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Multiplicative Updating of the Rotation Tensor in the Finite Element Analysis of Rods and Shells - A Path Independent Approach

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Abstract

Rotation tensors play a pre dominant role in many engineering applications. They exhibit a pronounced multiplicative structure, the various aspects of which must be dealt with carefully in order to arrive at a numerically efficient and physically sound treatment. A method of multiplicative updating of rotations in the frame of finite element analysis of rods was suggested by Simo and Vu-Quoc which proved to be path-dependent, even in purely elastic problems, as observed by Jelenic and Crisfield. In this paper a path-independent treatment of rotations is developed which proves to be numerically efficient, physically sound, and preserves the multiplicative structure of rotations. In addition, a unified treatment of rod and shell theories is established which considers them from the point of view of Cosserat continua with same degrees of freedom. In the shell case, the formulation allows in a natural way for the inclusion of drill rotations.

Keywords: Rotation group, multiplicative updating, path independency, rods, shells, finite elements

1 Introduction

Rotation tensors play a pre dominant role in many engineering applications. They appear explicitly in geometrically exact shell and rod theories, in extended theories of three-dimensional continua, and are fundamental within the area of multi-body dynamics. Typically, the rotation tensor defines a highly non-linear field over a certain domain where, in general, closed solutions cease to exist. Accordingly, interpolations within a numerical approach, such as that of the finite element method, are to be carried out. Whereas the updating procedure of displacement vectors is straightforward and additive in nature, that of the rotation tensors differs in a fundamental way. First, rotation tensors depend on three rotation parameters, the components of a rotation vector. Accordingly, the rotation tensor itself cannot be directly interpolated. Although rotation parameters can be equipped with

an *Euclidean* structure and hence can be updated additively (see e.g. Cardona and Geradin [4], Sansour and Bufler [22], Sansour and Bednarczyk [21], Borri and Bottasso [3]), physically one is motivated to deal with the rotation tensors as a *Lie* group with a multiplicative structure. This is mathematically more convenient and allows for a direct physical interpretation of the quantities involved. The multiplicative structure gives rise to an incremental rotation vector, the components of which can be interpolated within a finite element procedure in a classical way. The question now arises of how to build up and update the rotation tensor itself. A method of multiplicative updating of rotations was suggested by Simo and Vu-Quoc [24] which was widely accepted and subsequently used in various finite element formulations of rod and shell theories. The updating strategy rests on the treatment of the rotation tensor as a history variable. Only the increments of the rotation vector are interpolated over the element. The rotation tensor itself is formulated only at the *Gauss* points and is updated multiplicatively using the incremental rotation tensor generated by the interpolated incremental rotation vector. Accordingly, rotation tensors exist only at the *Gauss* points and not at element nodes. Recently, Jelenic and Crisfield [15] have shown that the methodology is in fact path-dependent. This is also true for problems which, as such, are path-independent as in the case of elasticity. They suggested a specific so-called co-rotational formulation which deviates from a classical continuum treatment such as a Lagrangian one, one would like to appeal to.

Based on the previous work by Sansour and Bednarcyzk [21], we systematically develop in this paper a multiplicative updating scheme for the rotation tensors which enjoys the following features:

1. The formulation is objective and path-independent.
2. The rotation tensors are well defined at the *Gauss*ian points but are not treated as history variables. They are also well defined at the element nodes.
3. The multiplicative structure of the rotational group and the updating scheme is preserved.
4. Classical finite element interpolations can be carried out in a classical manner.

As an application we discuss the formulation of elastic rod and shell theories. These formulations exhibit the following features:

1. The treatment of one- as well as two-dimensional models is carried out using the same approach and resulting in the same number of degrees of freedom.
2. As to a shell, drilling rotations are included directly and naturally in the formulation.

The content of the paper is as follows. First, we give a short outline of the three-dimensional theory. The strain measures of the classical continuum, as well as those of the *Cosserat* continuum are given and discussed. The direct approach is then applied to achieve dimensional reduction. Two cases are considered: the reduction to one dimension resulting in a general theory of rods and the reduction to two dimensions resulting in a general theory

of shells. The theories are geometrically exact. An important feature is the consideration of a three parametric rotation tensor contrasting the rotation tensor involved in theories based on the *Green* strain measures. The inclusion of drilling degrees of freedom is inherent in the theoretical framework itself and hence is achieved in a completely natural way. For the two-dimensional case a finite-element formulation is briefly discussed. The formulation is based on a partially hybrid variational principle.

2 The direct approach to rod and shell theories

2.1 Preface

Historically, it is remarkable that dimensionally reduced theories of elasticity were available before the three-dimensional theory was developed at all. Specifically, one-dimensional theories of rods and two-dimensional theories of plates had very early gained access to applications and, to a great extent established a basis for engineering. Nowadays, although a well developed three-dimensional theory is available, it is generally accepted that the treatment of problems of elasticity on thin domains is best carried out at a dimensionally reduced level. The dimensionally reduced problem is easier to solve, as well as being free of ill-conditioning.

The reduction of dimension can be achieved either prior to the numerical treatment of the problem, or within, and as a part of the numerical discretisation itself. In the former case, one is led to theories of rods, plates, and shells, the concern of this paper.

There are two approaches for the derivation of dimensionally reduced theories: the three-dimensional approach and the direct approach. In the first approach, the three-dimensional governing equations are reduced via assumptions on the displacement field (or other physical fields) resulting in one- or two-dimensional theories of rods and shells. A frequently adopted assumption is that of a linearly varying displacement field over the thickness of the thin three-dimensional body.

In the second approach, the direct approach, the governing equations are derived by considering a manifold of a dimension less than three, but with more degrees of freedom attached to its points. A classical (in one or two directions thin) three-dimensional continuum is modelled directly as a non-classical continuum of reduced dimension. By a classical continuum we mean a continuum with the degrees of freedom being displacements. On the other hand, the non-classical continuum is considered to be a *Cosserat* continuum, which is characterized by a displacement vector as well as an independent rotation vector attached to every particle of the continuum. The dimension of the *Cosserat* continuum is taken to be one or two, depending on the kind of theory one is interested in, a rod or shell theory. The stored energy function of the three-dimensional body is then assumed to depend on the strain measures of the *Cosserat* continuum.

Even in the case of a *Cosserat* continuum, the strain measures may take completely different forms. On the one hand, metric-based quantities can be taken as strain measures, e.g. the right Cauchy Green tensor; on the other hand, the strain measures can be stretch type measures which, in fact, result in completely different expressions motivating different

numerical treatments.

Theories of shells derived by means of the direct approach and based on the *Green* strain tensor as a strain measure, that is on metric based quantities, were the concern of Cohen and DeSilva [6], Green et al. [10], and NAGHDI [18]; see also Rubin [20] for a general account. In these theories so-called directors are attached to every point of the *Cosserat* surface or line. The kinematics of the directors thereby constitute the additional degrees of freedom, which for a three-dimensional body take into account typical effects such as bending. A finite-element formulation and rotational parameterization of the corresponding geometrically exact shell theory was given by Simo and Fox [23] (see also Basar and Ding [2]). Within these theories the rotation tensor is only two-parametric, reflecting the fact that the rotation tensor is constrained and belongs to the subgroup $SO(3)/SO(2)$, with SO(3) being the special orthogonal group, that is the three-parametric group of orthogonal tensors with positive determinant, while SO(2)is the group of rotations of the plane given by only one-parametric rotations. Rotations which are elements of $SO(3)/SO(2)$ exclude drilling rotations.

Alternatively, the dimensionally reduced theories can depend on stretch type strain tensors based on a different philosophy and formalism, which makes the same approach directly applicable whatever the dimension of the continuum may be. Essentially the same degrees of freedom and the same type of strain measures are considered for both rods and shells, it is only the dimension of the continuum which differs. A basic difference to the director based formulations lies in the fact that the rotation tensor is actually an element of the group $SO(3)$, which implies that all three rotational parameters are independent and drilling rotations are naturally considered.

It is interesting to note that as far as one-dimensional theories are concerned, the theory to be developed here is equivalent to a model known in the literature as formulated by Reissner [19], Antmann [1], and Simo and Vu-Quoc [24]. The model has been dealt with intensively in the literature (see e.g. Cardona and Geradin [4], Borri and Bottasso [3]), Ibrahimbegovic [14], Gruttmann et al. [11], McRobie and Lasenby [17], Trindade and Sampaio [26], to mention few). Nevertheless, of special interest is the different methodology we are following here to arrive at a rod theory which makes the strong relation to two-dimensional theories apparent as well.

2.2 Strain measures of the Cosserat continuum

Let $\mathcal{B} \subset \mathbb{R}^3$, where $\mathcal{B}$ is a three-dimensional manifold defining a material body. The map $\boldsymbol{\varphi}(t) : \mathcal{B} \to \mathbb{R}^3$ is an embedding depending on a well chosen parameter $t \in \mathbb{R}$. Hereby, $\boldsymbol{\varphi_0} = \boldsymbol{\varphi}(t = t_0)$ defines a reference configuration, which enables the identification of the material points. We take $\boldsymbol{\varphi_0}$ to be the identity map. Writing $\mathcal{B}$ for $\boldsymbol{\varphi_0}\mathcal{B}$ and $\mathcal{B}_t$ for $\boldsymbol{\varphi}(t)\mathcal{B}$ we get $\boldsymbol{\varphi}(t) : \mathcal{B} \to \mathcal{B}_t$. For $\mathbf{X} \in \mathcal{B}$ and $\mathbf{x} \in \mathcal{B}_t$ we have

$$\mathbf{x}(t) = \boldsymbol{\varphi}(\mathbf{X}, t) \qquad \text{and} \qquad \mathbf{X}(t) = \boldsymbol{\varphi}^{-1}(\mathbf{x}, t). \tag{1}$$

Further, let ϑ^i, $i = 1, 2, 3$ be co-ordinate charts in $\mathcal{B}$, which we choose to be attached to the body (convected). With $\mathcal{TB}$, $\mathcal{TB}_t$ being the tangent spaces of $\mathcal{B}$ and $\mathcal{B}_t$, the covariant

base vectors are

$$\mathbf{G}_i = \partial \mathbf{X}/\partial \vartheta^i \qquad \text{with} \qquad \mathbf{G}_i \in \mathcal{TB}\,, \tag{2}$$

and

$$\mathbf{g}_i = \partial \mathbf{x}/\partial \vartheta^i \qquad \text{with} \qquad \mathbf{g}_i \in \mathcal{TB}_t. \tag{3}$$

Here, and in what follows, latin indices take the values $1, 2$ or 3.

The *Riemannian* metric in either configuration is given by

$$G_{ij} = \mathbf{G}_i \cdot \mathbf{G}_j \qquad \text{and} \qquad g_{ij} = \mathbf{g}_i \cdot \mathbf{g}_j\,, \tag{4}$$

respectively, where scalar products of vectors are denoted by a dot. The determinants of the metrics are denoted by G and g, respectively, their inverse as usual by G^{ij} and g^{ij}. Further, we consider a *Cartesian* frame denoted by $\mathbf{e}_i$ and define the quantities

$$c_{ij} = \mathbf{G}_i \cdot \mathbf{e}_j \tag{5}$$

such that the relations hold

$$\mathbf{G}_i = c_{ij}\mathbf{e}_j, \qquad \mathbf{e}_i = c_{ji}\mathbf{G}^j. \tag{6}$$

Note that c_{ij} is not symmetric. The basic skew-symmetric three-dimensional *Levi-Civita* tensor (permutation tensor) is denoted by $\boldsymbol{\epsilon}$. Its Cartesian components are defined as

$$e^{ijk} = e_{ijk} = \begin{cases} +1 & \text{for odd permutations of } i,j,k \\ -1 & \text{for even permutations of } i,j,k\,. \end{cases} \tag{7}$$

The tangent of the map $\boldsymbol{\varphi}$ is called the deformation gradient and is denoted by $\mathbf{F}$. It maps the tangent space of $\mathcal{B}$ at the reference configuration to that at the actual configuration and is given by

$$\mathbf{F} = \mathbf{g}_i \otimes \mathbf{G}^i. \tag{8}$$

Introducing the displacement field

$$\mathbf{u} = \mathbf{x} - \mathbf{X} \tag{9}$$

and denoting partial derivatives by a comma, we get with (3)

$$\mathbf{g}_i = \mathbf{G}_i + \mathbf{u}_{,i} \tag{10}$$

and with (8)

$$\mathbf{F} = (\mathbf{G}_i + \mathbf{u}_{,i}) \otimes \mathbf{G}^i. \tag{11}$$

The polar decomposition applies to give

$$\mathbf{F} = \mathbf{QU} \qquad \mathbf{Q} \in SO(3) \quad \text{and} \quad \mathbf{U} = \mathbf{U}^T \tag{12}$$

$$\mathbf{F} = \mathbf{VQ} \qquad \mathbf{Q} \in SO(3) \quad \text{and} \quad \mathbf{V} = \mathbf{V}^T. \tag{13}$$

$\mathbf{U}$ and $\mathbf{V}$ are called the stretch tensors. They define objective strain measures. Their computation necessitates the use of a rotation tensor which is fully determined by one of the symmetry conditions

$$\mathbf{Q}^T\mathbf{F} = \mathbf{F}^T\mathbf{Q}, \qquad \mathbf{F}\mathbf{Q}^T = \mathbf{Q}\mathbf{F}^T\,, \tag{14}$$

included in (12) or (13). In other words, the rotation tensor is not an independent variable, but is completely determined by the deformation itself as described by the map $\boldsymbol{\varphi}$. This point is crucial for understanding the difference between classical and non-classical continua.

For comparison we include strain measures which do not necessitate the explicit use of rotation tensors. Frequently used examples are the right *Cauchy-Green* tensor

$$\mathbf{C} = \mathbf{F}^T\mathbf{F} = \mathbf{1} + (\mathbf{u}_{,i} \cdot \mathbf{G}_j + \mathbf{u}_{,j} \cdot \mathbf{G}_i + \mathbf{u}_{,i} \cdot \mathbf{u}_{,j})\mathbf{G}^j \otimes \mathbf{G}^i \tag{15}$$

and the corresponding *Green* strain tensor $\mathbf{E} = \frac{1}{2}(\mathbf{C} - \mathbf{1})$ which are directly expressed in terms of the displacement field.

We emphasize again that the strain and stress state of a classical continuum is fully determined by one strain measure. It is given in terms of the displacement field alone since the rotation field does not define an independent kinematical variable.

On the contrary, the *Cosserat* continuum, which is the simplest possible continuum of a wide class of non-classical continua, is characterized by the fact that displacements as well as independent rotations are assigned to its points . That is, attached to every point of the *Cosserat* continuum are the degrees of freedom of a rigid body. Since the rotation field is considered independent, the strain measures of the continuum are not fully described by the stretch tensor alone, therefore a further strain tensor is needed.

Let $\mathbf{R} \in SO(3)$. In order to get explicit formulas, the parameterization of the rotation tensor $\mathbf{R}$ is carried out with the help of the exponential map as follow ([5, 7])

$$\mathbf{R} = \exp(\boldsymbol{\Gamma}) = \mathbf{1} + \boldsymbol{\Gamma} + \frac{\boldsymbol{\Gamma}^2}{2!} + \frac{\boldsymbol{\Gamma}^3}{3!} + \cdots \tag{16}$$

with

$$\boldsymbol{\Gamma} = -\boldsymbol{\Gamma}^T. \tag{17}$$

Denoting the axial vector of $\boldsymbol{\Gamma}$ by $\boldsymbol{\gamma}$, one has the closed expression

$$\mathbf{R} = \mathbf{1} + \frac{\sin|\boldsymbol{\gamma}|}{|\boldsymbol{\gamma}|}\boldsymbol{\Gamma} + \frac{1 - \cos|\boldsymbol{\gamma}|}{|\boldsymbol{\gamma}|^2}\boldsymbol{\Gamma}^2 \,. \tag{18}$$

Moreover, the relation $\mathbf{R}\boldsymbol{\gamma} = \boldsymbol{\gamma}$ holds, that is, the rotation vector in an eigen vector of the rotation tensor.

Now, by the relation $\mathbf{R}^T\mathbf{R} = \mathbf{1}$ we have

$$\mathbf{R}^T\mathbf{R}_{,i} + \mathbf{R}_{,i}^T\mathbf{R} = \mathbf{0} \tag{19}$$

from which we infer that $\mathbf{R}^T\mathbf{R}_{,i} \in so(3)$, where $so(3)$ is the tangent space of $SO(3)$ consisting of all skew-symmetric tensors. Let the axial vector of the skew-product $\mathbf{R}^T\mathbf{R}_{,i}$ be $\mathbf{k}_i$, one may elaborate the relation

$$\mathbf{k}_i = \frac{\sin|\boldsymbol{\gamma}|}{|\boldsymbol{\gamma}|}\boldsymbol{\gamma}_{,i} + \frac{1 - \cos|\boldsymbol{\gamma}|}{|\boldsymbol{\gamma}|^2}\boldsymbol{\gamma}_{,i} \times \boldsymbol{\gamma} + \left(\frac{1}{|\boldsymbol{\gamma}|} - \frac{\sin|\boldsymbol{\gamma}|}{|\boldsymbol{\gamma}|^2}\right)\frac{(\boldsymbol{\gamma} \cdot \boldsymbol{\gamma}_{,i})}{|\boldsymbol{\gamma}|}\boldsymbol{\gamma} \tag{20}$$

which relates $\mathbf{k}_i$ to $\boldsymbol{\gamma}$.

With the rotation tensor $\mathbf{R} \in SO(3)$ being independent from the deformation gradient, the strain measures are then defined as (see Eringen and Kafadar [9], Hjalmars [13]):
The first *Cosserat* strain tensor

$$\mathbf{U} := \mathbf{R}^T\mathbf{F}\,, \tag{21}$$

and the second *Cosserat* strain tensor

$$\mathbf{K} := -\mathbf{k}_i \otimes \mathbf{G}^i. \tag{22}$$

Alternatively, $\mathbf{K}$ may be written with the help of the permutation tensor in terms of the rotation tensor directly as

$$\mathbf{K} = \frac{1}{2}\boldsymbol{\epsilon} : \mathbf{R}^T\mathbf{R}_{,i} \otimes \mathbf{G}^i, \tag{23}$$

where (:) denotes double contraction. The fact that $\boldsymbol{\epsilon}$ is a three-dimensional tensor reveals the product $\boldsymbol{\epsilon} : \mathbf{R}^T\mathbf{R}_{,i}$ to a vector and hence $\mathbf{K}$ to a two-dimensional tensor. The tensor $\mathbf{H} = \mathbf{U} - \mathbf{1}$ can be defined so as to arrive at a strain measure vanishing at the reference configuration. It is important to note that since $\mathbf{R}$ is independent, the stretch tensor $\mathbf{U}$ is not symmetric in general.

2.3 Rod and shell strain measures

2.3.1 Rod theory

We consider a one-dimensional manifold $\mathcal{S}$, understood as an arbitrary material curve to which we refer as a *Cosserat* curve, embedded in a three-dimensional *Euclidean* space. The curve may be represented by the line of centroids of cross-sections of a three-dimensional body considered in two directions to be thin. We assume the curve is parameterized with the help of a length parameter s. In order to make use of the formulas given for the three-dimensional case, we set $s \equiv \vartheta^1$. The most important step in the development of the dimensionally reduced theory (in this section one-dimensional) is actually simple: The tangent space $\mathcal{TS}$ of the *Cosserat* curve $\mathcal{S}$ at the reference as well as the tangent space $\mathcal{TS}_t$ of the *Cosserat* curve $\mathcal{S}_t$ at the actual configuration consist of the tangent vectors given by

$$\mathbf{G}_1 = \partial\mathbf{X}/\partial\vartheta^1, \quad \text{and} \quad \mathbf{g}_1 = \partial\mathbf{x}/\partial\vartheta^1\,, \tag{24}$$

respectively. Hence, the deformation gradient is given by the one map

$$\mathbf{F} = \mathbf{g}_1 \otimes \mathbf{G}^1. \tag{25}$$

Analogously, and in view of (19)and (20), there exists only one skew-symmetric product $\mathbf{R}^T\mathbf{R}_{,1}$ with one axial vector given by

$$\mathbf{k}_1 = \frac{\sin|\boldsymbol{\gamma}|}{|\boldsymbol{\gamma}|}\boldsymbol{\gamma}_{,1} + \frac{1-\cos|\boldsymbol{\gamma}|}{|\boldsymbol{\gamma}|^2}\boldsymbol{\gamma}_{,1}\times\boldsymbol{\gamma} + \left(\frac{1}{|\boldsymbol{\gamma}|} - \frac{\sin|\boldsymbol{\gamma}|}{|\boldsymbol{\gamma}|^2}\right)\frac{(\boldsymbol{\gamma}\cdot\boldsymbol{\gamma}_{,1})}{|\boldsymbol{\gamma}|}\boldsymbol{\gamma}. \tag{26}$$

With the displacement field $\mathbf{u} = \mathbf{x} - \mathbf{X}$ we have

$$\mathbf{F} = (\mathbf{G}_1 + \mathbf{u}_{,1}) \otimes \mathbf{G}^1. \tag{27}$$

The strain measures of the *Cosserat* curve now read:

$$\mathbf{H} = \mathbf{R}^T\mathbf{F} - \mathbf{1} = \mathbf{R}^T(\mathbf{G}_1 + \mathbf{u}_{,1}) \otimes \mathbf{G}^1 - \mathbf{G}_1 \otimes \mathbf{G}^1. \tag{28}$$

and

$$\mathbf{K} = -\mathbf{k}_1 \otimes \mathbf{G}^1. \tag{29}$$

With (6), (18), (26), (27), and with the adequate choice of Cartesian components of $\mathbf{u}$ and $\boldsymbol{\gamma}$,

$$\mathbf{u} = u_k\mathbf{e}_k, \quad \boldsymbol{\gamma} = \gamma_k\mathbf{e}_k\,, \tag{30}$$

we can explicitly calculate

$$\begin{aligned}
\mathbf{H} &= \Big\{c_{nk}\,u_{k,1} + (c_{1k} + u_{k,1})c_{nj} \\
&\quad \times \left[\frac{\sin|\boldsymbol{\gamma}|}{|\boldsymbol{\gamma}|}\,e_{ijk}\,\gamma_i + \frac{1-\cos|\boldsymbol{\gamma}|}{|\boldsymbol{\Gamma}|^2}\,(\gamma_k\gamma_j - \gamma_i\gamma_i\delta_{jk})\right]\Big\}\,\mathbf{G}^n \otimes \mathbf{G}^1 \qquad (31)\\
\mathbf{K} &= -c_{nk}\left(\frac{\sin|\boldsymbol{\gamma}|}{|\boldsymbol{\gamma}|}\,\gamma_{k,1} + \frac{1-\cos|\boldsymbol{\gamma}|}{|\boldsymbol{\gamma}|^2}\,e_{ijk}\gamma_{i,1}\gamma_j\right. \\
&\quad \left. + \frac{|\boldsymbol{\gamma}| - \sin|\boldsymbol{\gamma}|}{|\boldsymbol{\gamma}|^2}\,|\boldsymbol{\gamma}|_{,1}\gamma_k\right)\mathbf{G}^n \otimes \mathbf{G}^1 \qquad (32)
\end{aligned}$$

2.3.2 Shell theory

Likewise, we consider now $\mathcal{M} \subset \mathbb{R}^3$ to be a two-dimensional manifold defining a material surface. By considering this surface to be a *Cosserat* continuum (*Cosserat* surface), a geometrically exact shell theory can be derived. We just need to specialize Eqs. (11), (20)-(22) to the two-dimensional case, as we have done in the one-dimensional case.

First, we let $\vartheta^\alpha, \alpha = 1, 2$ be co-ordinate charts in $\mathcal{M}$, which we choose again to be attached to the surface (convected). With $\mathcal{T}\mathcal{M}$, $\mathcal{T}\mathcal{M}_t$ being the tangent spaces of $\mathcal{M}$ and $\mathcal{M}_t$ the covariant base vectors are

$$\mathbf{G}_\alpha = \partial\mathbf{X}/\partial\vartheta^\alpha \qquad \text{with} \qquad \mathbf{G}_\alpha \in \mathcal{T}\mathcal{B}\,, \tag{33}$$

and

$$\mathbf{g}_\alpha = \partial\mathbf{x}/\partial\vartheta^\alpha \qquad \text{with} \qquad \mathbf{g}_\alpha \in \mathcal{T}\mathcal{B}_t\,. \tag{34}$$

Here and in the rest of the paper Greek indices take the values of 1 or 2. At the reference surface the normal vector is defined by $\mathbf{N} = 1/\sqrt{G}\,e^{\alpha\beta 3}\mathbf{G}_\alpha \times \mathbf{G}_\beta$, where it is always understood that $\mathbf{N} \equiv \mathbf{G}_3$. The components $B_{\alpha\beta}$ of the curvature tensor $\mathbf{B} = B_{\alpha\beta}\mathbf{G}^\alpha \otimes \mathbf{G}^\beta$ are then given by $B_{\alpha\beta} = -\mathbf{N}_{,\alpha} \cdot \mathbf{G}_\beta$.

The *Riemannian* metric in either configuration is given by

$$G_{\alpha\beta} = \mathbf{G}_\alpha \cdot \mathbf{G}_\beta \qquad \text{and} \qquad g_{\alpha\beta} = \mathbf{g}_\alpha \cdot \mathbf{g}_\beta\,, \tag{35}$$

respectively.

In analogy to the one-dimensional case the deformation gradient is completely determined by (the two maps)

$$\mathbf{F} = \mathbf{g}_\alpha \otimes \mathbf{G}^\alpha \tag{36}$$

which, with the displacement field $\mathbf{u} = \mathbf{x} - \mathbf{X}$ can be written in the form

$$\mathbf{F} = (\mathbf{G}_\alpha + \mathbf{u}_{,\alpha}) \otimes \mathbf{G}^\alpha. \tag{37}$$

In the two-dimensional case there exist two skew-symmetric products $\mathbf{R}^T\mathbf{R}_{,\alpha}$ with two corresponding axial vectors $\mathbf{k}_\alpha$. The counter part of (20) is then

$$\mathbf{k}_\alpha = \frac{\sin|\boldsymbol{\gamma}|}{|\boldsymbol{\gamma}|}\boldsymbol{\gamma}_{,\alpha} + \frac{1-\cos|\boldsymbol{\gamma}|}{|\boldsymbol{\gamma}|^2}\boldsymbol{\gamma}_{,\alpha}\times\boldsymbol{\gamma} + \left(\frac{1}{|\boldsymbol{\gamma}|} - \frac{\sin|\boldsymbol{\gamma}|}{|\boldsymbol{\gamma}|^2}\right)\frac{(\boldsymbol{\gamma}\cdot\boldsymbol{\gamma}_{,\alpha})}{|\boldsymbol{\gamma}|}\boldsymbol{\gamma}. \tag{38}$$

In view of (21),(22), and (37), the corresponding strain measures of the shell read

$$\mathbf{H} = \mathbf{R}^T\mathbf{F} - \mathbf{1} = \mathbf{R}^T(\mathbf{G}_\alpha + \mathbf{u}_{,\alpha}) \otimes \mathbf{G}^\alpha - \mathbf{G}_\alpha \otimes \mathbf{G}^\alpha\,, \tag{39}$$

$$\mathbf{K} = -\mathbf{k}_\alpha \otimes \mathbf{G}^\alpha\,, \tag{40}$$

which, with the decompositions (6) as well as with (38), can be explicitly written as

$$\begin{aligned}
\mathbf{H} \;=\; & \Big\{c_{\beta k}\,u_{k,\alpha} + (c_{\alpha k} + u_{k,\alpha})c_{\beta j} \\
& \times \left[\frac{\sin|\boldsymbol{\gamma}|}{|\boldsymbol{\gamma}|}\,e_{ijk}\,\gamma_i + \frac{1-\cos|\boldsymbol{\gamma}|}{|\boldsymbol{\gamma}|^2}\,(\gamma_k\gamma_j - \gamma_i\gamma_i\delta_{jk})\right]\Big\}\,\mathbf{G}^\beta \otimes \mathbf{G}^\alpha \\
& + \Big\{c_{3k}u_{k,\alpha} + (c_{\alpha k} + u_{k,\alpha})c_{3j} \\
& \times \left[\frac{\sin|\boldsymbol{\gamma}|}{|\boldsymbol{\gamma}|}\,e_{ijk}\,\gamma_i + \frac{1-\cos|\boldsymbol{\gamma}|}{|\boldsymbol{\gamma}|^2}\,(\gamma_k\gamma_j - \gamma_i\gamma_i\delta_{jk})\right]\Big\}\,\mathbf{N} \otimes \mathbf{G}^\alpha
\end{aligned} \tag{41}$$

$$\begin{aligned}
\mathbf{K} \;=\; & -c_{\beta k}\left(\frac{\sin|\boldsymbol{\gamma}|}{|\boldsymbol{\gamma}|}\,\gamma_{k,\alpha} + \frac{1-\cos|\boldsymbol{\gamma}|}{|\boldsymbol{\gamma}|^2}\,e_{ijk}\gamma_{i,\alpha}\gamma_j\right. \\
& \qquad \left. + \frac{|\boldsymbol{\gamma}| - \sin|\boldsymbol{\gamma}|}{|\boldsymbol{\gamma}|^2}\,|\boldsymbol{\gamma}|_{,\alpha}\gamma_k\right)\mathbf{G}^\beta \otimes \mathbf{G}^\alpha \\
& -c_{3k}\left(\frac{\sin|\boldsymbol{\gamma}|}{|\boldsymbol{\gamma}|}\,\gamma_{k,\alpha} + \frac{1-\cos|\boldsymbol{\gamma}|}{|\boldsymbol{\gamma}|^2}\,e_{ijk}\gamma_{i,\alpha}\gamma_j + \frac{|\boldsymbol{\gamma}| - \sin|\boldsymbol{\gamma}|}{|\boldsymbol{\gamma}|^2}\,|\boldsymbol{\gamma}|_{,\alpha}\gamma_k\right)\mathbf{N} \otimes \mathbf{G}^\alpha
\end{aligned} \tag{42}$$

The following features of these strain measures may be pointed out:

- Only first derivatives are involved. Within a finite-element formulation only C^0-continuity is required.
- The rotation tensor is three-parametric. In-plane rotations are naturally included and the continuity of the kinematical fields, even at points with discontinuous geometric data (sharp edges), is guaranteed.

- Compared with the tensor of change of curvature emanating from a *Green* type strain measure, the tensor $\mathbf{K}$ exhibits a simpler and more practicable form. In one-dimensional deformations (e.g. axi-symmetric deformations), $K_{\alpha\beta}$ depends even linearly on the derivative of the rotation (in this case, the direction of the rotation vector is fixed).

- No symmetry conditions are employed on the stretch tensor. Such conditions appear when the shell theory is derived by means of the three-dimensional approach which rests on the polar decomposition theorem (see [22]). From a numerical point of view, symmetry conditions are subsidiary conditions which have to be taken into account, seriously complicating the numerical procedure. In light of this, the direct approach appears as an elegant method to circumvent such conditions.

2.4 The multiplicative structure of the rotation group

As a *Lie* group, $SO(3)$ exhibits a certain multiplicative structure which has been a source of misunderstandings and misinterpretations, but also objective difficulties in the numerical treatment of rotational parameters. In this section we discuss the basic multiplicative structure of the rotational group, where we confine ourselves to the quasi static case. Accordingly, it is sufficient to deal with variations.

Let us be given the rotation tensor $\mathbf{R}$, Variations of $\mathbf{R}$ can be given by left or by right multiplications in the form

$$\delta\mathbf{R} = \mathbf{W}\mathbf{R} = \mathbf{R}\mathbf{Y}, \tag{43}$$

where $\mathbf{W}$ and $\mathbf{Y}$ are elements of $so(3)$, that is both are skew-symmetric. The relation holds $\mathbf{W} = \mathbf{R}\mathbf{Y}\mathbf{R}^T$. One says that $\mathbf{W}\mathbf{R}$ defines a left tangent vector in the tangent space of SO(3), while $\mathbf{R}\mathbf{Y}$ defines a right one.

By denoting the axial vector of $\mathbf{W}$ by $\mathbf{w}$, that of $\mathbf{Y}$ by $\mathbf{y}$, one can derive expressions relating the variation of $\mathbf{k}_\alpha$ to $\mathbf{w}$, or $\mathbf{y}$:

$$\delta\mathbf{k}_\alpha = \text{axial}[\delta(\mathbf{R}^T\mathbf{R}_{,\alpha})] = \text{axial}[\delta\mathbf{R}^T\mathbf{R}_{,\alpha} + \mathbf{R}^T\delta\mathbf{R}_{,\alpha}]\,, \tag{44}$$

which, with (43), gives

$$\begin{aligned} \delta\mathbf{k}_\alpha &= \text{axial}[-\mathbf{Y}\mathbf{R}^T\mathbf{R}_{,\alpha} + \mathbf{R}^T\mathbf{R}_{,\alpha}\mathbf{Y} + \mathbf{Y}_{,\alpha}], \\ &= -\mathbf{y}\times\mathbf{k}_\alpha + \mathbf{y}_{,\alpha}. \end{aligned} \tag{45}$$

Alternatively, using left variations one arrives at the relation

$$\delta\mathbf{k}_\alpha = \mathbf{R}^T\mathbf{w}_{,\alpha}\,, \tag{46}$$

which is obtained by straightforward calculations using $\mathbf{w} = \mathbf{R}\mathbf{y}$. From this equation it is evident that it is simpler to deal with a left vector field when taking variations of the materially defined second *Cosserat* deformation tensor determined with the help of $\mathbf{k}_i$ according to (22). Accordingly we will concentrate on left multiplications. In any case, the treatment is equally valid for right multiplications.

3 The variational formulation

In this section the functionals which form the basis for a finite element formulation will be given. In addition, the field equations will be derived. For the sake of brevity, we will do this for the case of the surface only. In the same framework, the functionals and field equations can be rephrased to describe the one- and three-dimensional cases.

3.1 Weak form and field equations

For hyperelastic materials, there exists an internal potential

$$\Psi_{int} = \int_{\mathcal{M}} \rho\psi_{int}(\mathbf{U},\mathbf{K})dA, \tag{47}$$

which is a function of both deformation tensors $\mathbf{U}$ and $\mathbf{K}$, such that the conjugate force and moment tensors, $\mathbf{n}$ and $\mathbf{m}$, are given by

$$\mathbf{n} = \rho\frac{\partial\psi_{int}(\mathbf{U},\mathbf{K})}{\partial\mathbf{U}}\,, \qquad \mathbf{m} = \rho\frac{\partial\psi_{int}(\mathbf{U},\mathbf{K})}{\partial\mathbf{K}}. \tag{48}$$

Here, ρ defines the density at the reference configuration.

The external virtual work is defined as

$$\mathcal{W}_{ext} = \int_{\mathcal{M}} \rho\mathbf{b}\cdot\delta\mathbf{u}dA + \int_{\mathcal{M}} \rho\mathbf{l}\cdot\mathbf{w}dA + \int_{\partial\mathcal{M}} \mathbf{t}\cdot\delta\mathbf{u}ds + \int_{\partial\mathcal{M}} \mathbf{q}\cdot\mathbf{w}ds\,, \tag{49}$$

where, dA denotes the area element of the surface and ds the corresponding line element of its boundary $\partial\mathcal{M}$, $\mathbf{b}$ and $\mathbf{l}$ are the surface forces and torques, while $\mathbf{t}$ and $\mathbf{q}$ are the corresponding quantities acting on the boundary. We note also that the virtual rotation vector conjugate to an external moment is given by the spatial quantity $\mathbf{w} = \mathbf{R}\mathbf{y}$ and not by the material one $\mathbf{y}$.

The equations of motion are the Euler-Lagrange equations of the functional

$$\delta\Psi_{int} - \mathcal{W}_{ext} = 0, \tag{50}$$

which, using (47), reads

$$\begin{aligned} &\int_{\mathcal{M}} \left[\rho\frac{\partial\psi_{int}(\mathbf{U},\mathbf{K})}{\partial\mathbf{U}} : \delta\mathbf{U} + \rho\frac{\partial\psi_{int}(\mathbf{U},\mathbf{K})}{\partial\mathbf{K}} : \delta\mathbf{K}\right] dA \\ &- \int_{\mathcal{M}} \rho\mathbf{b}\cdot\delta\mathbf{x}dA - \int_{\mathcal{M}} \rho\mathbf{l}\cdot\mathbf{w}dA - \int_{\partial\mathcal{M}} \mathbf{t}\cdot\delta\mathbf{x}ds - \int_{\partial\mathcal{M}} \mathbf{q}\cdot\mathbf{w}ds \;=\; 0\,. \end{aligned} \tag{51}$$

With the help of (48), we first rewrite the functional as

$$\int_{\mathcal{B}} [\mathbf{n} : \delta\mathbf{U} + \mathbf{m} : \delta\mathbf{K}]\, dA - \int_{\mathcal{B}} \rho\mathbf{b}\cdot\delta\mathbf{u}dA - \int_{\mathcal{B}} \rho\mathbf{l}\cdot\mathbf{w}dA - \int_{\partial\mathcal{B}} \mathbf{t}\cdot\delta\mathbf{u}ds - \int_{\partial\mathcal{B}} \mathbf{q}\cdot\mathbf{w}ds = 0\,. \tag{52}$$

Now the variations of the strain measures can be established with the help of (39), (40), (43), and (46). One gets

$$\begin{aligned} &\int_{\mathcal{B}} \left[\mathbf{R}\mathbf{n} : (\delta\mathbf{u}_{,\alpha}\otimes\mathbf{G}^{\alpha}) - \mathbf{R}\mathbf{n}\mathbf{F}^{T} : \mathbf{W} - \mathbf{m}^{T} : \mathbf{R}\mathbf{w}_{,\alpha}\otimes\mathbf{G}^{\alpha})\right] dA \\ &- \int_{\mathcal{B}} \rho\mathbf{b}\cdot\delta\mathbf{u}dA - \int_{\mathcal{B}} \rho\mathbf{l}\cdot\mathbf{w}dA - \int_{\partial\mathcal{B}} \mathbf{t}\cdot\delta\mathbf{u}ds - \int_{\partial\mathcal{B}} \mathbf{q}\cdot\mathbf{w}ds \;=\; 0. \end{aligned} \tag{53}$$

At this point we introduce for reasons of compact notation the following vectors

$$\mathbf{n}^\alpha = \mathbf{n}\mathbf{G}^\alpha, \qquad \mathbf{m}^\alpha = \mathbf{m}\mathbf{G}^\alpha\,, \tag{54}$$

with the help of which the above functional is rewritten as

$$\begin{aligned} &\int_{\mathcal{B}} \left[\mathbf{R}\mathbf{n}^\alpha \cdot \delta\mathbf{u}_{,\alpha} - \mathbf{R}\mathbf{n}\mathbf{F}^T : \mathbf{W} - \mathbf{R}\mathbf{m}^\alpha \cdot \mathbf{w}_{,\alpha}\right] dA \\ &- \int_{\mathcal{B}} [\rho\mathbf{b} \cdot \delta\mathbf{u} + \rho\mathbf{l} \cdot \mathbf{w}] dA - \int_{\partial\mathcal{B}} [\mathbf{t} \cdot \delta\mathbf{u} + \mathbf{q} \cdot \mathbf{w}] ds \;\; = \;\; 0\,. \end{aligned} \tag{55}$$

Applying the divergence theorem, we get

$$\begin{aligned} &\int_{\mathcal{B}} \left[\frac{1}{\sqrt{G}}(\sqrt{G}\mathbf{R}\mathbf{n}^\alpha)_{,\alpha} \cdot \delta\mathbf{u} + \mathbf{R}\mathbf{n}\mathbf{F}^T : \mathbf{W} - \frac{1}{\sqrt{G}}(\sqrt{G}\mathbf{R}\mathbf{m}^\alpha)_{,\alpha} \cdot \mathbf{w}\right] dA \\ &+ \int_{\mathcal{B}} [\rho\mathbf{b} \cdot \delta\mathbf{u} + \rho\mathbf{l} \cdot \mathbf{w}] dA - \int_{\partial\mathcal{B}} \left[\mathbf{R}\mathbf{n}^\alpha \nu_\alpha \cdot \delta\mathbf{u} - \mathbf{R}\mathbf{m}^\alpha \nu_\alpha \cdot \mathbf{w} + \mathbf{t} \cdot \delta\mathbf{u} + \mathbf{q} \cdot \mathbf{w}\right] ds \;\; = \;\; 0, \end{aligned} \tag{56}$$

where ν_α denotes the components of the external normal vector at the boundary $\partial\mathcal{B}$. The expression $\mathbf{R}\mathbf{n}\mathbf{F}^T : \mathbf{W}$ can be reformulated using some algebraic manipulations as follows

$$\mathbf{R}\mathbf{n}\mathbf{F}^T : \mathbf{W} \;\; = \;\; -(\mathbf{W}\mathbf{R}\mathbf{n}^\alpha \otimes \mathbf{x}_{,\alpha}) : \mathbf{1} = -(\mathbf{w} \times \mathbf{R}\mathbf{n}^\alpha) \cdot \mathbf{x}_{,\alpha} = (\mathbf{x}_{,\alpha} \times \mathbf{R}\mathbf{n}^\alpha) \cdot \mathbf{w}. \tag{57}$$

Taking into account that $\delta\mathbf{u}, \mathbf{w}$ are free variations, we arrive at the localized form of the governing equations, the Euler-Lagrange equations of the above functional. They read

$$\frac{1}{\sqrt{G}}(\sqrt{G}\mathbf{R}\mathbf{n}^\alpha)_{,\alpha} + \rho\mathbf{b} = \mathbf{0}, \tag{58}$$

$$\mathbf{x}_{,\alpha} \times \mathbf{R}\mathbf{n}^\alpha - \frac{1}{\sqrt{G}}(\sqrt{G}\mathbf{R}\mathbf{m}^\alpha)_{,\alpha} + \rho\mathbf{l} = \mathbf{0}. \tag{59}$$

The corresponding boundary conditions are

$$\mathbf{R}\mathbf{n}^\alpha \nu_\alpha = \mathbf{t}, \quad \mathbf{R}\mathbf{m}^\alpha \nu_\alpha = -\mathbf{q}, \quad \text{on} \quad \partial\mathcal{B}_\sigma. \tag{60}$$

$\partial\mathcal{B}_\sigma$ is the part of the boundary $\partial\mathcal{B}$ with prescribed natural boundary conditions.

If the variation of the rotation tensor is carried out using right multiplications, that is with the help of $\mathbf{Y}$ instead of $\mathbf{W}$, only the second Euler-Lagrange equation (59) takes a modified form reflecting the material nature of the equation. The equation will then read

$$\mathbf{R}^T\mathbf{x}_{,\alpha} \times \mathbf{n}^\alpha - \frac{1}{\sqrt{G}}(\sqrt{G}\mathbf{m}^\alpha)_{,\alpha} - \mathbf{k}_\alpha \times \mathbf{m}^\alpha + \rho\mathbf{R}^T\mathbf{l} = \mathbf{0}. \tag{61}$$

Note that (61) is nothing but the pull-back of (59) under $\mathbf{R}$.

3.2 A hybrid functional

In this section we will formulate the functional on which the finite element formulation and the numerical calculations are based. At this stage it is constructive to write down the

constitutive relations, which are used in our model. These are the classical linear equations. The main difference is that the tensors are generally not symmetric:

$$n^{\alpha\beta} = \frac{Eh}{(1-\nu^2)}\Pi^{\alpha\beta\gamma\lambda}(U_{\gamma\lambda} - G_{\gamma\lambda}), \quad n^{\alpha 3} = \frac{Eh}{2(1+\nu)}G^{\alpha\beta}U_{\beta 3} \tag{62}$$

$$m^{\alpha\beta} = \frac{Eh^3}{12(1-\nu^2)}\Pi^{\alpha\beta\gamma\lambda}K_{\gamma\lambda}, \quad m^{\alpha 3} = \frac{Eh^3}{12(1+\nu)}G^{\alpha\beta}K_{\beta 3}, \tag{63}$$

where

$$\Pi^{\alpha\beta\gamma\lambda} = \nu G^{\alpha\beta}G^{\gamma\lambda} + (1-\nu)G^{\alpha\gamma}G^{\beta\lambda}\,. \tag{64}$$

E denotes Young's Modulus, ν Poisson ratio, and h is an internal length which we identify with the shell thickness.

It is well known that displacement-based functionals, as formulated in (51), lead to poor performance when subjected to a finite element discretization in case of thin shells. For this reason we follow [21] in constructing a hybrid-type functional.

For an uncoupled linear elastic Material law, the internal potential is quadratic in $\mathbf{U}$ and $\mathbf{K}$:

$$\psi_{int}(\mathbf{U},\mathbf{K}) = \psi^1_{int}(\mathbf{U}) + \psi^2_{int}(\mathbf{K}). \tag{65}$$

Since $\psi^1_{int}(\mathbf{U})$ is convex in $\mathbf{U}$, there exists a Legendre transformation such that the complementary potential $\tilde{\psi}_{int}(\mathbf{n})$ is given by

$$\rho\psi^1_{int}(\mathbf{U}) + \rho\tilde{\psi}_{int}(\mathbf{n}) = \mathbf{n} : \mathbf{U}\,. \tag{66}$$

With (66) we can reformulate (51) to get

$$\begin{aligned}\int_{\mathcal{B}}\left[-\rho\frac{\partial\tilde{\psi}_{int}(\mathbf{n})}{\partial\mathbf{n}} : \delta\mathbf{n} + \mathbf{U} : \delta\mathbf{n} + \delta\mathbf{U} : \mathbf{n} + \rho\frac{\partial\psi^2_{int}(\mathbf{K})}{\partial\mathbf{K}} : \delta\mathbf{K}\right]dA \\ - \int_{\mathcal{B}}\rho\mathbf{b}\cdot\delta\mathbf{u}dA - \int_{\mathcal{B}}\rho\mathbf{l}\cdot\mathbf{w}dA - \int_{\partial\mathcal{B}}\mathbf{t}\cdot\delta\mathbf{u}ds - \int_{\partial\mathcal{B}}\mathbf{q}\cdot\mathbf{w}ds \;=\; 0,\end{aligned} \tag{67}$$

On the basis of this functional the finite element formulation will be given later.

4 Path-independent updating of the rotation tensor

4.1 Multiplicative updating

At a certain loading step i we have a stage of equilibrium defined by the displacement field $\mathbf{u}_i$ and the rotation field $\mathbf{R}_i$. By changing the external loading, the body will attain from this state of equilibrium a new one characterized by the new kinematical fields $\mathbf{u}_{i+1}$ and $\mathbf{R}_{i+1}$.

Within an iteration process in a finite element analysis the resulting field equations are to be linearized leading to linear equations for incremental quantities of the kinematical fields. Computationally, to get from a load step i to another one $i+1$, several linear computations

(iterations) are performed which lead in each iteration to incremental displacements $\Delta\mathbf{u}^j$ and incremental rotations $\Delta\mathbf{W}^j$, where j denotes the iteration step. While it is evident how to construct the displacement field at the end of an iteration step by simply relying on the additive structure of the displacement vectors to obtain

$$\mathbf{u}_{i+1}^{j} = \mathbf{u}_{i+1}^{(j-1)} + \Delta\mathbf{u}\,, \tag{68}$$

it is by no means clear how to build up a rotation tensor, given the incremental rotation. Note that according to the above notation we must have $\mathbf{u}_{i+1}^{(0)} = \mathbf{u}_i$.

The first idea is the following. Let the linearisation of the rotation tensor be carried out multiplicatively either by left or right multiplications. That is, the linearisation is of the form $\Delta\mathbf{R} = \Delta\mathbf{W}\mathbf{R} = \mathbf{R}\Delta\mathbf{Y}$ (by simply replacing the variations by the increments), where the rotational increments are also skew symmetric. Then, it is natural to build up the rotation tensor according to

$$\mathbf{R}_{i+1}^{j} = \exp(\Delta\mathbf{W})\,\mathbf{R}_{i+1}^{(j-1)} = \mathbf{R}_{i+1}^{(j-1)}\exp(\Delta\mathbf{Y})\,. \tag{69}$$

In other words, given a rotation tensor $\mathbf{R}_{i+1}^{(j-1)}$ corresponding to the $(j-1)$-iteration at the $(i+1)$-load step, one builds an incremental rotation tensor $\Delta\mathbf{R} = \exp(\boldsymbol{\Delta}\mathbf{W})$ and multiplies it with the rotation tensor $\mathbf{R}_{i+1}^{(j-1)}$.

The above multiplicative scheme pertains to the general structure of the rotational group, but it does not tell us how to interpolate rotational parameters. Recall that the rotation tensor itself cannot be interpolated, only rotational parameters can. The rotation vector of $\Delta\mathbf{R}$ is $\Delta\mathbf{w}$, that of any rotation tensor $\mathbf{R}$ will be the corresponding $\boldsymbol{\gamma}$, and only these quantities can be interpolated.

A first method for multiplicative updating was assigned in [24] (see also Simo et al. [25] where the elaborations on the method are more explicit), which is based on the idea that only $\Delta\mathbf{w}$ is interpolated such that the incremental rotation vector is defined at every *Gauss* point. Given this rotation vector, one constructs the corresponding rotation tensor at the *Gauss* points which is then multiplied with that existing from the previous step and the result is stored as a history variable. In other words, the operation documented in (69) is carried out at *Gauss* points and $\mathbf{R}_{i+1}^{(j)}$ is stored as a history variable. At the nodes, only $\Delta\mathbf{W}$ is defined and, hence, only the increment of the rotation vector is interpolated. Note that at the reference configuration we have $\mathbf{R} = \mathbf{1}$.

The above method was widely accepted and used and it is only recently that Jelenic and Crisfield [15] have observed its path-dependency. In contrast, we will device in the following a path-independent multiplicative scheme for rotational parameters which is actually based on the first author's work in [21]. The key to making a scheme path-independent is the observation that the method must interpolate total rotational parameters, not only the incremental ones. In order to preserve the multiplicative structure and not end up in an additive one, a special scheme is needed in order to construct the total rotational parameters which have to be defined at the nodal points. The concept now is therefore as follows. Let the rotation vector $\boldsymbol{\gamma}_{j+1}^{i-1}$ be given at nodal points (at the reference configuration we have simply $\boldsymbol{\gamma} = \mathbf{0}$). The linear iteration step provides us with an incremental rotation vector $\Delta\mathbf{w}$. Accordingly, we have $\Delta\mathbf{R}$ and $\mathbf{R}_{i+1}^{j-1}$ defined at nodal points. Now we build up multiplicatively

$\mathbf{R}_{i+1}^{j} = \Delta\mathbf{R}\mathbf{R}_{i+1}^{(j-1)}$, also at nodal points, and extract from $\mathbf{R}_{i+1}^{j}$ the corresponding rotation vector $\boldsymbol{\gamma}_{i+1}^{j}$. The latter can now be interpolated to arrive at the rotation vector, and hence rotation tensor, at *Gauss* points. Accordingly, both quantities $\Delta\mathbf{w}$ as well as $\boldsymbol{\gamma}_{i+1}^{j}$ are defined at nodal points and can be interpolated in the classical way. The method is simple and efficient as well, since one does not need to carry out the tensor multiplications explicitly. Based on the notion of quaternions, one can directly generate the vector $\boldsymbol{\gamma}_{i+1}^{j}$ from given $\Delta\mathbf{w}$ and $\boldsymbol{\gamma}_{i+1}^{j-1}$. In the following we briefly describe the basic computational steps.

4.2 Updating method using quaternions

For a readable amount on quaternions we refer to Hestens [12], see also McRobie and Lasenby [17], who entirely reformulated the rod equations in terms of quaternions. Let $\mathbf{a}$ be any vector in $\mathbb{R}^3$ and let i be defined as a complex number with $i^2 = -1$. The '$\wedge$'-product (wedge product) of two *Euclidean* vectors $\mathbf{a}$ and $\mathbf{b}$ is defined as

$$\mathbf{a} \wedge \mathbf{b} = i(\mathbf{a} \times \mathbf{b})\,, \tag{70}$$

where $\mathbf{a} \times \mathbf{b}$ is the usual cross product of vectors.

The geometric product of two vectors is now defined as

$$\mathbf{ab} = \mathbf{a} \cdot \mathbf{b} + \mathbf{a} \wedge \mathbf{b} = \mathbf{a} \cdot \mathbf{b} + i(\mathbf{a} \times \mathbf{b})\,. \tag{71}$$

Note that the result consists of a scalar and a vector. The operation $(+)$ is not to be confused with the usual addition of scalars or vectors.

Using the above terminology any rotation tensor, say $\mathbf{R}$ with corresponding rotation vector $\boldsymbol{\gamma}$, can be described as

$$\mathbf{R} = \alpha + i\boldsymbol{\beta}\,, \tag{72}$$

where α and $\boldsymbol{\beta}$ are defined according to

$$\alpha = \cos(\frac{|\boldsymbol{\gamma}|}{2})\,, \tag{73}$$

$$\boldsymbol{\beta} = \sin(\frac{|\boldsymbol{\gamma}|}{2})\frac{\boldsymbol{\gamma}}{|\boldsymbol{\gamma}|}\,. \tag{74}$$

The relations hold

$$\mathbf{R}^T = \alpha - i\boldsymbol{\beta} \tag{75}$$

and

$$\mathbf{R}^T\mathbf{R} = 1\,, \tag{76}$$

since we have, using (72) and (75),

$$\mathbf{R}^T\mathbf{R} = \alpha^2 + \boldsymbol{\beta}^2 = 1\,, \tag{77}$$

which shows that the four parameters α and $\boldsymbol{\beta}$ are not independent but have to fulfill the side condition (77).

One of the features of the representation in quaternions is that it is unique for arbitrary rotations, while the rotation vector representation is not unique for a rotation angle greater than 2π. From a computational point of view this would be a less important issue. The real advantage lies in the simple multiplication of rotations.

Now, given two rotation vectors $\boldsymbol{\gamma}_i$ and $\Delta\mathbf{w}$, what is the rotation vector which corresponds to the multiplicative product of the corresponding rotation tensors? The computation goes as follows. From (73) and (74) one has

$$\alpha_1 = \cos(\frac{|\Delta\mathbf{w}|}{2}) \,, \tag{78}$$

and

$$\boldsymbol{\beta}_1 = \sin(\frac{|\Delta\mathbf{w}|}{2})\frac{\Delta\mathbf{w}}{|\Delta\mathbf{w}|} \,. \tag{79}$$

Similarly, the relations are valid

$$\alpha_2 = \cos(\frac{|\boldsymbol{\gamma}_i|}{2}) \,, \tag{80}$$

and

$$\boldsymbol{\beta}_2 = \sin(\frac{|\boldsymbol{\gamma}_i|}{2})\frac{\boldsymbol{\gamma}_i}{|\boldsymbol{\gamma}_i|} \,. \tag{81}$$

The geometric product of both quaternions reads:

$$\begin{aligned} \mathbf{R}_{i+1} &= \Delta\mathbf{R}\mathbf{R}_i \\ &= (\alpha_1 + i\boldsymbol{\beta}_1)(\alpha_2 + i\boldsymbol{\beta}_2) \\ &= \alpha_1\alpha_2 + \alpha_1 i\boldsymbol{\beta}_2 + \alpha_2 i\boldsymbol{\beta}_1 + i^2(\boldsymbol{\beta}_1\boldsymbol{\beta}_2) \\ &= \alpha_1\alpha_2 + \alpha_1 i\boldsymbol{\beta}_2 + \alpha_2 i\boldsymbol{\beta}_1 + i^2(\boldsymbol{\beta}_1\cdot\boldsymbol{\beta}_2 + i(\boldsymbol{\beta}_1\times\boldsymbol{\beta}_2)) \\ &= (\alpha_1\alpha_2 - \boldsymbol{\beta}_1\cdot\boldsymbol{\beta}_2) + i(\alpha_1\boldsymbol{\beta}_2 + \alpha_2\boldsymbol{\beta}_1 - \boldsymbol{\beta}_1\times\boldsymbol{\beta}_2) \\ &= \alpha_{i+1} + i\boldsymbol{\beta}_{i+1} \,. \end{aligned} \tag{82}$$

From the last equation we read

$$\boldsymbol{\beta}_{i+1} = (\alpha_1\boldsymbol{\beta}_2 + \alpha_2\boldsymbol{\beta}_1 - \boldsymbol{\beta}_1\times\boldsymbol{\beta}_2) \tag{83}$$

Using (74), the rotation vector corresponding to $\mathbf{R}_{i+1}$ is recovered as

$$\boldsymbol{\gamma}_{i+1} = \boldsymbol{\beta}_{i+1}\frac{2\arcsin|\boldsymbol{\beta}_{i+1}|}{|\boldsymbol{\beta}_{i+1}|} \,, \tag{84}$$

which can now be classically interpolated.

5 The finite-element approach

Following [21], the finite element formulation of the theory presented in the previous sections is developed on the basis of the functional (67). Accordingly, the kinematical fields, as well as the components of $\mathbf{n}$, are to be interpolated. While all components of $\mathbf{u}$ and $\boldsymbol{\gamma}$, respectively

$\Delta\mathbf{w}$, are interpolated using the well known bi-linear interpolation functions, the components of $\mathbf{n}$ are given by

$$\begin{aligned} n^{11}(\xi,\eta) &= S_1 + \eta S_2 \\ n^{22}(\xi,\eta) &= S_3 + \xi S_4 \\ n^{12}(\xi,\eta) &= S_5 \\ n^{21}(\xi,\eta) &= S_6 \\ n^{13}(\xi,\eta) &= S_7 + \eta S_8 \\ n^{23}(\xi,\eta) &= S_9 + \xi S_{10}. \end{aligned} \tag{85}$$

Here ξ, η are the coordinates at the element level corresponding to ϑ^1, ϑ^2 respectively and $S_1, S_2 ...$ are some constants determining the stress field within the element. The interpolation functions for $\mathbf{n}$ are assumed to be discontinuous over elements and hence can be eliminated at the element level.

In the case of the one-dimensional rod, the above interpolations reduce to linear interpolations for the kinematical fields and to constant interpolations for the components of $\mathbf{n}$.

6 Numerical examples

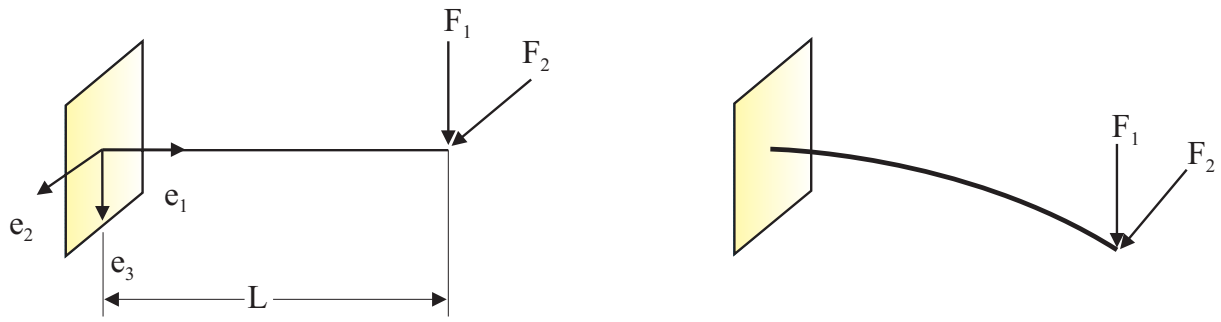
We consider two numerical examples, the first one-dimensional and the second two-dimensional, to illustrate the path independent approach discussed in the paper.

6.1 A cantilever beam under the action of combined loading

As sketched in Fig. 1, a cantilever beam is subject to two concentrated single forces at its end. We consider three different load histories: i) first F_2 is applied and then F_1, ii) F_1 is applied and then F_2, and iii) both forces are applied together. The beam is discretized using 8 one-dimensional elements and the displacements at the tip for all three cases are summarized in Table 1. As is clearly seen, the method of Simo et al. does exhibit path-dependency while the new suggested method is in fact path-independent.

Method	u_1	u_2	u_3
Simo et al. (i)	-21.9129215	35.4090103	35.1574601
Simo et al. (ii)	-21.9129215	35.1574601	35.4090103
Simo et al. (iii)	-21.9130795	35.2835694	35.2835694
present (i)	-21.9130795	35.2835694	35.2835694
present (ii)	-21.9130795	35.2835694	35.2835694
present (iii)	-21.9130795	35.2835694	35.2835694

Table 1: Tip displacements for cantilever beam with different load sequences



Material Properties	E	=	$1 \cdot 10^7$	ν	=	0.3
Length, Cross section	L	=	80	A	=	1×1
Forces	F_1	=	300	F_2	=	300

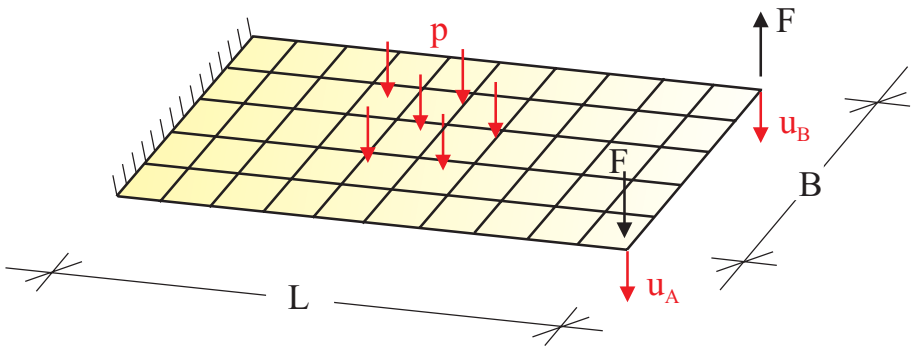
Figure 1: Cantilever beam with different load sequences

6.2 A plate under the action of combined loading

In this two-dimensional example (Fig. 2), a plate is fully clamped at one side and is subjected to a combined loading consisting of dead loading acting in the field and two concentrated single forces acting at the edges of the opposing side. Two load histories are considered: (i) first the whole load is applied at the same time and is gradually increased to arrive the maximum, (ii) second the dead loading is applied first until its maximum value is reached; after that the concentrated forces are increased until its maximum value is reached as well. The plate is discretized using 10×5 elements. The results of the vertical displacement of the points A and B under the concentrated forces are included in Table 2. Here too, the load history influences the results of the method of Simo et al., while it is not affecting the results of the new one. The differences are less pronounced in comparison with the beam case as the absolute values of the rotations in the two-dimensional case remain rather limited. Nevertheless, it is expected that the differences will increase once computations are run for long times as is the case in structural dynamics.

Method	u_A	u_B
Simo et al. (i)	40.7013072466	2.21994675864
Simo et al. (ii)	40.7701046574	2.29383969869
present (i)	40.6841610528	2.19769883927
present (ii)	40.6841610528	2.19769883927

Table 2: Displacements for clamped plate with different load sequences



Material Properties	E	=	$3.10275 \cdot 10^4$	ν	=	0.3		
Length,Width,Thickness	L	=	100	B	=	50	h =	1.27
Forces	F_{max}	=	500	p_{max}	=	0.025		

Figure 2: Clamped plate with different load sequences

7 Closure

In this paper, a method of multiplicative updating of rotations in the frame of finite element analysis of rods and shells was developed. Contrasting some established multiplicative updating schemes (e.g. the method of Simo and Vu-Quoc), the new formulation is path-independent. Altogether, the method is numerically efficient, physically sound, and preserves the multiplicative structure of rotations.

The rotation tensor appears as a kinematical variable within rod and shell formulations which are established based on a direct approach for the development of dimensionally reduced theories for elastic problems on thin domains. The three-dimensional classical continuum is replaced by a two- or one-dimensional *Cosserat* continuum avoiding any kinematical assumptions. In both theories, the one-dimensional as well as the two-dimensional theory, the approach is straightforwardly applied allowing for an equal treatment in either case. The rotation tensor involved is three-parametric allowing for naturally inclusion of drilling degrees of freedom.

Computations are carried out using a hybrid 4-node finite element (respectively 2-node element in the one-dimensional case) which is based on a partially mixed functional.

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