i = \alpha \bar{p}^t n_i \quad (\bar{p}^t \text{ specified}) \tag{6}$$

Computed quantities: (αn_i), and $\frac{\partial (\alpha n_i)}{\partial \hat{u}_{kb}}$.

Additional traction types for consideration:

(e) "Follower" Piola traction

$$\bar{p}_i = \bar{p}^p n_i + \bar{\tau}^p s_i \quad (\bar{p}^p \text{ and } \bar{\tau}^p \text{ specified}) \tag{7}$$

Computed quantities: n_i, $\frac{\partial n_i}{\partial \hat{u}_{kb}}$, s_i, and $\frac{\partial s_i}{\partial \hat{u}_{kb}}$.

(f) "Follower" Cauchy traction

$$\bar{p}_i = \alpha(\bar{p}^t n_i + \bar{\tau}^t s_i) \quad (\bar{p}^t \text{ and } \bar{\tau}^t \text{ specified}) \tag{8}$$

Computed quantities: (αn_i), $\frac{\partial (\alpha n_i)}{\partial \hat{u}_{kb}}$, (αs_i), and $\frac{\partial (\alpha s_i)}{\partial \hat{u}_{kb}}$.

Where $s_i s_i = 1$, $n_i s_i = 0$.

4 Isoparametric Transformations for Facet Elements

We require two things from the isoparametric mapping:

1. Integration weights at quadrature points (ratio of areas in the physical space to areas in the parent space)
2. Shape function gradients with respect to physical coordinates (in-plane gradients defined on the surface of the facet)

The fundamental issue: mapping between an $n-1$ dimensional parent space and an n dimensional physical space.

Consider the isoparametric mapping for a facet element in three dimensions:

$$X_i = \sum_a \varphi_a(\xi,\, \eta) X_{ia} \tag{9}$$

We can construct the Jacobian mapping $\mathbf{J}$ which relates material vectors $d\xi_\alpha$ in parent space to material vectors dX_i in physical space ($dX_i = J_{i\alpha} d\xi_\alpha$):

$$\mathbf{J} = \begin{bmatrix} X_{1,\xi} & X_{1,\eta} \\ X_{2,\xi} & X_{2,\eta} \\ X_{3,\xi} & X_{3,\eta} \end{bmatrix} \tag{10}$$

For continuum elements, shape function gradients are computed as

$$\varphi_{a,j} = J^{-1}_{j\alpha} \varphi_{a,\alpha} \tag{11}$$

but for facet elements, $\mathbf{J}$ is not invertible.

We can supplement the Jacobian mapping with an additional column corresponding to $\mathbf{X}_{,\zeta}$, even though the isoparametric mapping for facets is parameterized by only ξ and η. Consider the following augmented mapping for a facet element:

$$X_i = \sum_a \varphi_a(\xi,\, \eta) X_{ia} + \zeta N_i(\xi,\, \eta) \tag{12}$$

where $\mathbf{N}$ is the unit normal of the surface in physical space, defined as

$$\mathbf{N} = \frac{\mathbf{X}_{,\xi} \times \mathbf{X}_{,\eta}}{|\mathbf{X}_{,\xi} \times \mathbf{X}_{,\eta}|} \tag{13}$$

It follows that $\mathbf{X}_{,\zeta}$ is simply $\mathbf{N}$, and the Jacobian mapping becomes

$$\mathbf{J} = \begin{bmatrix} X_{1,\xi} & X_{1,\eta} & N_1 \\ X_{2,\xi} & X_{2,\eta} & N_2 \\ X_{3,\xi} & X_{3,\eta} & N_3 \end{bmatrix} \tag{14}$$

Qualitatively, we can interpret this agumentation to our original mapping as simply an extrusion of our two-dimensional facet, so that it now has bi-unit thickness in the normal direction.

We may now invert $\mathbf{J}$ in the usual fashion to obtain *in-plane* shape function gradients. Since $\varphi_{a,\zeta} = 0$, the resulting gradients with respect to physical coordinates will lie only in the plane of the facet, such that

$\varphi_{a,j} N_j = 0 \; \forall a$. Therefore, the shape function gradients $\varphi_{a,j}$ constitute a collection of *covariant derivatives* on the 2-manifold defined by the facet.

To compute quadrature weights, the usual approach for continuum elements involves computing $J = \det(\mathbf{J})$ (the Jacobian determinant) at corresponding quadrature points. J may be thought of as a ratio of differential volumes between physical and parent space, such that we may write $dV = J d\xi d\eta d\zeta$. However, since we have insisted that our facet retain bi-unit thickness in both parent space and physical space, the Jacobian determinant equivalently represents the ratio of differential surface areas between physical and parent space, such that $dA = J d\xi d\eta$.

5 Deficiencies of the Deformation Gradient for Facet Elements

The deformation gradient $\mathbf{F}$ as defined for continuum elements may be expressed as

$$F_{ij} = \delta_{ij} + \sum_a \varphi_{a,j} u_{ia} \tag{15}$$

Alternatively,

$$\mathbf{F} = \mathbf{I} + \sum_a \mathbf{u}_a \otimes \frac{\partial \varphi_a}{\partial \mathbf{X}} \tag{16}$$

In essence, $\mathbf{F}$ maps material vectors $d\mathbf{X}$ in the reference configuration to material vectors $d\mathbf{x}$ in the current configuration ($d\mathbf{x} = \mathbf{F} d\mathbf{X}$). One can cocieve of $d\mathbf{X}$ as a small spherical material region surrounding a given point in space which is both stretched and rotated (under the action of $\mathbf{F}$) into an ellipsoidal material region corresponding to $d\mathbf{x}$. Put another way, $\mathbf{F}$ should map vectors $d\mathbf{X} \in \mathbb{R}^3$ to vectors $d\mathbf{x} \in \mathbb{R}^3$.

For facet elements, it is no longer appropriate to consider a mapping between material vectors which exist in $\mathbb{R}^3$, as the material region surrounding a point on a facet should correspond to $d\mathbf{X} \in \mathcal{S}_r$, where $\mathcal{S}_r \subset \mathbb{R}^3$ is the two-dimensional subspace defining the surface of the facet in the reference configuration. $\mathbf{F}$ should therefore map material vectors $d\mathbf{X} \in \mathcal{S}_r$ to material vectors $d\mathbf{x} \in \mathcal{S}_c$, where $\mathcal{S}_c \subset \mathbb{R}^3$ is a *different* two-dimensional subspace for the facet in the current configuration.

As we have currently written $\mathbf{F}$ in equations (15) and (16), the appropriate mapping of in-plane material vectors is indeed obtained, but the action of $\mathbf{F}$ upon out-of-plane vectors that exist in $\mathbb{R}^3$ is ill-defined. In truth, the mapping of such out-of-plane vectors is irrelevant for our purposes, but it does result in one important consequence: $\mathbf{F}$ (for facet elements) may not be invertible in all cases. In particular, if the deformation includes a 90 degree rotation about any axis that lies in the plane of the reference configuration, then all vectors $d\mathbf{X} \in \mathbb{R}^3$ will be mapped to $d\mathbf{x} \in \mathcal{S}_c$. Since $\mathbf{F}$ in this case will not be a one-to-one mapping, we cannot obtain its inverse.

This deficiency is relevant because we might have otherwise been able to use Namson's equation to relate differential areas $d\mathbf{A}$ in the reference configuration to areas $d\mathbf{a}$ in the current configuration via

$$d\mathbf{a} = J\mathbf{F}^{-T} d\mathbf{A} \tag{17}$$

If $d\mathbf{A} = \mathbf{N}dA$ and $d\mathbf{a} = \mathbf{n}da$, then we may write

$$\alpha\mathbf{n} = J\mathbf{F}^{-T}\mathbf{N} \tag{18}$$

where $\alpha = \frac{da}{dA}$. This would provide us with a means of computing the necessary quantities α, $\mathbf{n}$, $\frac{\partial\alpha}{\partial\hat{u}_{kb}}$, and $\frac{\partial\mathbf{n}}{\partial\hat{u}_{kb}}$. Feasibly, this method could still be used when $\mathbf{F}$ is invertible ($J > 0$), with an alternative strategy employed when J is close to 0.

In the following section, we propose such an alternative scheme for computing the desired deformation quantities in the presence of a singular $\mathbf{F}$.

6 A Method for Computing α, n, $\frac{\partial\alpha}{\partial\hat{u}_{kb}}$, $\frac{\partial\mathbf{n}}{\partial\hat{u}_{kb}}$

Fundamentally, we seek an expression for $d\mathbf{a} = \mathbf{n}da$. Based on the foregoing arguments, this may be obtained via Namson's relation if $\mathbf{F}$ is non-singular. For the special case when $\mathbf{F}$ is not invertible, we may consider the following approach:

Suppose we have identified two arbitrary material vectors $d\mathbf{X}_1 \in S_r$ and $d\mathbf{X}_2 \in S_r$, such that

$$d\mathbf{A} = d\mathbf{X}_1 \times d\mathbf{X}_2 = \mathbf{N}dA \tag{19}$$

If we prescribe $d\mathbf{X}_1$ and $d\mathbf{X}_2$ to be an orthonormal basis of $\mathcal{S}_r$, then $dA = 1$, and we may write

$$d\mathbf{a} = d\mathbf{x}_1 \times d\mathbf{x}_2 = \mathbf{F}d\mathbf{X}_1 \times \mathbf{F}d\mathbf{X}_2 = \mathbf{n}da = \alpha\mathbf{n} \tag{20}$$

Cleary,

$$\alpha = |\mathbf{F}d\mathbf{X}_1 \times \mathbf{F}d\mathbf{X}_2| \tag{21}$$

and

$$\mathbf{n} = \frac{1}{\alpha}(\mathbf{F}d\mathbf{X}_1 \times \mathbf{F}d\mathbf{X}_2) \tag{22}$$