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On the Relation Between Different Parametrizations of Finite Rotations for Shells*

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Abstract

In this work we present interrelations between different finite rotation parametrizations for geometrically exact classical shell models (i.e. models without drilling rotation). In these kind of models the finite rotations are unrestricted in size but constrained in the 3-d space. In the finite element approximation we use interpolation that restricts the treatment of rotations to the finite element nodes. Mutual relationships between different parametrizations are very clearly established and presented by informative commutative diagrams. The pluses and minuses of different parametrizations are discussed and the finite rotation terms arising in the linearization are given in their explicit forms.

*Dedicated to the memory of Professor Frano B. Damjanić

Key words: shell theory, constrained finite rotations, constrained finite rotation vector

1. Introduction

We consider nonlinear shell theories which are capable to handle the problems where rotations are very large. Such theories are frequently referred to as geometrically exact (see e.g. Simo and Fox (1989), Simo *et al.* (1990), Ibrahimbegović (1997)), since the geometric nonlinearities, including rotations, are treated without any simplifications. However, related computational models may exhibit singularity problems, which are closely related to the chosen parametrization of finite rotations.

One way to handle finite rotations of shells is to develop models which incorporate so-called drilling rotation, i.e. rotation around the shell director vector (e.g. see Chroscielewski *et al.* (1992), Sansour and Buefer (1992) or Ibrahimbegović (1994)). In this case, finite rotations can be treated in the same manner as for the beams, and one can draw from the very rich experience on the subject; see e.g. Argyris (1982), Simo and Vu-Quoc (1986) or Ibrahimbegović *et al.* (1995), (1998). When working with geometrically exact shell models of more classical form, where drilling rotation is set to zero (see e.g. Simo and Fox (1989), Büchter and Ramm (1992), Bařar and Ding (1997) or Brank *et al.* (1997)), we have to deal with rotations which are on one hand unrestricted in size, and on the other hand constrained in the 3-d space in the direction of the shell director. Therefore we may speak about the *constrained finite rotation* and the corresponding *constrained rotation vector*. It is only these kinds of models that are considered in the present work.

In geometrically exact shell theories of classical form one needs to model motion of a single vector (i.e. a shell director vector), which does not rotate around the axis defined by that vector. It was recognized long ago (e.g. see Ramm and Matzenmiller (1986) and references therein) that such a rotation can be described by two rotation parameters only, thus leading to the shell finite elements with 5 dof/node. A large variety of possibilities exist for the choice of those two independent parameters (see e.g. Betsch *et al.* (1998) for a recent review), however, three types of parameters are typically preferred in the computational mechanics literature:

- (i) *Euler-like angles* (also called spherical coordinates) which can be updated

additively, e.g. see Ramm and Matzenmiller (1986), Bařar and Ding (1997), Gruttmann and Wagner (1994) or Brank *et al.* (1995);

- (ii) Components of the *iterative constrained rotation vector* along with the multiplicative update of constrained finite rotation tensor at each solution iteration, see e.g. Simo *et al.* (1990), Brank *et al.* (1998);
- (iii) Components of the *total constrained rotation vector* which can be updated additively, e.g. Brank *et al.* (1997), (2000), Betsch *et al.* (1998) or Ibrahimbegović *et al.* (2001).

The main aim of this work is directed towards derivation of mutual relationships between frequently used rotation parameters mentioned in the points (ii) and (iii) above. In particular, we present the so-called commutative diagrams, which relate, on one hand, *multiplicative* and *additive* rotation parameters, and, on the other hand, *spatial* and *material* versions of those parameters.

Although the parameters that allow for an additive update are very attractive, such formulations cannot avoid singularity problems. For example, parametrization of the shell director motion with the total constrained rotation vector is singularity-free when the norm of the total constrained rotation vector is smaller than π (see e.g. Betsch *et al.* (1998), Ibrahimbegović *et al.* (2001)). In formulations with Euler-like angles singularity occurs for certain values of one of the angles (see e.g. Büchter and Ramm (1992), Betsch *et al.* (1998)). Additive parametrization can bypass the singularity problem only if the total quantities are replaced with their incremental versions, thus allowing for a additive update only within each solution increment. For the components of the constrained rotation vector this has been recently proposed by Ibrahimbegović *et al.* Ibrahimbegović *et al.* (2001), Brank *et al.* (2000).

The outline of the paper is as follows. In section 2 we briefly recall governing equations for the stress resultant geometrically exact shell finite element model. Equations are given in terms of the shell director vector and no particular rotation parameters are yet associated with its rotation. In section 3 we recall the relationships between possible parametrizations of the rotation tensor in 3-d space. In section 4 we derive mutual relationships for constrained rotation parameters, and we relate those parameters with the shell director vector. We also address linearization aspects and a geometric view of constrained rotation parameters. Numerical example is presented in section 5 and conclusions are given in section 6.

2. Geometrically exact finite element shell formulation

2.1. Governing equations

In this work we model a shell as a 2-d surface in the 3-d space which has at each point attached a single vector, called shell director vector. The position vector in any deformed configuration of the shell is then defined by the following expression

$$\boldsymbol{\varphi}(\xi^1, \xi^2) + \zeta \mathbf{t}(\xi^1, \xi^2); \quad (\xi^1, \xi^2) \in \mathcal{A}, \quad \zeta \in \mathcal{F} \quad (2.1)$$

Here \mathcal{A} defines the domain of the shell middle surface parameterization and $\mathcal{F} := \{h^-, h^+\}$, with $h = h^+ - h^-$, defining its thickness. In (2.1) above, ξ^1 and ξ^2 are convected coordinates, which are typically employed in the classical works on shells. In the finite element computation we can think of ξ^1 and ξ^2 as of the isoparametric coordinates of a shell finite element. The shell director vector \mathbf{t} is assumed to remain a unit vector for any deformed configuration

$$\|\mathbf{t}\| = 1 \quad (2.2)$$

It follows from (2.1) that all deformed configurations of the shell are completely determined by pairs $(\boldsymbol{\varphi}, \mathbf{t})$, where $\boldsymbol{\varphi}$ defines the shell mid-surface and \mathbf{t} the shell director vector field. The configuration space for a shell, denoted by \mathcal{C} , is then defined by

$$\mathcal{C} = \{(\boldsymbol{\varphi}, \mathbf{t}) : \mathcal{A} \rightarrow \mathbb{R}^3 \times S^2 \mid \boldsymbol{\varphi}|_{\partial\varphi\mathcal{A}} = \bar{\boldsymbol{\varphi}}, \mathbf{t}|_{\partial\Lambda\mathcal{A}} = \bar{\mathbf{t}}\} \quad (2.3)$$

where $\partial\varphi\mathcal{A}$ and $\partial\Lambda\mathcal{A}$ are the parts of the boundary where the displacement and the director field are specified, respectively, and S^2 is a unit sphere, i.e. a space of all vectors of unit length.

Following the classical expositions on the subject, we define at each point of the mid-surface in shell deformed configuration the convected frame as

$$\{\mathbf{t}_1, \mathbf{t}_2, \mathbf{t}_3\} := \{\boldsymbol{\varphi}_{,1}, \boldsymbol{\varphi}_{,2}, \mathbf{t}\} \quad (2.4)$$

where $(\circ)_{,\alpha} = \partial(\circ)/\partial\xi^\alpha$. It is considered that such a basis is convected by the motion from the natural frame constructed in the shell reference configuration

$$\{\mathbf{g}_1, \mathbf{g}_2, \mathbf{g}_3\} := \{\boldsymbol{\varphi}_{0,1}, \boldsymbol{\varphi}_{0,2}, \mathbf{g}\} \quad (2.5)$$

In (2.5) above, $(\boldsymbol{\varphi}_0, \mathbf{g}) \in \mathcal{C}$ are initial positions of the mid-surface and the shell director vector field. Without loss of generality it is assumed that any shell director

vector is at the reference configuration orthogonal to the shell mid-surface, i.e. vector \mathbf{g} is parallel to $\boldsymbol{\varphi}_{0,1} \times \boldsymbol{\varphi}_{0,2}$.

We can define the relative deformation gradient at $\boldsymbol{\varphi}_0$ as a linear map $\mathbf{F} : T_{\boldsymbol{\varphi}_0}\mathcal{C} \rightarrow T_{\boldsymbol{\varphi}}\mathcal{C}$, which is mapping a vector field of the reference shell surface onto a vector field defined on the current shell surface. Relative deformation gradient is given by

$$\mathbf{F} = \mathbf{t}_\alpha \otimes \mathbf{g}^\alpha + \mathbf{t}_3 \otimes \mathbf{g}^3 \quad (2.6)$$

where \mathbf{g}^i are the dual base vectors defined through the relationship $\mathbf{g}_i \cdot \mathbf{g}^j = \delta_i^j$, with δ_i^j as the Kronecker symbol. We note that $\mathbf{g}_3 = \mathbf{g}^3$. With this form of the deformation gradient we can write the Lagrangian strain measures for the shell as

$$\mathbf{E}^{m,s} = \frac{1}{2} [\mathbf{F}^T \mathbf{F} - \mathbf{1}] \quad (2.7)$$

where $\mathbf{1} = \mathbf{g}_\alpha \otimes \mathbf{g}^\alpha + \mathbf{g}_3 \otimes \mathbf{g}^3$ is a unit tensor relative to the reference configuration. It follows from (2.4) and (2.5) that the components of such a strain tensor may be written as

$$\begin{aligned} \varepsilon_{\alpha\beta} &= \frac{1}{2} (\boldsymbol{\varphi}_{,\alpha} \cdot \boldsymbol{\varphi}_{,\beta} - \boldsymbol{\varphi}_{0,\alpha} \cdot \boldsymbol{\varphi}_{0,\beta}) \\ 2\varepsilon_{\alpha 3} &= \gamma_\alpha = \boldsymbol{\varphi}_{,\alpha} \cdot \mathbf{t} - \underbrace{\boldsymbol{\varphi}_{0,\alpha} \cdot \mathbf{g}}_0 \end{aligned} \quad (2.8)$$

where $\varepsilon_{\alpha\beta}$ and γ_α are the classical expressions for the shell membrane and the shell transverse shear strains (e.g. see Naghdi (1972)). The Lagrangian strain measures for the bending strains can be developed by making use of the shell director vector gradient. By defining tensor $\mathbf{G} = \mathbf{t}_{,\alpha} \otimes \mathbf{g}^\alpha$ we may write

$$\mathbf{E}^b = [\mathbf{F}^T \mathbf{G} - \mathbf{B}] \quad (2.9)$$

where $\mathbf{B} = \mathbf{g}_\alpha \cdot \mathbf{g}_{,\beta} \mathbf{g}^\alpha \otimes \mathbf{g}^\beta$ is the curvature tensor (second fundamental form) of the shell surface at the reference configuration. The components of such strain tensor are

$$\kappa_{\alpha\beta} = \boldsymbol{\varphi}_{,\alpha} \cdot \mathbf{t}_{,\beta} - \boldsymbol{\varphi}_{0,\alpha} \cdot \mathbf{g}_{,\beta} \quad (2.10)$$

which are the classical expressions for the shell bending strains (e.g. see Naghdi (1972)).

With strain measures (2.8) and (2.10) we can define the shell strain energy function

$$\Psi (\varepsilon_{\alpha\beta}, \gamma_\alpha, \kappa_{\alpha\beta}, \circ) \quad (2.11)$$

where an empty slot in (2.11) indicates that such a strain energy function should also depend, in general, upon the first and the second fundamental forms of the reference shell surface (i.e. metric tensor and curvature tensor, respectively), along with an eventual presence of internal variables for elastoplastic shells. For small strains, but large displacements and large rotations of elastic isotropic shells, one can assume a quadratic form of the strain energy Ψ , so that the effective stress resultants can be obtained as the corresponding partial derivatives of the strain energy, i.e.

$$n^{\alpha\beta} = \frac{\partial \Psi}{\partial \varepsilon_{\alpha\beta}} \quad q^\alpha = \frac{\partial \Psi}{\partial \gamma_\alpha} \quad m^{\alpha\beta} = \frac{\partial \Psi}{\partial \kappa_{\alpha\beta}} \quad (2.12)$$

It was shown by Budiansky (1968) that the symmetry of the effective stress resultants is the consequence of the balance of angular momentum.

The weak form of the shell balance equation of linear momentum can be written as

$$\begin{aligned} G(\boldsymbol{\varphi}, \mathbf{t}, \delta\boldsymbol{\varphi}, \delta\mathbf{t}) &= \int_A [n^{\alpha\beta} (\delta\boldsymbol{\varphi}_{,\alpha} \cdot \boldsymbol{\varphi}_{,\beta}) + q^\alpha (\delta\boldsymbol{\varphi}_{,\alpha} \cdot \mathbf{t} + \boldsymbol{\varphi}_{,\alpha} \cdot \delta\mathbf{t}) \\ &+ m^{\alpha\beta} (\delta\boldsymbol{\varphi}_{,\alpha} \cdot \mathbf{t}_{,\beta} + \boldsymbol{\varphi}_{,\alpha} \cdot \delta\mathbf{t}_{,\beta})] dA - G_{ext} = 0 \end{aligned} \quad (2.13)$$

where A defines the shell surface at the reference configuration, $\delta\boldsymbol{\varphi}$ is the virtual displacement vector, whereas $\delta\mathbf{t}$ is the variation of the director vector, which has to satisfy condition

$$\delta\mathbf{t} \cdot \mathbf{t} = 0 \quad (2.14)$$

arising from the inextensibility of the shell director vector in (2.2).

In solving the finite element approximation of equations (2.13) by the Newton incremental-iterative method, one makes use of the linearized form of the last

expression given as

$$\begin{aligned}
\text{Lin}[G(\cdot)] &= [G(\cdot)] + \int_A \left[(\delta\varphi_{,\alpha} \cdot \varphi_{,\beta}) \frac{\partial^2 \Psi}{\partial \varepsilon_{\alpha\beta} \partial \varepsilon_{\gamma\delta}} (\Delta\varphi_{,\gamma} \cdot \varphi_{,\delta}) \right. \\
&+ (\delta\varphi_{,\alpha} \cdot \mathbf{t} + \varphi_{,\alpha} \cdot \delta\mathbf{t}) \frac{\partial^2 \Psi}{\partial \gamma_\alpha \partial \gamma_\beta} (\Delta\varphi_{,\beta} \cdot \mathbf{t} + \varphi_{,\beta} \cdot \Delta\mathbf{t}) \\
&+ (\delta\varphi_{,\alpha} \cdot \mathbf{t}_{,\beta} + \varphi_{,\alpha} \cdot \delta\mathbf{t}_{,\beta}) \frac{\partial^2 \Psi}{\partial \kappa_{\alpha\beta} \partial \kappa_{\gamma\delta}} (\Delta\varphi_{,\gamma} \cdot \mathbf{t}_{,\delta} + \varphi_{,\gamma} \cdot \Delta\mathbf{t}_{,\delta}) \left. \right] dA \\
&+ \int_A \left\{ [n^{\alpha\beta} (\delta\varphi_{,\alpha} \cdot \Delta\varphi_{,\beta}) + q^\alpha (\delta\varphi_{,\alpha} \cdot \Delta\mathbf{t} + \Delta\varphi_{,\alpha} \cdot \delta\mathbf{t}) \right. \\
&+ m^{\alpha\beta} (\delta\varphi_{,\alpha} \cdot \Delta\mathbf{t}_{,\beta} + \Delta\varphi_{,\alpha} \cdot \delta\mathbf{t}_{,\beta}) \left. \right] \\
&+ [q^\alpha (\varphi_{,\alpha} \cdot \Delta\delta\mathbf{t}) + m^{\alpha\beta} (\varphi_{,\alpha} \cdot \Delta\delta\mathbf{t}_{,\beta})] \left. \right\} dA = 0
\end{aligned} \tag{2.15}$$

where $\Delta\varphi$ is the incremental displacement vector and $\Delta\mathbf{t}$ is the increment of the director vector, constrained by $\Delta\mathbf{t} \cdot \mathbf{t} = 0$. Note, that $\Delta\delta\varphi$ is zero, while $\Delta\delta\mathbf{t}$ is in general not. We note that the integrals given in (2.15) above provide the basis for computing the material and the geometric part of the tangent operator.

To provide the tangent stiffness matrix for the shell finite element, we choose the following interpolation of the shell deformed configuration

$$\varphi(\xi^1, \xi^2) = \sum_{a=1}^{n_{en}} N_a(\xi^1, \xi^2) \varphi_a \quad \mathbf{t}(\xi^1, \xi^2) = \sum_{a=1}^{n_{en}} N_a(\xi^1, \xi^2) \mathbf{t}_a \tag{2.16}$$

where $N_a(\xi_1, \xi_2)$ are the corresponding shape functions for a shell element with n_{en} nodes, whereas $(\cdot)_a$ are the corresponding nodal values. The virtual and the incremental quantities are interpolated in the same manner

$$\delta\varphi(\xi^1, \xi^2) = \sum_{a=1}^{n_{en}} N_a(\xi^1, \xi^2) \delta\varphi_a \quad \delta\mathbf{t}(\xi^1, \xi^2) = \sum_{a=1}^{n_{en}} N_a(\xi^1, \xi^2) \delta\mathbf{t}_a \tag{2.17}$$

$$\Delta\varphi(\xi^1, \xi^2) = \sum_{a=1}^{n_{en}} N_a(\xi^1, \xi^2) \Delta\varphi_a \quad \Delta\mathbf{t}(\xi^1, \xi^2) = \sum_{a=1}^{n_{en}} N_a(\xi^1, \xi^2) \Delta\mathbf{t}_a \tag{2.18}$$

Derivations of (2.16) to (2.18) with respect to ξ^α coordinates can be obtained trivially.

REMARK 1: Finite element interpolations of this kind are referred to as continuum-consistent, since we interpolate the shell surface and the shell director field with the same interpolation functions. Moreover, we interpolate the

components of the varied and linearized shell director rather than the rotational parameters themselves. In that case the linearization and the discretization commute, i.e. are interchangeable. Another possibility for the interpolation - namely, to directly interpolate the rotation parameters - will not be discussed here.

REMARK 2: The shell model, completely equivalent to the present 2-d surface model, can be derived from the 3-d continuum by employing standard assumptions on the distribution of the displacement field on the shell body and by approximating the terms describing the shell strains; see e.g. Büchter and Ramm (1992), Parisch (1992), Başar and Ding (1997), Brank *et al.* (1997), (1998).

2.2. Description of the problem addressed

Up to now the finite rotation parameters were not yet explicitly introduced in the above equations; this will be done below in section 4. Once such parameters are chosen, one has to compute variation, $\delta\mathbf{t}$, and linearization, $\Delta\mathbf{t}$ and $\Delta\delta\mathbf{t}$, in accordance with the chosen parameters. Rotation degrees of freedom in the finite element computations are then associated with the linearization of the shell director with respect to the chosen rotation parameters. By using the continuum-consistent interpolation (2.16), we need to derive those quantities only at the *nodal points* of the finite element mesh. Therefore, formulations with different parameters (with different types of rotation degrees of freedom) should produce the same results.

The problem that we address in the following may be stated as: Derive variation, linearization and linearization of the variation of the shell director vector at a finite element node with respect to different rotation parameters and establish mutual relationships between those parameters.

3. Unconstrained rotations in the 3-d space (beam case)

In this section we summarize some expressions for finite rotations in the 3-d space which we need in subsequent developments.

3.1. Representation of rotation tensor

A space of all rotations (orthogonal tensors) in the 3-d space is defined as

$$SO(3) = \{\Lambda \mid \Lambda\Lambda^T = \mathbf{I}, \det \Lambda = 1\} \quad (3.1)$$

For any $\Lambda \in SO(3)$ there exists a vector $\boldsymbol{\vartheta} \in \mathbb{R}^3$ which is not affected by the rotation Λ . This is an eigenvector or a rotation vector of Λ . Since Λ is a two-point tensor which maps quantities from the reference into the current configuration, one may use the following notation (Ibrahimbegović *et al.* (1995))

$$\begin{aligned}\boldsymbol{\theta} &= \Lambda \boldsymbol{\vartheta} \\ &= \mathbf{I} \boldsymbol{\vartheta}\end{aligned}\tag{3.2}$$

We refer to $\boldsymbol{\vartheta}$ as the material rotation vector and to $\boldsymbol{\theta}$ as its spatial counterpart. If we choose one fixed frame \mathbf{e}_i ($\mathbf{e}_3 \equiv \mathbf{e}$) for both configurations, we have

$$\vartheta^i \mathbf{e}_i = \theta^i \mathbf{e}_i$$

Knowing rotation vector $\boldsymbol{\vartheta}$, one can reconstruct the corresponding orthogonal matrix Λ by using the Rodrigues formula

$$\Lambda(\boldsymbol{\vartheta}) = \cos \vartheta \mathbf{I} + \frac{\sin \vartheta}{\vartheta} \Theta + \frac{1 - \cos \vartheta}{\vartheta^2} \boldsymbol{\vartheta} \otimes \boldsymbol{\vartheta}\tag{3.3}$$

or the exponential mapping formula

$$\Lambda(\boldsymbol{\vartheta}) = \exp[\Theta]\tag{3.4}$$

where $\Theta \in so(3)$ is a skew-symmetric tensor defined as $\Theta \mathbf{b} = \boldsymbol{\vartheta} \times \mathbf{b}$ for any $\mathbf{b} \in \mathbb{R}^3$, $\vartheta = \|\boldsymbol{\vartheta}\|$ and \otimes is a tensor product of two vectors. One also calls $\boldsymbol{\vartheta}$ the axial vector of Θ .

In the following we will use representations (3.3) and (3.4) of the rotation tensor Λ to describe the motion of the shell director vector \mathbf{t} and to derive the corresponding variations and linearizations needed in the linearized form of shell balance equation (2.15).

3.2. Rotation parameters and commutative diagram

With the use of exponential mapping (3.4), a variation of rotation tensor Λ can be presented in either material or spatial version

$$\begin{aligned}\delta \Lambda &= \left. \frac{d}{dt} \Lambda \exp[t\delta\Psi] \right|_{t=0} = \Lambda \delta\Psi \\ &= \left. \frac{d}{dt} \exp[t\delta\mathbf{W}] \Lambda \right|_{t=0} = \delta\mathbf{W} \Lambda\end{aligned}\tag{3.5}$$

respectively, where $\delta\Psi$ and $\delta\mathbf{W}$ are material and spatial skew-symmetric tensors which represent infinitesimal rotations. From (3.5) it follows that

$$\delta\Psi = \Lambda^T \delta\mathbf{W} \Lambda \quad \delta\mathbf{W} = \Lambda \delta\Psi \Lambda^T \quad (3.6)$$

It can be shown from (3.6) that their corresponding axial vectors $\delta\mathbf{w}$ and $\delta\boldsymbol{\psi}$ are related as

$$\delta\mathbf{w} = \Lambda \delta\boldsymbol{\psi} \quad \delta\boldsymbol{\psi} = \Lambda^T \delta\mathbf{w} \quad (3.7)$$

One can also compute variation of Λ in terms of vector-like rotation parameters, i.e. in terms of rotation vector. By exploiting (3.3) and by using additive update of rotation parameters

$$\begin{aligned} \delta\Lambda &= \left. \frac{d}{dt} \Lambda(\boldsymbol{\vartheta} + t\delta\boldsymbol{\vartheta}) \right|_{t=0} \\ &= \left. \frac{d}{dt} \Lambda(\boldsymbol{\theta} + t\delta\boldsymbol{\theta}) \right|_{t=0} \end{aligned} \quad (3.8)$$

we can obtain explicit expressions for $\delta\Lambda$ in terms of rotation vector.

By comparing (3.5) and (3.8) we can obtain the following relationships

$$\delta\boldsymbol{\psi} = \mathbf{T}^T(\boldsymbol{\vartheta}) \delta\boldsymbol{\vartheta} \quad \delta\mathbf{w} = \mathbf{T}(\boldsymbol{\theta}) \delta\boldsymbol{\theta} \quad (3.9)$$

where

$$\mathbf{T}(\boldsymbol{\vartheta}) = \frac{\sin \vartheta}{\vartheta} \mathbf{I} + \frac{1 - \cos \vartheta}{\vartheta^2} \Theta + \frac{\vartheta - \sin \vartheta}{\vartheta^3} \boldsymbol{\vartheta} \otimes \boldsymbol{\vartheta} \quad (3.10)$$

and $\mathbf{T}(\boldsymbol{\theta})$ is defined analogously. It can be shown (Ibrahimbegović *et al.* (1995)) that $\mathbf{T}(\boldsymbol{\vartheta})$ and $\mathbf{T}(\boldsymbol{\theta})$ will exhibit a singularity problem whenever the norm or rotation vector $\vartheta = \|\boldsymbol{\vartheta}\| = \|\boldsymbol{\theta}\| = \theta$ reaches multiple of 2π . For overcoming this deficiency, Ibrahimbegović (1997) introduced so-called incremental rotation vector, which is reset at the beginning of each solution increment; see also Ibrahimbegović *et al.* (1995), Ibrahimbegović and Al Mikdad (1998).

The above relations can be summarized in a commutative diagram for unconstrained 3-d rotations (see Figure 3.1) which interrelates variations $(\delta\boldsymbol{\psi}, \delta\mathbf{w}, \delta\boldsymbol{\vartheta}, \delta\boldsymbol{\theta})$ of all four possible parametrizations within representation of Λ in forms (3.3) and (3.4).

4. Constrained rotations in the 3-d space (classical shell case)

In this section we construct commutative diagrams for classical shell models.

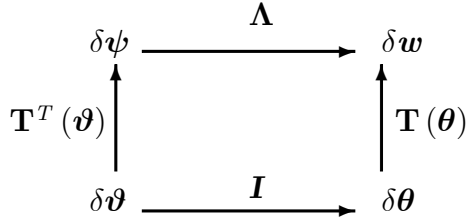


Figure 3.1: Commutative diagram of admissible variations for unconstrained 3-d finite rotation parameters (beam case).

4.1. Definition of material and spatial rotation

Let us define position of the shell director vector at a particular point of the shell mid-surface by a finite rotation of the global base vector (see Fig. 4.1)

$$\mathbf{g} = \Lambda_0 \mathbf{e} \quad \mathbf{e}_3 \equiv \mathbf{e} = \{0, 0, 1\}^T \quad (4.1)$$

where Λ_0 is initial rotation tensor. In an analogous manner, its position at the deformed configuration may be obtained by using rotation tensor Λ

$$\mathbf{t} = \Lambda \mathbf{e} \quad (4.2)$$

Orthogonal tensor Λ may be viewed as a composition of two orthogonal tensors, e.g. one taking us from fixed global basis to the local basis in the reference configuration and another taking us further to the current configuration. Equation (4.2) may be then rewritten as

$$\begin{aligned} \mathbf{t} = \Lambda \mathbf{e} &= \Lambda_0 \tilde{\Lambda}(\vartheta) \mathbf{e} \\ &= \tilde{\Lambda}(\theta) \Lambda_0 \mathbf{e} = \tilde{\Lambda}(\theta) \mathbf{g} \end{aligned} \quad (4.3)$$

where $\tilde{\Lambda}(\circ)$ is rotation expressed either in form (3.3) or (3.4).

It can be seen from Fig. 4.1 that we have material and spatial version of rotation vector for both rotations $\tilde{\Lambda}(\vartheta)$ and $\tilde{\Lambda}(\theta)$; altogether four rotation vectors. In the following we will identify ϑ as a material rotation vector associated with

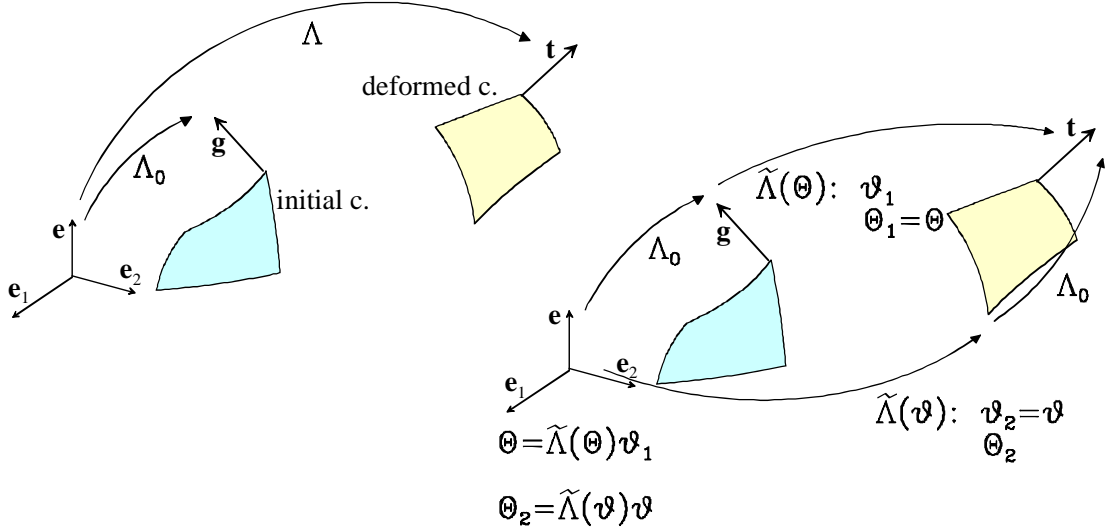


Figure 4.1: Shell director at initial and deformed configuration. Material and spatial rotation vector.

$\tilde{\Lambda}(\boldsymbol{\vartheta})$ and $\boldsymbol{\theta}$ as a spatial rotation vector associated with $\tilde{\Lambda}(\boldsymbol{\theta})$, see Fig. 4.1. Relation between those two vectors may be obtained from (4.3)

$$\tilde{\Lambda}(\boldsymbol{\theta}) = \Lambda_0 \tilde{\Lambda}(\boldsymbol{\vartheta}) \Lambda_0^T \quad \Rightarrow \quad \boldsymbol{\theta} = \Lambda_0 \boldsymbol{\vartheta} \quad \boldsymbol{\vartheta} = \Lambda_0^T \boldsymbol{\theta} \quad (4.4)$$

Position of rotation vectors in \mathbb{R}^3 is restricted by the assumption that Λ rotates \mathbf{e} into \mathbf{t} without drilling rotation, and, similarly, Λ_0 rotates \mathbf{e} into \mathbf{g} with no rotation about that vector. In other words, rotations Λ and Λ_0 are constrained by requiring that the rotation component along the shell director vector plays no role in the theory. We may then write the following constraints (see eqs. (4.3))

$$\begin{aligned} \mathbf{t} = \Lambda_0 \tilde{\Lambda}(\boldsymbol{\vartheta}) \mathbf{e} &\Rightarrow \boldsymbol{\vartheta} \cdot \mathbf{e} = 0; \quad \boldsymbol{\vartheta} \cdot \Lambda_0^T \mathbf{t} = 0 \\ \mathbf{t} = \tilde{\Lambda}(\boldsymbol{\theta}) \mathbf{g} &\Rightarrow \boldsymbol{\theta} \cdot \mathbf{g} = 0; \quad \boldsymbol{\theta} \cdot \mathbf{t} = 0 \end{aligned} \quad (4.5)$$

It is because of the above constraints (4.5) that we talk about the constrained rotation tensor and about the constrained rotation vector. Due to (4.1) and (4.4) we have

$$\begin{aligned} \boldsymbol{\vartheta} \cdot \mathbf{e} &= 0 \iff \boldsymbol{\theta} \cdot \mathbf{g} = 0 \\ \boldsymbol{\vartheta} \cdot \Lambda_0^T \mathbf{t} &= 0 \iff \boldsymbol{\theta} \cdot \mathbf{t} = 0 \end{aligned}$$

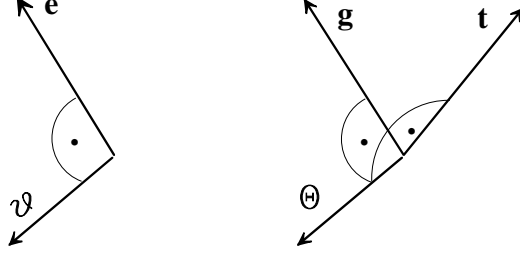


Figure 4.2: Constraints on material and spatial rotations.

4.2. Variation of the shell director rotation

In this section we derive variation of the shell director which we need in the weak form of shell balance equation of linear momentum, (2.13). Formally it may be obtained as

$$\delta \mathbf{t} = \left. \frac{d}{dt} \right|_{t=0} \mathbf{t}_t = \left. \frac{d}{dt} \right|_{t=0} \Lambda_t \mathbf{e} \quad (4.6)$$

where altogether four possibilities exist to construct Λ_t within the use of (3.3) and (3.4).

By exploiting (3.5), we can obtain the first two possibilities in terms of multiplicative parameters $\delta \boldsymbol{\psi}$ and $\delta \mathbf{w}$

$$\mathbf{t}_t = \Lambda_t \mathbf{e} = \Lambda \exp [t \delta \Psi] \mathbf{e} \quad \Rightarrow \quad \delta \mathbf{t} = \Lambda (\delta \boldsymbol{\psi} \times \mathbf{e}) \quad (4.7)$$

$$\mathbf{t}_t = \Lambda_t \mathbf{e} = \exp [t \delta \mathbf{W}] \Lambda \mathbf{e} = \exp [t \delta \mathbf{W}] \mathbf{t} \quad \Rightarrow \quad \delta \mathbf{t} = \delta \mathbf{w} \times \mathbf{t} \quad (4.8)$$

Since $\exp [t \delta \Psi]$ rotates \mathbf{e} and $\exp [t \delta \mathbf{W}]$ rotates \mathbf{t} without drilling rotation, we have from (4.7) and (4.8) the following constraints

$$\delta \boldsymbol{\psi} \cdot \mathbf{e} = 0 \quad \delta \mathbf{w} \cdot \mathbf{t} = 0 \quad (4.9)$$

By exploiting (3.3) and (3.8), we can derive another two expressions in terms of additive parameters

$$\mathbf{t}_t = \Lambda_t \mathbf{e} = \Lambda_0 \tilde{\Lambda} (\boldsymbol{\vartheta} + t \delta \boldsymbol{\vartheta}) \mathbf{e} \quad \Rightarrow \quad \delta \mathbf{t} = \Lambda_0 \mathbf{A} (\boldsymbol{\vartheta}) \delta \boldsymbol{\vartheta} \quad (4.10)$$

$$\mathbf{t}_t = \Lambda_t \mathbf{e} = \tilde{\Lambda}(\boldsymbol{\theta} + t\delta\boldsymbol{\theta}) \Lambda_0 \mathbf{e} \quad \Rightarrow \quad \delta\mathbf{t} = \mathbf{A}(\boldsymbol{\theta})\delta\boldsymbol{\theta} \quad (4.11)$$

Tensor $\mathbf{A}(\boldsymbol{\vartheta})$ in (4.10) is defined as

$$\mathbf{A}(\boldsymbol{\vartheta}) = -\frac{\sin \vartheta}{\vartheta} (\mathbf{e} \otimes \boldsymbol{\vartheta} + \mathbf{E}) + \frac{\vartheta \cos \vartheta - \sin \vartheta}{\vartheta^3} (\boldsymbol{\vartheta} \times \mathbf{e}) \otimes \boldsymbol{\vartheta} \quad (4.12)$$

where \mathbf{E} is skew-symmetric tensor with the property $\mathbf{E}\mathbf{b} = \mathbf{e} \times \mathbf{b}$ for any $\mathbf{b} \in \mathbb{R}^3$. Tensor $\mathbf{A}(\boldsymbol{\theta})$ in (4.11) is defined in a similar way as

$$\mathbf{A}(\boldsymbol{\theta}) = -\frac{\sin \theta}{\theta} (\mathbf{g} \otimes \boldsymbol{\theta} + \mathbf{G}) + \frac{\theta \cos \theta - \sin \theta}{\theta^3} (\boldsymbol{\theta} \times \mathbf{g}) \otimes \boldsymbol{\theta} \quad (4.13)$$

where $\mathbf{G}\mathbf{b} = \mathbf{g} \times \mathbf{b}$ for any $\mathbf{b} \in \mathbb{R}^3$. Since the norm of the rotation vector is $\vartheta = \theta$ and $\mathbf{G} = \Lambda_0 \mathbf{E} \Lambda_0^T$, it can be shown by using (4.4) that

$$\mathbf{A}(\boldsymbol{\theta}) = \Lambda_0 \mathbf{A}(\boldsymbol{\vartheta}) \Lambda_0^T \quad (4.14)$$

Further details about the derivation of tensors $\mathbf{A}(\boldsymbol{\vartheta})$ or $\mathbf{A}(\boldsymbol{\theta})$ may be found in Parisch (1992), Brank *et al.* (1997), Betsch *et al.* (1998), Ibrahimbegović *et al.* (2001).

4.3. Position of the shell director vector

By using (3.3) and (4.5), we may express position of the shell director vector at the deformed configuration, (4.3), in terms of rotation vector simply as

$$\begin{aligned} \mathbf{t} &= \Lambda_0 \tilde{\Lambda}(\boldsymbol{\vartheta}) \mathbf{e} = \Lambda_0 \left(\cos \vartheta \mathbf{e} + \frac{\sin \vartheta}{\vartheta} \boldsymbol{\vartheta} \times \mathbf{e} \right) \\ \mathbf{t} &= \tilde{\Lambda}(\boldsymbol{\theta}) \mathbf{g} = \cos \theta \mathbf{g} + \frac{\sin \theta}{\theta} \boldsymbol{\theta} \times \mathbf{g} \end{aligned} \quad (4.15)$$

Note, that norm $\|\boldsymbol{\vartheta}\| = \vartheta = \theta = \|\boldsymbol{\theta}\|$, and that vectors $\boldsymbol{\vartheta}$ and $\boldsymbol{\theta}$ are the total material and the total spatial rotation vector, respectively. In other words, they measure the total rotation of the shell director from the reference configuration.

By using (4.7) and (4.8) we may express shell director position at the $i+1$ -th iteration of the n -th solution increment as

$$\begin{aligned} \mathbf{t}_n^{i+1} &= \Lambda_n^i \exp[\Delta\Psi_n^{i+1}] \mathbf{e} \\ \mathbf{t}_n^{i+1} &= \exp[\Delta\mathbf{W}_n^{i+1}] \mathbf{t}_n^i = \exp\left[\widehat{\mathbf{t}_n^i \times \Delta\mathbf{t}_n^{i+1}}\right] \mathbf{t}_n^i \end{aligned}$$

where $\Delta\Psi_n^{i+1}$, $\Delta\mathbf{W}_n^{i+1}$ and $\widehat{(\circ)}$ are skew-symmetric tensors.

4.4. Rotation vectors and related tensors in coordinate representation

By observing constraints (4.5), we conclude that $\boldsymbol{\vartheta}$ may be determined by 2 components only in $\{\mathbf{e}_1, \mathbf{e}_2, \mathbf{e}\}$ frame, while $\boldsymbol{\theta}$ has 3 components which are not mutually independent

$$\boldsymbol{\vartheta}^T = \{\vartheta_1, \vartheta_2\} \quad \boldsymbol{\theta}^T = \{\theta_1, \theta_2, \theta_3\} \quad (4.16)$$

For example, by using (4.15) we can define \mathbf{t} in terms of $\boldsymbol{\vartheta}$ components simply as

$$\mathbf{t} = \Lambda_0 \left\{ \frac{\sin \vartheta}{\vartheta} \vartheta_2, -\frac{\sin \vartheta}{\vartheta} \vartheta_1, \cos \vartheta \right\}^T \quad (4.17)$$

Similar conclusion can be done for $\delta\boldsymbol{\psi}$ and $\delta\mathbf{w}$: the former vector can be presented by 2 components only and the latter has 3 components constrained by (4.9)₂

$$\delta\boldsymbol{\psi}^T = \{\delta\psi_1, \delta\psi_2\} \quad \delta\mathbf{w}^T = \{\delta w_1, \delta w_2, \delta w_3\} \quad (4.18)$$

Let us further write the coordinate representation of $\mathbf{A}(\boldsymbol{\vartheta})$ and check if this operation is bijective

$$\mathbf{A}(\boldsymbol{\vartheta}) = \begin{bmatrix} (c_2\vartheta_1\vartheta_2) & (c_1 + c_2\vartheta_2^2) \\ (-c_1 - c_2\vartheta_1^2) & -c_2\vartheta_1\vartheta_2 \\ (-c_1\vartheta_1) & (-c_1\vartheta_2) \end{bmatrix}_{(3 \times 2)}$$

$$c_1 = \frac{\sin \vartheta}{\vartheta} \quad c_2 = \frac{\vartheta \cos \vartheta - \sin \vartheta}{\vartheta^3}$$

It can be seen that for any rotation value with $\vartheta = k\pi; k = 1, 2, \dots$, which implies $c_1 = 0$, the matrix $\mathbf{A}(\boldsymbol{\vartheta})$ would only have rank one, i.e. only one column will be independent, since the second column can be obtained by multiplying the first with ϑ_2/ϑ_1 . This implies that the mapping between the director vector and the corresponding rotation vector is no longer bijective. It is not possible to uniquely define variation of \mathbf{t} when $\vartheta = \pi$ (see 4.10), so that the finite rotation formulations based on the total rotation vector $\boldsymbol{\vartheta}$ are restricted to solution of the problems where rotations of the shell directors are less than π . How to avoid this singularity problem will be addressed in section 4.7. According to (4.14), $\mathbf{A}(\boldsymbol{\theta})$ is a (3×3) matrix obtained as

$$[\mathbf{A}(\boldsymbol{\theta})]_{(3 \times 3)} = [\Lambda_0]_{(3 \times 3)} [\mathbf{A}(\boldsymbol{\vartheta})]_{(3 \times 2)} [\Lambda_0^T]_{(2 \times 3)} \quad (4.19)$$

4.5. Interrelations between different parametrizations

In this section we establish relationships between different chosen parametrizations.

First, from (4.4) it follows that a relation between the variation of constrained material rotation vector and the variation of constrained spatial rotation vector can be written as

$$\delta\boldsymbol{\theta} = \Lambda_0\delta\boldsymbol{\vartheta} \quad \delta\boldsymbol{\vartheta} = \Lambda_0^T\delta\boldsymbol{\theta} \quad (4.20)$$

Next, we obtain by comparing (4.7) with (4.10) the relation between the material multiplicative parameters, $\delta\boldsymbol{\psi}$, and the material additive parameters, $\delta\boldsymbol{\vartheta}$. We have

$$\Lambda(\delta\boldsymbol{\psi} \times \mathbf{e}) = \Lambda_0\mathbf{A}(\boldsymbol{\vartheta})\delta\boldsymbol{\vartheta} \quad (4.21)$$

By using $\Lambda = \Lambda_0\tilde{\Lambda}(\boldsymbol{\vartheta})$, see (4.3), it follows from (4.21) that $\delta\boldsymbol{\psi}$ may be expressed as

$$\delta\boldsymbol{\psi} = \mathbf{E} \left[\tilde{\Lambda}(\boldsymbol{\vartheta}) \right]^T \mathbf{A}(\boldsymbol{\vartheta})\delta\boldsymbol{\vartheta} = \mathbf{B}(\boldsymbol{\vartheta})\delta\boldsymbol{\vartheta} \quad (4.22)$$

where \mathbf{E} is skew-symmetric matrix associated with the base vector \mathbf{e} . A product $\left[\tilde{\Lambda}(\boldsymbol{\vartheta}) \right]^T \mathbf{A}(\boldsymbol{\vartheta})$, which appears in eq. (4.22), may be, with the use of (3.3) and after some manipulations, written as

$$\begin{aligned} \tilde{\mathbf{B}}(\boldsymbol{\vartheta}) = \left[\tilde{\Lambda}(\boldsymbol{\vartheta}) \right]^T \mathbf{A}(\boldsymbol{\vartheta}) &= \left(-\frac{\sin^2 \vartheta}{\vartheta^2} \mathbf{I} + \frac{\vartheta - \sin \vartheta \cos \vartheta}{\vartheta^3} \Theta \right) \mathbf{e} \otimes \boldsymbol{\vartheta} \\ &- \frac{\sin \vartheta}{\vartheta} \left[\cos \vartheta \mathbf{I} - \frac{\sin \vartheta}{\vartheta} \Theta + \frac{1 - \cos \vartheta}{\vartheta^2} \boldsymbol{\vartheta} \otimes \boldsymbol{\vartheta} \right] \end{aligned} \quad (\mathbf{E.23})$$

where Θ is skew-symmetric matrix associated with vector $\boldsymbol{\vartheta}$. The component form of the above product is

$$\tilde{\mathbf{B}}(\boldsymbol{\vartheta}) = \begin{bmatrix} (\vartheta_1\vartheta_2(d_2 - d_3)) & (d_1 + d_2\vartheta_2^2 + d_3\vartheta_1^2) \\ (-d_1 - d_2\vartheta_1^2 - d_3\vartheta_2^2) & (\vartheta_1\vartheta_2(d_3 - d_2)) \end{bmatrix}_{(2 \times 2)} \quad (4.24)$$

$$d_1 = \frac{\sin \vartheta \cos \vartheta}{\vartheta} \quad d_2 = \frac{\vartheta - \sin \vartheta \cos \vartheta}{\vartheta^3} \quad d_3 = \frac{\sin \vartheta (1 - \cos \vartheta)}{\vartheta^3}$$

By multiplication of (4.24) with \mathbf{E} from the left hand side, we obtain a symmetric matrix

$$\mathbf{B}(\boldsymbol{\vartheta}) = \mathbf{E}\tilde{\mathbf{B}}(\boldsymbol{\vartheta}) = \begin{bmatrix} (d_1 + d_2\vartheta_1^2 + d_3\vartheta_2^2) & (\vartheta_1\vartheta_2(d_2 - d_3)) \\ (\vartheta_1\vartheta_2(d_2 - d_3)) & (d_1 + d_2\vartheta_2^2 + d_3\vartheta_1^2) \end{bmatrix}_{(2 \times 2)} \quad (4.25)$$

with the determinant equal to $(\sin \vartheta/\vartheta)$, which implies that the singularity occurs at $\vartheta = k\pi; k = 1, 2, \dots$, as in the case of $\mathbf{A}(\boldsymbol{\vartheta})$.

Analogously, we obtain the relation between the spatial multiplicative parameters, $\delta\mathbf{w}$, and the spatial additive parameters, $\delta\boldsymbol{\theta}$, by comparing (4.8) with (4.11)

$$\delta\mathbf{w} = \mathbf{T}\mathbf{A}(\boldsymbol{\theta})\delta\boldsymbol{\theta} = \mathbf{D}(\boldsymbol{\theta}) \quad (4.26)$$

where $\mathbf{T}\mathbf{b} = \mathbf{t} \times \mathbf{b}$ for any $\mathbf{b} \in \mathbb{R}^3$. By using transformation (4.14) and relation $\mathbf{T} = \Lambda\mathbf{E}\Lambda^T$, we can show that

$$[\mathbf{D}(\boldsymbol{\theta})]_{(3 \times 3)} = \Lambda_{(3 \times 2)} [\mathbf{B}(\boldsymbol{\vartheta})]_{(2 \times 2)} [\Lambda_0^T]_{(2 \times 3)} \quad (4.27)$$

which implies the singularity of $\mathbf{D}(\boldsymbol{\theta})$ for $\theta = \vartheta = k\pi; k = 1, 2, \dots$

The above relations are summarized on the commutative diagram of Figure 4.3 of admissible variations of constrained rotation parameters $(\delta\boldsymbol{\psi}, \delta\mathbf{w}, \delta\boldsymbol{\vartheta}, \delta\boldsymbol{\theta})$. The diagram is also valid for the iterative $(\Delta\boldsymbol{\psi}_n^i, \Delta\mathbf{w}_n^i, \Delta\boldsymbol{\vartheta}_n^i, \Delta\boldsymbol{\theta}_n^i)$ quantities with i defining iteration at n -th solution increment. As such it can be useful for the transformation of one finite rotation shell finite element formulation into the another. The diagram namely relates, on one hand, the multiplicative $(\Delta\boldsymbol{\psi}_n^i, \Delta\mathbf{w}_n^i)$ with the additive $(\Delta\boldsymbol{\vartheta}_n^i, \Delta\boldsymbol{\theta}_n^i)$ constrained rotation parameters, and on the other hand, the spatial $(\Delta\mathbf{w}_n^i, \Delta\boldsymbol{\theta}_n^i)$ with the material $(\Delta\boldsymbol{\psi}_n^i, \Delta\boldsymbol{\vartheta}_n^i)$ version of those parameters.

4.6. Interrelations between different parametrizations for an alternative form of variation of the shell director rotation

On can use eqs. (4.7) and (4.8) and take vector product $\delta\boldsymbol{\psi} \times \mathbf{e}$ instead of $\delta\boldsymbol{\psi}$ as an admissible variation of material rotation variables, and, similarly, vector product $\delta\mathbf{w} \times \mathbf{t}$ instead of $\delta\mathbf{w}$ as an admissible variation of spatial rotation variables. The commutative diagram from Figure 4.3 has then an alternative form which is

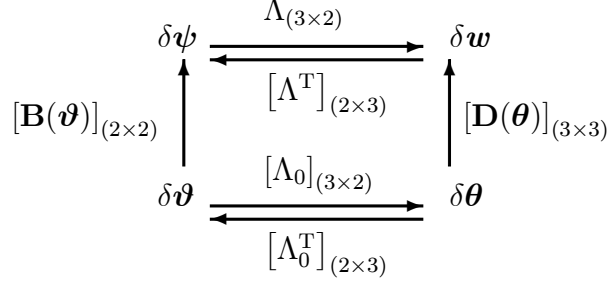


Figure 4.3: Commutative diagram of admissible variations for constrained finite rotation parameters. Vectors $\delta\boldsymbol{\psi}$ and $\delta\boldsymbol{\vartheta}$ have two components, while vectors $\delta\mathbf{w}$ and $\delta\boldsymbol{\theta}$ have three components which are not mutually independent.

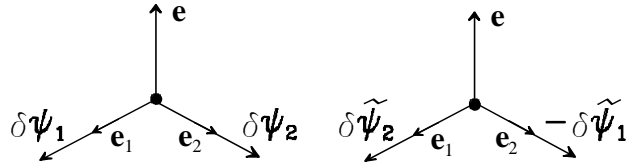


Figure 4.4: Direction of variations of material rotation parameters for multiplicative update of rotations.

presented in Figure 4.5. Note, that $\|\delta\boldsymbol{\psi} \times \mathbf{e}\| = \|\delta\boldsymbol{\psi}\|$ and that the component representation of $\delta\boldsymbol{\psi} \times \mathbf{e}$ is

$$\delta\boldsymbol{\psi} \times \mathbf{e} = \{\delta\psi_2, -\delta\psi_1\}^T = \delta\tilde{\boldsymbol{\psi}} = \{\delta\tilde{\psi}_1, \delta\tilde{\psi}_2\}^T \quad (4.28)$$

This approach was used in the works of Simo *et al.* (1989), (1990) and Brank *et al.* (1998). Rotational degrees of freedom are then $\Delta\tilde{\psi}_{n,1}^i = \Delta\psi_{n,2}^i$ and $\Delta\tilde{\psi}_{n,2}^i = -\Delta\psi_{n,1}^i$.

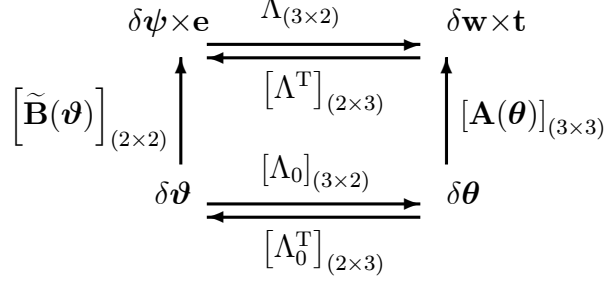


Figure 4.5: An alternative form of commutative diagram of admissible variations for constrained finite rotations. Multiplicative parameters are retained in a form of vector product. Vectors $\delta\boldsymbol{\psi} \times \mathbf{e}$ and $\delta\boldsymbol{\vartheta}$ have two components, while vectors $\delta\mathbf{w} \times \mathbf{t}$ and $\delta\boldsymbol{\theta}$ have three components which are not mutually independent.

4.7. Solution for singularity problem: Constrained incremental rotation vector

For overcoming the singularity problem of $\mathbf{A}(\boldsymbol{\vartheta})$, described in section 4.4, the constrained incremental rotation vector was introduced in Ibrahimbegović *et al.* (2001) and Brank *et al.* (2000). It is fully consistent with the standard incremental solution scheme for nonlinear problems.

Let us denote this vector as $\boldsymbol{\vartheta}_{n+1}$ (material version) and as $\boldsymbol{\theta}_{n+1}$ (spatial version) for a typical increment $n + 1$. It is reset to zero at the beginning of each increment, so that in accordance with (4.19) the singularity would occur when its value reaches $\vartheta_{n+1} = \|\boldsymbol{\vartheta}_{n+1}\| = \theta_{n+1} = k\pi; k = 1, 2, \dots$. In practice this is never the case, since the incremental shell director rotation is limited to much smaller value by the solution procedure.

Incremental rotation vectors $\boldsymbol{\vartheta}_{n+1}$ and $\boldsymbol{\theta}_{n+1}$ are defined by relations (see Fig. 4.6)

$$\Lambda_{n+1} = \tilde{\Lambda}(\boldsymbol{\theta}_{n+1}) \Lambda_n = \Lambda_n \tilde{\Lambda}(\boldsymbol{\vartheta}_{n+1}) \quad (4.29)$$

We can conclude from (4.29) that

$$\tilde{\Lambda}(\boldsymbol{\theta}_{n+1}) = \Lambda_n \tilde{\Lambda}(\boldsymbol{\vartheta}_{n+1}) \Lambda_n^T, \quad \tilde{\Lambda}(\boldsymbol{\vartheta}_{n+1}) = \Lambda_n^T \tilde{\Lambda}(\boldsymbol{\theta}_{n+1}) \Lambda_n \quad (4.30)$$

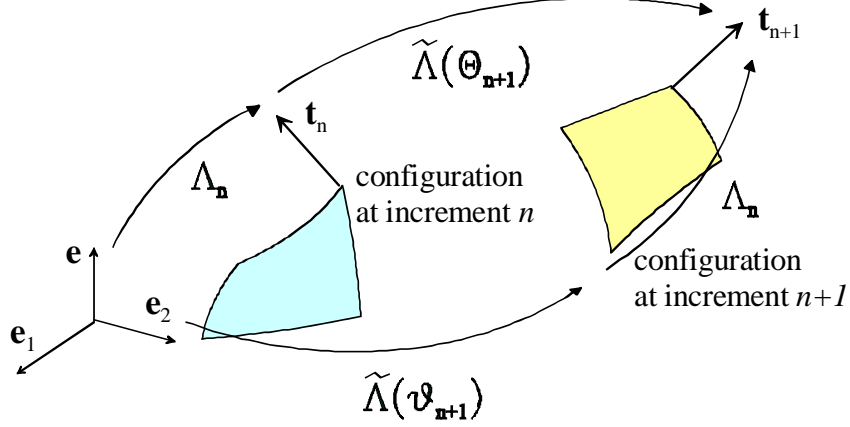


Figure 4.6: Shell director position at increments n and $n+1$. Material and spatial incremental rotation vectors.

and that

$$\boldsymbol{\theta}_{n+1} = \Lambda_n \boldsymbol{\vartheta}_{n+1}, \quad \boldsymbol{\vartheta}_{n+1} = \Lambda_n^T \boldsymbol{\theta}_{n+1} \quad (4.31)$$

Without going through the detailed proofs, we can show that the relations given in section 4 above, also hold for the corresponding incremental rotation vector, simply by making the following substitutions

$$\begin{aligned} \boldsymbol{\vartheta}, \Delta \boldsymbol{\vartheta} &\rightarrow \boldsymbol{\vartheta}_{n+1}, \Delta \boldsymbol{\vartheta}_{n+1} \\ \boldsymbol{\theta}, \Delta \boldsymbol{\theta} &\rightarrow \boldsymbol{\theta}_{n+1}, \Delta \boldsymbol{\theta}_{n+1} \\ \mathbf{g}, \mathbf{t} &\rightarrow \mathbf{t}_n, \mathbf{t}_{n+1} \\ \Lambda_0, \Lambda &\rightarrow \Lambda_n, \Lambda_{n+1} \end{aligned} \quad (4.32)$$

Note, that the following constraints (see (4.5), (4.6) and (4.32)) hold

$$\begin{aligned} \boldsymbol{\vartheta}_{n+1} \cdot \mathbf{e} &= 0 \iff \boldsymbol{\theta}_{n+1} \cdot \mathbf{t}_n = 0 \\ \boldsymbol{\vartheta}_{n+1} \cdot \Lambda_n^T \mathbf{t}_{n+1} &= 0 \iff \boldsymbol{\theta}_{n+1} \cdot \mathbf{t}_{n+1} = 0 \end{aligned}$$

By using substitutions (4.32) in Figure 4.3, the commutative diagram for the finite rotation incremental parameters is then of the form given in Figure 4.7. In Figure 4.7 we present interrelations between iterative quantities with superscript i denoting i -th iteration in the $n+1$ increment. In the same way we can modify

the diagram of Figure 4.5 to be used for the incremental constrained rotational parameters.

Constrained material rotation parameters for shells, which were treated so far, are summarized in Table 1.

Table 1. Constrained material rotation parameters

Rotation parameter	Singularity point	Update of the shell director rotation
Iterative, $\Delta\boldsymbol{\psi}_n^i$	/	Multiplicative
Incremental, $\boldsymbol{\vartheta}_{n+1}$	$\vartheta_{n+1} = \pi$	Additive at each increment
Total, $\boldsymbol{\vartheta}$	$\vartheta = \pi$	Additive

$$\begin{array}{ccc}
 \Delta\boldsymbol{\psi}_{n+1}^i & \begin{array}{c} \xrightarrow{[\Lambda_{n+1}^i]_{(3 \times 2)}} \\ \xleftarrow{[\Lambda_{n+1}^i]^T_{(2 \times 3)}} \end{array} & \Delta\mathbf{w}_{n+1}^i \\
 \uparrow [\mathbf{B}(\boldsymbol{\vartheta}_{n+1}^i)]_{(2 \times 2)} & & \uparrow [\mathbf{D}(\boldsymbol{\theta}_{n+1}^i)]_{(3 \times 3)} \\
 \Delta\boldsymbol{\vartheta}_{n+1}^i & \begin{array}{c} \xrightarrow{[\Lambda_n]_{(3 \times 2)}} \\ \xleftarrow{[\Lambda_n]^T_{(2 \times 3)}} \end{array} & \Delta\boldsymbol{\theta}_{n+1}^i
 \end{array}$$

Figure 4.7: Commutative diagram of incremental constrained rotational parameters. Vectors $\Delta\boldsymbol{\psi}_{n+1}$ and $\Delta\boldsymbol{\vartheta}_{n+1}$ have two components, while vectors $\Delta\mathbf{w}_{n+1}$ and $\Delta\boldsymbol{\theta}_{n+1}$ have three components which are not mutually independent.

4.8. Comparison of different parametrizations

In this section we present pluses and minuses of different above discussed parametrizations.

Multiplicative parameters (material $\Delta\boldsymbol{\psi}_n^i$, $\Delta\boldsymbol{\psi}_n^i \times \mathbf{e}$ and spatial $\Delta\mathbf{w}_n^i$, $\Delta\mathbf{w}_n^i \times \mathbf{t}_n^i$) Theory (-): The theory which uses multiplicative rotation parameters is relatively complicated because of the nonlinear structure of the shell configuration space.

FE implementation (+): (i) The terms related to the shell director vector in the linearized weak form of the equilibrium equations are of simple form and easy to derive; (ii) There are no problems regarding singularity, i.e. there is one to one correspondence between the shell director vector and the multiplicative shell rotation parameters.

FE implementation (-): (i) Rotation degrees of freedom are not treated in the same way as displacement ones, therefore, special procedures need to be developed for the update of the shell director vector. (ii) A 3×3 rotation matrix (or 4 quaternions) need to be stored at each solution iteration at each node for the later use at the next iteration.

Dynamic analysis (-): Time-stepping schemes (e.g. Newmark family of implicit time-stepping schemes) have to be considerably and non-trivially changed to be used for rotation degrees of freedom.

Additive parameters (material ϑ and spatial θ) *Theory (+)*: The theory preserves linear vector structure of the shell configuration space, since we use vector-like parameters for parametrization of shell finite rotations.

FE implementation (+): (i) Displacement and rotation degrees of freedom are treated in the same way; they are additively updated at each solution iteration. (ii) No storage for rotation matrix or quaternions is needed.

FE implementation (-): (i) Linearization of the shell director vector terms which appear in the linearized weak form of the equilibrium equations is relatively complicated. (ii) We have a singularity problem when the norm of any shell director vector rotation approaches to π .

Dynamic analysis (+): No modification at all (for material parameter) or trivial modification (for spatial parameter) of classical displacement time-stepping schemes are needed for rotation degrees of freedom.

Incremental additive parameters (material ϑ_{n+1} and spatial θ_{n+1}) *Theory (+)*: The theory is a combination of the two approaches mentioned above in this section, however it preserves linear vector structure of the shell configuration space.

FE implementation (+): (i) Displacement and rotation degrees of freedom are treated in the same way. Rotations are additively updated during each solution increment. (ii) There are no singularity problems, since singularities are very clearly restricted.

FE implementation (−): A 3×3 rotation matrix (or 4 quaternions) need to be stored at the last iteration of each solution increment to be later used in the next solution increment.

Dynamic analysis (+): No modification at all (for material parameter) or trivial modification (for spatial parameter) of classical displacement time-stepping schemes are needed for rotation degrees of freedom.

Material parameters *Theory and FE implementation* (+): Two material rotation parameters define an optimum number of rotation parameters.

Dynamic analysis (+): Direct application of classical time-stepping schemes (e.g. Newmark formula) is possible for rotation degrees of freedom.

Applications (−): Connection with 3-d beams is not directly possible, since beams have three rotation degrees of freedom.

Spatial parameters *Theory and FE implementation* (−): Three spatial rotation parameters are not mutually independent. This can produce singular stiffness matrix of a structure if the adjacent finite elements are lying on the same plane. It can happen even when the mesh of a curved structure is very fine and the slopes of two adjacent elements are similar.

Dynamic analysis (−): For the application of classical time-stepping schemes some modifications are necessary.

Applications (+): Direct connection with 3-d beams is possible.

REMARK 3: Care has to be taken when defining external moments, since different rotation parameters relate to different energy conjugate external moments.

4.9. Geometric view on constrained rotation parameters

In this section we discuss geometric representation of additive rotation parameters. For that purpose, let us first define local Cartesian frame at each point of the shell surface in the reference configuration. The orthonormal base vectors of such a frame are denoted as

$$\{\mathbf{x}_1, \mathbf{x}_2, \mathbf{x}_3 \equiv \mathbf{g}\} \tag{4.33}$$

Vectors \mathbf{x}_1 and \mathbf{x}_2 span the same tangent plane to the shell reference surface as vectors \mathbf{g}_1 and \mathbf{g}_2 , see (2.5), and vector $\mathbf{x}_3 = \mathbf{g}$ has a direction of normal to that

surface. They define rotation matrix $\Lambda_0 = [\mathbf{x}_1, \mathbf{x}_2, \mathbf{g}]$ which rotates fixed base vectors

$$\{\mathbf{e}_1, \mathbf{e}_2, \mathbf{e}_3 \equiv \mathbf{e}\} \quad (4.34)$$

into vectors (4.33). Note that in the finite element computations we need to define local Cartesian frames only at the nodes of the finite element mesh.

In section 4 above we were thinking of eq. (4.1) as of an operation which rotates fixed vector of unit length \mathbf{e} into the shell director at the reference configuration \mathbf{g} . However, this equation can have another picture: it can represent transformation of the components of vector \mathbf{g} , defined with respect to the shell surface basis $\{\mathbf{x}_i\}$, into the global basis $\{\mathbf{e}_i\}$. Since \mathbf{g} is of unit length and normal to the shell surface at the reference configuration, it has $\{0, 0, 1\}$ components with respect to the $\{\mathbf{x}_i\}$ basis. The global components of this vector are defined by multiplication of local components with the transformation matrix Λ_0 , see (4.1).

By analogy, we can think of two components of the total material rotation vector $\boldsymbol{\vartheta} = \{\vartheta_1, \vartheta_2\}^T$ as of local rotation parameters which are related to the basis $\{\mathbf{x}_i\}$. Three components of the spatial rotation vector $\boldsymbol{\theta} = \{\theta_1, \theta_2, \theta_3\}^T$ are then global rotation parameters given with respect to the fixed basis (4.34) with equation (4.4) transforming local rotation components to the global ones. In the same manner, we can think of all tensors associated with material rotation vector $\boldsymbol{\vartheta}$ (e.g. $\mathbf{A}(\boldsymbol{\vartheta})$, $\mathbf{B}(\boldsymbol{\vartheta})$, etc.) to have their component representation with respect to the local basis $\{\mathbf{x}_i\}$ and of all the tensors associated with the spatial rotation vector $\boldsymbol{\theta}$ (e.g. $\mathbf{A}(\boldsymbol{\theta})$, $\mathbf{Y}(\boldsymbol{\theta})$, etc.) to have their component representation with respect to the fixed basis $\{\mathbf{e}_i\}$. The transformation of the tensor components from one basis into another is performed by using standard transformation rules, i.e. by using transformation matrix Λ_0 as in equation (4.19).

When working with the incremental rotation vector, we can think of two components of the incremental material rotation vector $\boldsymbol{\vartheta}_{n+1} = \{\vartheta_{1,n+1}, \vartheta_{2,n+1}\}^T$ as of local rotation parameters which are related to basis $\{\mathbf{x}_i\}_n$, i.e. orthogonal basis defined at each point of the shell surface in the configuration obtained at the solution increment n . Three components of the spatial counterpart $\boldsymbol{\theta}_{n+1} = \{\theta_{1,n+1}, \theta_{2,n+1}, \theta_{3,n+1}\}^T$ are then global rotation parameters given with respect to the fixed basis (4.34) with equation (4.31) transforming local rotation components to the global ones.

4.10. Linearization aspects

In this section we derive linearization of variation of the shell director, $\Delta\delta\mathbf{t}$, with respect to the corresponding constrained rotation parameters. Doing so, we exploit the fact that in the linearized weak form of the balance equations, (2.15), $\Delta\delta\mathbf{t}$ always appears in a scalar product.

By linearizing (4.7) and (4.8) and by multiplying resulting $\Delta\delta\mathbf{t}$ with an arbitrary vector $\mathbf{b} \in \mathbb{R}^3$ we can express product $\Delta\delta\mathbf{t} \cdot \mathbf{b}$ in terms of the multiplicative parameters as

$$\Delta\delta\mathbf{t} \cdot \mathbf{b} = \Lambda [\Delta\boldsymbol{\psi} \times (\delta\boldsymbol{\psi} \times \mathbf{e})] \cdot \mathbf{b} = (-\mathbf{t} \cdot \mathbf{b}) [\delta\boldsymbol{\psi} \mathbf{I} \Delta\boldsymbol{\psi}] \quad (4.35)$$

$$\Delta\delta\mathbf{t} \cdot \mathbf{b} = \delta\mathbf{w} \times (\Delta\mathbf{w} \times \mathbf{t}) \cdot \mathbf{b} = (-\mathbf{t} \cdot \mathbf{b}) [\delta\mathbf{w} \mathbf{I} \Delta\mathbf{w}] \quad (4.36)$$

It can be also shown that by using (4.28) as a variation of rotation parameters one has

$$\Delta\delta\mathbf{t} \cdot \mathbf{b} = (-\mathbf{t} \cdot \mathbf{b}) \left[\delta\tilde{\boldsymbol{\psi}} \mathbf{I} \Delta\tilde{\boldsymbol{\psi}} \right] = (-\mathbf{t} \cdot \mathbf{b}) [(\delta\boldsymbol{\psi} \times \mathbf{e}) \mathbf{I} (\Delta\boldsymbol{\psi} \times \mathbf{e})] \quad (4.37)$$

We can further express $\Delta\delta\mathbf{t}$ in terms of additive parameters. If we perform direct linearization of (4.10) we obtain $\Delta\delta\mathbf{t}$ in terms of the total material rotation vector $\boldsymbol{\vartheta}$ as

$$\begin{aligned} \Delta\delta\mathbf{t} &= \frac{\vartheta \cos \vartheta - \sin \vartheta}{\vartheta^3} \Lambda_0 \left[-(\delta\boldsymbol{\vartheta} \cdot \boldsymbol{\vartheta}) (\boldsymbol{\vartheta} \cdot \Delta\boldsymbol{\vartheta}) \mathbf{e} + (\delta\boldsymbol{\vartheta} \cdot \Delta\boldsymbol{\vartheta}) \boldsymbol{\vartheta} \times \mathbf{e} \right] \\ &- \frac{\sin \vartheta}{\vartheta} (\delta\boldsymbol{\vartheta} \cdot \Delta\boldsymbol{\vartheta}) \Lambda_0 \mathbf{e} + \frac{\sin \vartheta (3 - \vartheta^2) - 3\vartheta \cos \vartheta}{\vartheta^5} (\delta\boldsymbol{\vartheta} \cdot \boldsymbol{\vartheta}) (\boldsymbol{\vartheta} \cdot \Delta\boldsymbol{\vartheta}) \Lambda_0 (\boldsymbol{\vartheta} \times \mathbf{e}) \\ &+ \frac{\vartheta \cos \vartheta - \sin \vartheta}{\vartheta^3} \Lambda_0 \left[(\boldsymbol{\vartheta} \cdot \Delta\boldsymbol{\vartheta}) \delta\boldsymbol{\vartheta} \times \mathbf{e} + (\boldsymbol{\vartheta} \cdot \delta\boldsymbol{\vartheta}) \Delta\boldsymbol{\vartheta} \times \mathbf{e} \right] \end{aligned} \quad (4.38)$$

Multiplication of the above expression (4.38) with any vector \mathbf{b} further leads to

$$\Delta\delta\mathbf{t} \cdot \mathbf{b} = \delta\boldsymbol{\vartheta} [\mathbf{Y}(\boldsymbol{\vartheta})] \Delta\boldsymbol{\vartheta} \quad (4.39)$$

where $\mathbf{Y}(\boldsymbol{\vartheta})$ is a (2×2) matrix defined as (see Brank *et al.* (1997) for the derivation details)

$$\begin{aligned} \mathbf{Y}(\boldsymbol{\vartheta}) &= \frac{\vartheta \cos \vartheta - \sin \vartheta}{\vartheta^3} \left(- \begin{bmatrix} \vartheta_1^2 & \vartheta_1 \vartheta_2 \\ \vartheta_1 \vartheta_2 & \vartheta_2^2 \end{bmatrix} (\Lambda_0 \mathbf{e} \cdot \mathbf{b}) + \mathbf{I}_{(2 \times 2)} (\Lambda_0 (\boldsymbol{\vartheta} \times \mathbf{e}) \cdot \mathbf{b}) \right) \\ &- \frac{\sin \vartheta}{\vartheta} \mathbf{I}_{(2 \times 2)} (\Lambda_0 \mathbf{e} \cdot \mathbf{b}) \\ &+ \frac{\sin \vartheta (3 - \vartheta^2) - 3\vartheta \cos \vartheta}{\vartheta^5} \begin{bmatrix} \vartheta_1^2 & \vartheta_1 \vartheta_2 \\ \vartheta_1 \vartheta_2 & \vartheta_2^2 \end{bmatrix} (\Lambda_0 (\boldsymbol{\vartheta} \times \mathbf{e}) \cdot \mathbf{b}) \\ &+ \frac{\vartheta \cos \vartheta - \sin \vartheta}{\vartheta^3} \left(\begin{bmatrix} 0 & \vartheta_1 \\ \vartheta_1 & 2\vartheta_2^2 \end{bmatrix} (\Lambda_0 \mathbf{e}_1 \cdot \mathbf{b}) - \begin{bmatrix} 2\vartheta_1^2 & \vartheta_2 \\ \vartheta_2 & 0 \end{bmatrix} (\Lambda_0 \mathbf{e}_2 \cdot \mathbf{b}) \right) \end{aligned} \quad (4.40)$$

where $\mathbf{e}_1 = \{1, 0, 0\}^T$, $\mathbf{e}_2 = \{0, 1, 0\}^T$ and $\mathbf{e} = \mathbf{e}_3 = \{0, 0, 1\}^T$. With the use of commutative diagrams from Figures 4.3 and 4.5 it follows from (4.35) and (4.37) that $\mathbf{Y}(\boldsymbol{\vartheta})$ should be equal to

$$\mathbf{Y}(\boldsymbol{\vartheta}) = (-\mathbf{t} \cdot \mathbf{b}) \tilde{\mathbf{B}}^T \tilde{\mathbf{B}} \quad (4.41)$$

With the linearization of (4.11) we can get $\Delta\delta\mathbf{t}$ expressed in terms of the total spatial rotation vector $\boldsymbol{\theta}$

$$\Delta\delta\mathbf{t} \cdot \mathbf{b} = \delta\boldsymbol{\theta} [\mathbf{Y}(\boldsymbol{\theta})] \Delta\boldsymbol{\theta} \quad (4.42)$$

where $\mathbf{Y}(\boldsymbol{\theta})$ is a (3×3) matrix which can be obtained by using material-spatial transformations

$$\mathbf{Y}(\boldsymbol{\theta}) = [\Lambda_0]_{(3 \times 2)} [\mathbf{Y}(\boldsymbol{\vartheta})]_{(2 \times 2)} [\Lambda_0^T]_{(2 \times 3)} \quad (4.43)$$

When the incremental rotation vectors $\boldsymbol{\vartheta}_{n+1}$ and $\boldsymbol{\theta}_{n+1}$ are used instead of the total rotation vectors $\boldsymbol{\vartheta}$ and $\boldsymbol{\theta}$, respectively, we have to use substitutions (4.32) in the above expressions. For example, equations (4.40) and (4.43) have then the following form

$$\Delta\delta\mathbf{t} \cdot \mathbf{b} = \delta\boldsymbol{\vartheta} [\mathbf{Y}(\boldsymbol{\vartheta}_{n+1})] \Delta\boldsymbol{\vartheta}_{n+1} \quad (4.44)$$

$$\Delta\delta\mathbf{t} \cdot \mathbf{b} = \delta\boldsymbol{\theta} [\mathbf{Y}(\boldsymbol{\theta}_{n+1})] \Delta\boldsymbol{\theta}_{n+1} \quad (4.45)$$

with $\mathbf{Y}(\boldsymbol{\vartheta}_{n+1})$ being of form (4.40) with substitutions (4.32) used.

5. Numerical example

The computations were carried out by a research version of the computer program FEAP, developed by Prof. R. L. Taylor at UC Berkeley (e.g. see Zienkiewicz and Taylor (1989)). We have implemented several four-node shell elements with 5 dof/node making use of standard displacement based interpolations for membrane and bending strains and assumed strain interpolations in the form given by Dvorkin and Bathe (1989) for transverse shear strains. The shell elements developed differ among themselves only with respect to the chosen rotation parameters: the shell element using the total rotation vector parameterization (denoted as *total rotation vector* as proposed by Brank *et al.* (1997)), the shell element using

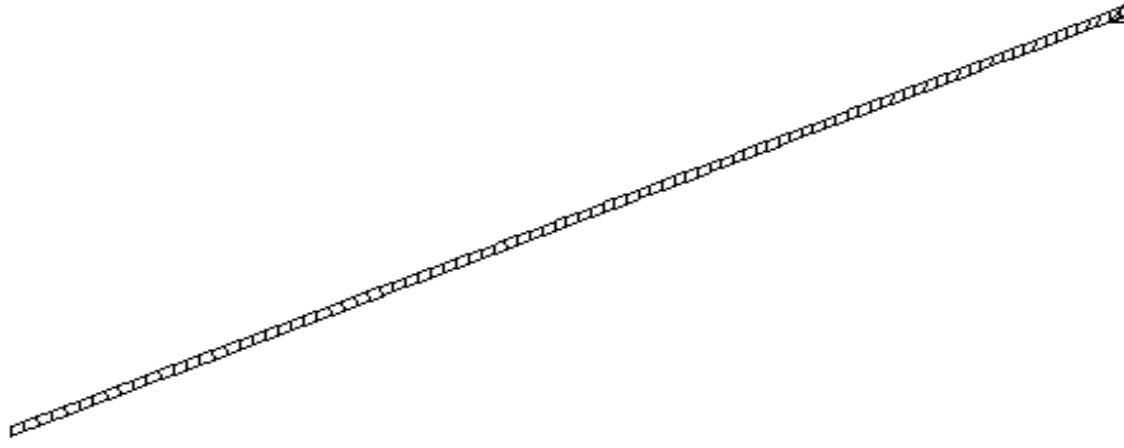


Figure 5.1: Initial and deformed configurations of the cantilever beam.

the incremental rotation vector (denoted as *incremental rotation vector*), the shell element using the multiplicative rotation update at each iteration, as proposed by Simo *et al.* (1990) (denoted as *orthogonal matrix*).

Since all the elements employ the same finite element interpolations, they all provide the same solution in terms of displacements, rotations and internal forces in the range of moderate rotations. In the range of large rotations, the *total rotation vector* element runs into singularity when the norm of rotation vector approaches to π .

This is illustrated with a modified version of the standard test problem of a cantilever beam under concentrated moment applied at its free end. The selected properties of the cantilever are : length $L = 100$, width $b = 1$, unit thickness $h = 1$, elastic modulus $E = 21000$ and Poisson's ratio $\nu = 0.2$. The value of the end moment increases linearly reaching the value $M = \frac{2\pi EI}{L}$ at $t = 2$, when a lateral force of $F = 0.03$ is applied at the cantilever free end which starts shifting the deformed cantilever out of the plane. The subsequent deformed configurations of the cantilever are provided in Figure (5.1).

Incremental rotation vector element and *orthogonal matrix* element pass this test without any singularity problems up to the final deformed configuration presented in Figure 5.1 where the total end rotation is equal to 4.04π . As expected, the *total rotation vector* element run into singularity problem at $t = \frac{1}{2}$.

6. Conclusions

Different parametrizations of finite rotations for smooth shells are compiled and their interrelations are described and illustrated in informative commutative diagrams. These diagrams may be used to transform one geometrically exact finite rotation shell formulation into the another. Minuses and pluses of different parametrizations are very clearly presented.

Since we use continuum-consistent interpolations in the finite element approximation, formulations with different rotation parameters (i.e. different rotation degrees of freedom) produce the same results before the singularity problem occurs for certain parametrizations. However, our preferred choice is parametrization in the form of incremental rotation vector with the main advantage of an additive update format at each iteration.

Care has to taken when defining external moments, since different rotation parameters relate to different energy conjugate external moments.

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