Kinematically Exact Beam Finite Elements Based on Quaternion Algebra

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***Abstract*—Rotations in three-dimensional Euclidean space can be represented by the use of quaternions numerically efficient and robust. In the present approach, rotational quaternions are used as the primary quantities to describe the rotational degrees of freedom for static and dynamic analysis of geometrically non-linear beam-like structures. The classical concept of parametrization of the rotation matrix by the rotational vector is thus completely abandoned. The consistent governing equations of the beam in terms of the quaternion algebra are presented and several quaternion-based numerical implementations are discussed.**

***Keywords*–beam theory; non-linear geometry; quaternion algebra; finite-element formulation, statics; dynamics**

I. Introduction

Beams are important load-carrying members of various engineering structures. A common characteristic of these structural elements is that one dimension is considerably longer than the other two, which allows us to employ relatively simple mathematical models to describe their geometry. Nevertheless, modern demands for such structures impose the need to predict accurately and efficiently large displacements and rotations and finite strains that can occur during the deformation. Therefore, the governing equations of the problem in general become non-linear and too demanding to be solved analytically.

Efficient numerical implementation of three-dimensional non-linear beam elements is still a challenge for researches. Most of the problems in non-linear beam formulations reported in literature stem from the properties of three-dimensional rotations that are directly or indirectly incorporated into the methods. The non-linearity of three-dimensional rotations requires a special treatment in parametrization, discretization, interpolation and iterative update. It is crucial for the overall efficiency of the finite element formulation that in all these procedures a sufficient attention is paid to the properties of rotations.

Among various existing non-linear beam theories we here study the 'geometrically exact beam theory' also denoted as 'Cosserat theory of rods' as introduced by Antman [1], Reissner [2], and Simo [3]. We will especially focus on the treatment of rotations in numerical implementation. There is a number of possible ways of choosing the suitable representation or parametrization of rotations. Widely used are the three-component parametrizations as we directly avoid any algebraic constraints. Among such parametrizations a 'rotational vector' [4] seems to be very popular. Simo [3], Bottasso and Borri [5], Jelenić and Crisfield [6] and many others employed the rotational vector as the members of the primary unknowns. In contrast to these models, Betsch and Steinmann [7] used the director triad with constraints. By the use of directors several disadvantages of the rotational vector, such as singularity and strain non-objectivity, are avoided with the additional cost of six constraint equations that need to be considered at each node. An interesting alternative is the algebra of quaternions that was only recently recognized as a suitable tool in three-dimensional beam formulations [8]–[12].

Quaternions are elements of the four-dimensional Euclidean space. By introducing an additional operation called 'quaternion multiplication' we are able to represent rotations with quaternions. Only one additional degree of freedom in such parametrization is sufficient to avoid singularities while it introduces only one algebraic constraint that needs to be satisfied. The equations of the beam need to be properly transformed and all the steps in the numerical procedure need to be taken in accord with the new configuration space. In this work, we therefore present the derivation of the dynamic governing equations of the three-dimensional beam in terms of quaternions using an energy-consistent approach and discuss the numerical implementation in terms of quaternion algebra for statics and dynamics.

This paper is structured in the following manner. Section 2 introduces quaternion algebra and its properties. In Section 3, we describe the mathematical model of the three-dimensional beam. Kinematic equations are reviewed in Section 4. Section 5 introduces the continuous governing equations in terms of quaternion algebra, while, in Sections 6 and 7, the finite-element implementations for static and dynamic problems are described, respectively, and some numerical examples are given. The paper ends with concluding remarks.

II. Quaternions

The set of quaternions $I\!H$ is a four-dimensional Euclidean linear space. Its elements are often presented as the sum of a scalar and a vector, i.e., $\widehat{x} = s + \vec{v} = \left(s, \vec{v}\right)$, $s \in I\!R$, $\vec{v} \in I\!R^3$. Addition and scalar multiplication are inherited from $I\!R^4$. We additionally introduce the *quaternion multiplication*

$$\widehat{x} \circ \widehat{y} = \left(s\,c - \vec{v} \cdot \vec{w}\right) + \left(c\vec{v} + s\vec{w} + \vec{v} \times \vec{w}\right), \qquad (1)$$

where $\widehat{y} = c + \vec{w} \in I\!H$. Here $(\cdot)$ denotes the scalar product and $(\times)$ denotes the cross-vector product in $I\!R^3$.

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Any quaternion q, with unit norm ($|\widehat{q}| = 1$) can be expressed in polar form as

$$\widehat{q} = \cos\frac{\vartheta}{2} + \sin\frac{\vartheta}{2}\,\vec{n}, \qquad \left|\vec{n}\right| = 1, \tag{2}$$

where ϑ is the angle of rotation and $\vec{n}$ is the unit vector on the axis of rotation. That is why we also call them *rotational quaternions*. Let $\vec{b} \in I\!R^3$ denote a three-dimensional vector obtained by rotating vector $\vec{a} \in I\!R^3$ by an angle ϑ about an axis, defined by unit vector $\vec{n}$. Then a relationship between the two vectors can be expressed as

$$\vec{b} = \widehat{q} \circ \vec{a} \circ \widehat{q}^*, \tag{3}$$

where $\widehat{q}^* = \cos\frac{\vartheta}{2} - \sin\frac{\vartheta}{2}\,\vec{n}$ is the conjugated quaternion.

III. Model of a three-dimensional beam

A three-dimensional beam, Fig. 1, is described by the family of position vectors $\vec{r}\,(x,t)$, $x \in [0, L]$, of the line of centroids and local orthonormal bases $\left\{\vec{G}_1\,(x,t)\,, \vec{G}_2\,(x,t)\,, \vec{G}_3\,(x,t)\right\}$ describing the inclination of cross-sections, which are assumed to preserve their shape and area during the deformation.

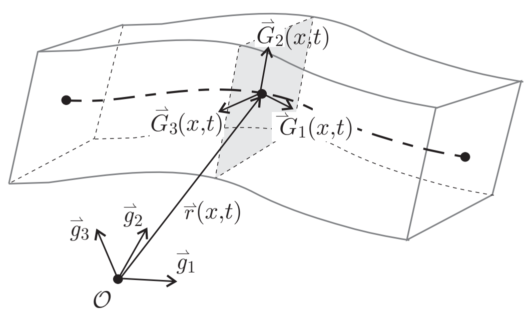

Figure 1. A three-dimensional beam.

After introducing a global orthonormal basis $\left\{\vec{g}_1, \vec{g}_2, \vec{g}_3\right\}$ each local basis can be defined by the rotation of the global one. In terms of the quaternion algebra, the relation between the moving and the fixed basis can be written as

$$\vec{G}_i\,(x,t) = \widehat{q}\,(x,t) \circ \vec{g}_i \circ \widehat{q}^*\,(x,t)\,, \qquad i = 1,2,3. \tag{4}$$

For computational purposes, vectors will be expressed with respect to either of the two bases and the component description will be denoted by bold face symbols. For quaternions a trivial extension of these two bases into quaternion space together with the fourth base vector - the identity element $\widehat{1} = 1 + \vec{0}$ will be used. An arbitrary quaternion, $\widehat{x} = s + \vec{v}$, can thus be expressed as

$$\widehat{x} = s\,\widehat{1} + v_1\vec{g}_1 + v_2\vec{g}_2 + v_3\vec{g}_3 = S\,\widehat{1} + V_1\vec{G}_1 + V_2\vec{G}_2 + V_3\vec{G}_3$$

and the components are represented by one-column matrices $\widehat{\mathbf{x}}$ and $\widehat{\mathbf{X}}$, respectively. The relationship between the two representations of any quaternion is given by

$$\widehat{\mathbf{X}} = \widehat{\mathbf{q}}^* \circ \widehat{\mathbf{x}} \circ \widehat{\mathbf{q}}, \qquad \widehat{\mathbf{x}} = \widehat{\mathbf{q}} \circ \widehat{\mathbf{X}} \circ \widehat{\mathbf{q}}^*. \tag{5}$$

We will identify vectors and quaternions with zero scalar part since any vector in $I\!R^3$ can be treated as an element of the four-dimensional Euclidean space:

$$\mathbf{v} \equiv \widehat{\mathbf{v}} = \left[\begin{array}{cccc} 0 & v_1 & v_2 & v_3 \end{array}\right]^T.$$

The hat over the symbol will be omitted when the first component equals zero since the appropriate size of one-column representation will always be evident from the context.

IV. Kinematic equations

In Reissner-Simo beam theory [2] – [3], the resultant strain measures at the centroid of each cross-section are directly introduced and expressed with kinematic variables by the first order differential equations. For describing the rate of change of the position vector we introduce the translational strain

$$\boldsymbol{\gamma} = \mathbf{r}' - \boldsymbol{\gamma}_0, \qquad \boldsymbol{\Gamma} = \widehat{\mathbf{q}}^* \circ \widehat{\mathbf{r}}' \circ \widehat{\mathbf{q}} + \boldsymbol{\Gamma}_0, \tag{6}$$

where $\boldsymbol{\gamma}_0$ and $\boldsymbol{\Gamma}_0$ are variational constants, determined from the initial configuration of the beam. The differentiation of equation (4) with respect to parameter x results in *rotational strain* vector. In terms of quaternions, the rotational strain, also called the curvature, is determined by

$$\boldsymbol{\kappa} = 2\widehat{\mathbf{q}}' \circ \widehat{\mathbf{q}}^*, \qquad \boldsymbol{K} = 2\widehat{\mathbf{q}}^* \circ \widehat{\mathbf{q}}'. \tag{7}$$

Analogously we have

$$\mathbf{v} = \dot{\mathbf{r}}, \qquad \mathbf{V} = \widehat{\mathbf{q}}^* \circ \dot{\mathbf{r}} \circ \widehat{\mathbf{q}}. \tag{8}$$

describing the velocity in both descriptions. The time-dependent analogy to curvature is the *angular velocity* vector:

$$\boldsymbol{\omega} = 2\dot{\widehat{\mathbf{q}}} \circ \widehat{\mathbf{q}}^*, \qquad \boldsymbol{\Omega} = 2\widehat{\mathbf{q}}^* \circ \dot{\widehat{\mathbf{q}}}. \tag{9}$$

Again, $\boldsymbol{\omega}$ denotes the angular velocity with respect to the fixed basis while $\boldsymbol{\Omega}$ is its local basis representation.

The weak or linearized form of kinematic equations (6) and (7) relating the variations of strains, displacements and rotational quaternions will also be needed. They can be derived by direct linearization of the strong form of kinematic equations, which leads to

$$\delta_{\rm rel}\boldsymbol{\Gamma} = (\widehat{\mathbf{q}}^* \circ \delta\widehat{\mathbf{r}}' \circ \widehat{\mathbf{q}}) + \; 2\widehat{\mathbf{q}}^* \circ (\widehat{\mathbf{r}}' \times (\delta\widehat{\mathbf{q}} \circ \widehat{\mathbf{q}}^*)) \circ \widehat{\mathbf{q}} \tag{10}$$

$$\delta_{\rm rel}\boldsymbol{K} = 2\widehat{\mathbf{q}}^* \circ (\delta\widehat{\mathbf{q}} \circ \widehat{\mathbf{q}}^*)' \circ \widehat{\mathbf{q}}. \tag{11}$$

Note that by (10)–(11) the relative or objective variations of strains are defined. The objective variations are variations of components with respect to the local basis where the changes of are not taken into account. It is also interesting to observe that the same equations can be obtained from the virtual work principle as presented in [13].

A result similar to (7) is obtained after we express the variation of the rotational vector $\boldsymbol{\vartheta} = \vartheta\mathbf{n}$ with the variation of rotational quaternion. After a short derivation we obtain

$$\delta\boldsymbol{\vartheta} = 2\delta\widehat{\mathbf{q}} \circ \widehat{\mathbf{q}}^*. \tag{12}$$

The above result is crucial for the replacement of rotational vectors with quaternions in any variational principle.

V. The continuous governing equations

Our goal is to express the governing equations in terms of quaternions as the only rotational degrees of freedom. Quaternions will serve as a suitable replacement for both rotational vector and matrix. We will start from the weak form of the dynamic equilibrium of a three-dimensional beam:

$$\begin{aligned}
&\int_0^L \Big[\mathbf{N}(x,t)\cdot\delta_{\rm rel}\boldsymbol{\Gamma}(x,t)+\mathbf{M}(x,t)\cdot\delta_{\rm rel}\boldsymbol{K}(x,t)\Big]dx\\
&=\int_0^L \Big[\tilde{\mathbf{n}}(x,t)-\rho A\ddot{\mathbf{r}}(x,t)\Big]\cdot\delta\mathbf{r}(x,t)\ dx\\
&+\int_0^L \Big[\tilde{\mathbf{m}}(x,t)-\mathbf{R}(x,t)\,\mathbf{J}_\rho\dot{\boldsymbol{\Omega}}(x,t)\\
&\qquad -\boldsymbol{\omega}(x,t)\times\mathbf{R}(x,t)\,\mathbf{J}_\rho\boldsymbol{\Omega}(x,t)\Big]\cdot\delta\boldsymbol{\vartheta}(x,t)\ dx\\
&+\boldsymbol{f}^L(t)\cdot\delta\mathbf{r}(L,t)+\boldsymbol{h}^L(t)\cdot\delta\boldsymbol{\vartheta}(L,t)\\
&-\boldsymbol{f}^0(t)\cdot\delta\mathbf{r}(0,t)+\boldsymbol{h}^0(t)\cdot\delta\boldsymbol{\vartheta}(0,t)\,, \qquad (13)
\end{aligned}$$

where the term on the left hand side denotes the virtual work of internal forces and the terms of the right hand side denote the virtual work of external (applied) and inertial forces and moments. $\mathbf{N}$ and $\mathbf{M}$ are the stress-resultant force and moment vectors of the cross-section; $\tilde{\mathbf{n}}$ and $\tilde{\mathbf{m}}$ are external distributed force and moment vectors per unit of the initial length; ρ denotes mass per unit of the initial volume; $\mathbf{R}$ is the rotation matrix; A is the area of the cross-section; $\mathbf{J}_\rho$ is the centroidal mass-inertia matrix of the cross-section; $\boldsymbol{f}^0$, $\boldsymbol{h}^0$, $\boldsymbol{f}^L$ and $\boldsymbol{h}^L$ are the external point forces and moments at the two boundaries, $x=0$ and $x=L$. For simplicity and clearness of the notation, the dependency on x and t will be omitted.

We will replace any rotation matrix acting on a vector by the quaternion-based rotation, see (3). Further, we will replace the variation of the three-parameter rotational vector by the variation of the four-parameter rotational quaternion using (12) and rearrange the scalar product in the following manner:

$$\mathbf{w}\cdot\delta\boldsymbol{\vartheta}=2\mathbf{w}\cdot\delta\widehat{\mathbf{q}}\circ\widehat{\mathbf{q}}^*=2\left(\mathbf{w}\circ\widehat{\mathbf{q}}\right)\cdot\delta\widehat{\mathbf{q}} \qquad (14)$$

for any vector $\mathbf{w}$.

The four components of the rotational quaternion are mutually dependent due to the unit norm condition. The unit norm constraint is enforced in the model by the method of Lagrangian multipliers. The constraint ($\widehat{\mathbf{q}}\cdot\widehat{\mathbf{q}}=1$) is first multiplied by an arbitrary unknown scalar function $\lambda(x,t)$, independent on the primary unknowns, varied and integrated along the length of the beam:

$$\int_0^L 2\lambda\widehat{\mathbf{q}}\cdot\delta\widehat{\mathbf{q}}\,dx+\int_0^L\left(\widehat{\mathbf{q}}\cdot\widehat{\mathbf{q}}-1\right)\delta\lambda\,dx. \qquad (15)$$

Equation (13) is rewritten in terms of quaternion algebra and (15) is added to finally get

$$\begin{aligned}
&\int_0^L \Big[\mathbf{N}\cdot\delta_{\rm rel}\boldsymbol{\Gamma}+\mathbf{M}\cdot\delta_{\rm rel}\boldsymbol{K}\Big]dx\\
&=\int_0^L\Big[\tilde{\mathbf{n}}-\rho A_r\ddot{\mathbf{r}}\Big]\cdot\delta\mathbf{r}\,dx\\
&+2\int_0^L\Big[\{\tilde{\mathbf{m}}-\widehat{\mathbf{q}}\circ\left(\mathbf{J}_\rho\dot{\boldsymbol{\Omega}}\right)\circ\widehat{\mathbf{q}}^*\\
&\qquad-\boldsymbol{\omega}\times\left(\widehat{\mathbf{q}}\circ(\mathbf{J}_\rho\boldsymbol{\Omega})\circ\widehat{\mathbf{q}}^*\right)\}\circ\widehat{\mathbf{q}}\Big]\cdot\delta\widehat{\mathbf{q}}\,dx\\
&-\int_0^L 2\lambda\widehat{\mathbf{q}}\cdot\delta\widehat{\mathbf{q}}\,dx-\int_0^L\left(\widehat{\mathbf{q}}\cdot\widehat{\mathbf{q}}-1\right)\delta\lambda\,dx+\boldsymbol{f}^L\cdot\delta\mathbf{r}^L\\
&+2\left(\boldsymbol{h}^L\circ\widehat{\mathbf{q}}\right)\cdot\delta\widehat{\mathbf{q}}^L-\boldsymbol{f}^0(t)\cdot\delta\mathbf{r}^0-2\left(\boldsymbol{h}^0\circ\widehat{\mathbf{q}}\right)\cdot\delta\widehat{\mathbf{q}}^0. \qquad (16)
\end{aligned}$$

A. The quaternion-based equations of dynamic equilibrium

Equation (16) represents the variational principle in which the variations $\delta_{\rm rel}\boldsymbol{\Gamma}$, $\delta_{\rm rel}\boldsymbol{K}$, $\delta\mathbf{r}$ and $\delta\widehat{\mathbf{q}}$ are not independent functions. The weak kinematic constraints (10)–(11) are therefore inserted into (16) to employ the fundamental lemma of the calculus of variations, which yields the continuous balance equations of a three-dimensional beam in quaternion notation:

$$\mathbf{n}'+\tilde{\mathbf{n}}-\rho A_r\ddot{\mathbf{r}}=\mathbf{0} \qquad (17)$$

$$\begin{aligned}
&\Big[\mathbf{m}'+\mathbf{r}'\times\mathbf{n}+\tilde{\mathbf{m}}-\widehat{\mathbf{q}}\circ\left(\mathbf{J}_\rho\dot{\boldsymbol{\Omega}}\right)\circ\widehat{\mathbf{q}}^*\\
&\qquad-\boldsymbol{\omega}\times\left(\widehat{\mathbf{q}}\circ(\mathbf{J}_\rho\boldsymbol{\Omega})\circ\widehat{\mathbf{q}}^*\right)-\lambda\widehat{\mathbf{1}}\Big]\circ\widehat{\mathbf{q}}=\widehat{\mathbf{0}} \qquad (18)
\end{aligned}$$

$$\widehat{\mathbf{q}}\cdot\widehat{\mathbf{q}}-1=0 \qquad (19)$$

together with the boundary conditions:

$$\mathbf{n}^0-\mathbf{f}^0=\mathbf{0} \qquad (20)$$

$$\left(\mathbf{m}^0-\mathbf{h}^0\right)\circ\widehat{\mathbf{q}}^0=\widehat{\mathbf{0}} \qquad (21)$$

$$\mathbf{n}^L-\mathbf{f}^L=\mathbf{0} \qquad (22)$$

$$\left(\mathbf{m}^L-\mathbf{h}^L\right)\circ\widehat{\mathbf{q}}^L=\widehat{\mathbf{0}}. \qquad (23)$$

Here, $\mathbf{n}$ and $\mathbf{m}$ represent stress-resultant force and moment vectors of the cross-section with respect to the fixed basis, i.e.

$$\boldsymbol{n}=\widehat{\mathbf{q}}\circ\mathbf{N}\circ\widehat{\mathbf{q}}^*,\qquad \boldsymbol{m}=\widehat{\mathbf{q}}\circ\mathbf{M}\circ\widehat{\mathbf{q}}^*. \qquad (24)$$

Equations (17)–(19) represent a system of eight governing equations for eight unknown functions – three components of displacement vector, four components of rotational quaternion and the Lagrangian multiplier. Equation (17) is identical to the standard linear momentum balance equation as it does not depend on rotation. In contrast, the balance equation (18) differs from the standard angular momentum balance equation. Using the notation $\mathcal{M}$ for the standard form of balance equation

$$\mathcal{M}=\mathbf{m}'+\mathbf{r}'\times\mathbf{n}+\tilde{\mathbf{m}}-\mathbf{R}\mathbf{J}_\rho\dot{\boldsymbol{\Omega}}-\boldsymbol{\omega}\times\mathbf{R}\mathbf{J}_\rho\boldsymbol{\Omega} \qquad (25)$$

and replacing rotation matrix with rotational quaternion (3) in (18), yields

$$\Big[\mathcal{M}-\lambda\widehat{\mathbf{1}}\Big]\circ\widehat{\mathbf{q}}=\widehat{\mathbf{0}}. \qquad (26)$$

Equation (26) represents the extension of the angular momentum balance equation to quaternion algebra as it follows from generalized d'Alembert principle. After (26) is multiplied on the right by $\widehat{\mathbf{q}}^*$ and the unity of quaternion $\widehat{\mathbf{q}}$ is considered, we get

$$\widehat{\mathcal{M}} - \lambda\widehat{\mathbf{1}} = \widehat{\mathbf{0}}$$

or, equivalently,

$$\lambda = 0 \tag{27}$$

$$\mathcal{M} = \mathbf{0}, \tag{28}$$

since $\mathcal{M}$ is a pure quaternion and λ is a scalar. Thus, Lagrangian multiplier λ vanishes for this problem and it could be eliminated from the set of unknown quantities iff the unity of quaternions is satisfied. Note that the unit-norm constraint is not neccessarily preserved after the discretization. When (19) is exactly preserved by the solution procedure the standard moment equilibrium equation can be used. Both approaches will be presented in numerical formulations.

VI. NUMERICAL IMPLEMENTATIONS FOR STATICS

In static analysis, inertial terms in governing equations vanish, which leads to a system of ordinary algebraic equations. In finite element approach, these differential equations are replaced by a set of non-linear algebraic equations and therefore the algebraic constraint for quaternions fits well into the numerical solution method. The consistent quaternion-based approach introduced eight equations (17)–(19) for eight primary unknowns $\mathbf{r}$, $\widehat{\mathbf{q}}$ and λ. The increments of the primary unknowns can be interpolated in a standard manner:

$$\Delta\mathbf{r}(x) = \sum_i P_i(x)\,\Delta\mathbf{r}^i, \qquad \Delta\mathbf{r}^i = \Delta\mathbf{r}(x_i) \tag{29}$$

$$\Delta\widehat{\mathbf{q}}(x) = \sum_i P_i(x)\,\Delta\widehat{\mathbf{q}}^i, \qquad \Delta\widehat{\mathbf{q}}^i = \Delta\widehat{\mathbf{q}}(x_i) \tag{30}$$

$$\Delta\lambda(x) = \sum_i P_i(x)\,\Delta\lambda^i, \qquad \Delta\lambda^i = \Delta\lambda(x_i), \tag{31}$$

where $x_i \in [0, L]$, $i = 0, 1, 2, ..., N+1$, with $x_0 = 0$ and $x_{N+1} = L$, are the *discretization points* and $P_i(x)$ are the interpolation functions. It is evident that such approach introduces additional degrees of freedom, but we should stress that the elements of the tangent-stiff matrix are computationally relatively inexpensive to evaluate. We could expect that the constraint (19) would enforce the unity of quaternions and that a standard additive update can be used. Unfortunately, the incremental quaternions are not unit, which leads to severe numerical problems observed at iteration procedure when solving discrete non-linear equations. The normalization of incremental quaternions does not result in considerably better convergence properties, but they are extremely improved after employing the kinematically consistent update. To obtain the updated rotational quaternion in a consistent manner, the following formula directly derived from (12) is used

$$D\widehat{\mathbf{q}}^i = \cos\left(\left|\Delta\widehat{\mathbf{q}}^i \circ \widehat{\mathbf{q}}^{*i}\right|\right) + \frac{\sin\left(\left|\Delta\widehat{\mathbf{q}}^i \circ \widehat{\mathbf{q}}^{*i}\right|\right)}{\left|\Delta\widehat{\mathbf{q}}^i \circ \widehat{\mathbf{q}}^{*i}\right|}\Delta\widehat{\mathbf{q}}^i \circ \widehat{\mathbf{q}}^{*i}. \tag{32}$$

The updated rotational quaternion is then obtained by multiplying two unit quaternions:

$$\widehat{\mathbf{q}}^{i[n+1]} = D\widehat{\mathbf{q}}^i \circ \widehat{\mathbf{q}}^{i[n]}. \tag{33}$$

The update procedure preserves the unity of rotational quaternions at interpolation points. Between the interpolation points the unity is enforced in the resultant sense as we demand $\int_0^L P_i\left(\widehat{\mathbf{q}} \cdot \widehat{\mathbf{q}} - 1\right) dx = 0$.

For comparison reasons a similar model was proposed but without introducing the additional Lagrangian multiplier λ and by omitting the constraint (19). Such approach reduces the number of degrees of freedom, but requires greater care since the unit norm constraint of rotational quaternions is preserved only pointwise at the interpolation nodes following (32)–(33). To increase the accuracy of numerical integration we employed the same update procedure also for the quaternions at the integration nodes, which were additionally stored during iteration.

Both approaches were proven to be computationally efficient and they both give very accurate results. It was observed, however, that the second approach might face some convergence problems, especially when a very high order of interpolation is used. The first approach does not suffer from such problems wich results in better efficiency and robustness.

A. Bending of 45° arch

We will present the results for the classical test problem by Bathe and Bolourchi [14], see Figure 2.

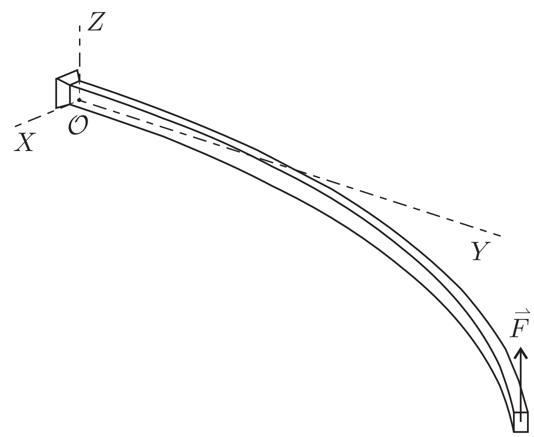

Figure 2. 45° arch.

The circular arch with the radius 100 is located in the horizontal plane and clamped at one end. The cross-section is taken to be a unit square. The arch is subjected to a vertical load $F = 600$ at the free end. The elastic and the shear moduli of material are $E = 10^7$ and $G = E/2$.

TABLE I. FREE-END POSITION OF THE 45° BEND CANTILEVER.

formulation	r_X	r_Y	r_Z
present, consistent, $N = 1$	15.29	47.42	53.47
present, consistent, $N = 3$	15.29	47.42	53.47
present, consistent, $N = 7$	15.29	47.42	53.47
present, consistent, $N = 15$	15.29	47.42	53.47
present, reduced, $N = 1$	15.91	46.98	53.94
present, reduced, $N = 3$	15.79	46.92	53.42
present, reduced, $N = 7$	15.74	47.15	53.43
present, reduced, $N = 15$	15.74	47.15	53.43
[14]	15.9	47.2	53.4
[3]	15.79	47.23	53.37

number of elements=8, N=number of internal points.

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In Table I, we compare the results for the position vector of the free end of the cantilever. Eight straight elements of various order were used to obtain the results of the present formulation. The present results agree well with the results of other authors. Slightly better behaviour of consistent formulation with additional degree of freedom can be observed.

VII. Numerical implementations for dynamics

In dynamics analysis, we base our model on the reduced set of equations (17) and (28). To avoid obtaining the system of the algebraic-differential equations we enforce the constraint (19) as a part of numerical algorithm. Primary unknowns are therefore only $\mathbf{r}(x,t)$ and $\widehat{\mathbf{q}}(x,t)$. They are replaced by a set of one-parameter functions $\mathbf{r}^i(t) = \mathbf{r}(x_i,t)$ and $\widehat{\mathbf{q}}^i(t) = \widehat{\mathbf{q}}(x_i,t)$ at $N+2$ discretization points from the interval $[0,L]$. Similarly as for static case it is suitable to introduce an interpolation of these functions with respect to parameter x:

$$\mathbf{r}(x,t) = \sum_i P_i(x)\,\mathbf{r}^i(t) \qquad \widehat{\mathbf{q}}(x,t) = \sum_i P_i(x)\,\widehat{\mathbf{q}}^i(t)\,. \tag{34}$$

Discretization with respect to x results in a system of $7(N+2)$ ordinary second-order scalar differential equations for dynamic analysis for $7(N+2)$ unknown scalar functions $\mathbf{r}^i(t)$ and $\widehat{\mathbf{q}}^i(t)$.

Several procedures are possible for the time discretization. We have successfully employed the methods of the Runge-Kutta family. Note that the standard methods for solving systems of ordinary differential equations do not automatically conserve the unit norm of the rotational quaternion. In order to obtain the kinematically admissible results, the rotational quaternions are normalized after each time step has been completed.

An interesting alternative is to derive time integrators specially designed for rotational quaternions. Based on the standard Newmark scheme on the additive configuration spaces:

$$\mathbf{r}^{[n+1]} = \mathbf{r}^{[n]} + \Delta t\,\mathbf{v}^{[n]} + \Delta t^2\left[\left(\frac{1}{2}-\beta\right)\dot{\mathbf{v}}^{[n]} + \beta\,\dot{\mathbf{v}}^{[n+1]}\right]$$
$$\mathbf{v}^{[n+1]} = \mathbf{v}^{[n]} + \Delta t\left[(1-\gamma)\,\dot{\mathbf{v}}^{[n]} + \gamma\,\dot{\mathbf{v}}^{[n+1]}\right]$$

and the kinematically consistent update of quaternions (32)–(33) the following scheme is obtained:

$$\begin{aligned}
\Delta\widehat{\mathbf{q}}^{[n]} &= \widehat{\mathbf{q}}^{[n]} \circ \frac{1}{2}\Big\{\Delta t\,\boldsymbol{\Omega}^{[n]} \\
&\quad + \Delta t^2\left[\left(\frac{1}{2}-\beta\right)\dot{\boldsymbol{\Omega}}^{[n]} + \beta\,\dot{\boldsymbol{\Omega}}^{[n+1]}\right]\Big\} \\
\widehat{\mathbf{q}}^{[n+1]} &= \Big[\cos\left|\Delta\widehat{\mathbf{q}}^{[n]} \circ \widehat{\mathbf{q}}^{[n]*}\right| \\
&\quad + \frac{\sin\left|\Delta\widehat{\mathbf{q}}^{[n]} \circ \widehat{\mathbf{q}}^{[n]*}\right|}{\left|\Delta\widehat{\mathbf{q}}^{[n]} \circ \widehat{\mathbf{q}}^{[n]*}\right|}\Delta\widehat{\mathbf{q}}^{[n]} \circ \widehat{\mathbf{q}}^{[n]*}\Big] \circ \widehat{\mathbf{q}}^{[n]} \\
\boldsymbol{\Omega}^{[n+1]} &= \boldsymbol{\Omega}^{[n]} + \Delta t\left[(1-\gamma)\,\dot{\boldsymbol{\Omega}}^{[n]} + \gamma\,\dot{\boldsymbol{\Omega}}^{[n+1]}\right].
\end{aligned}$$

For both schemes $\beta \in \left[0, \frac{1}{2}\right]$ and $\gamma \in [0,1]$. The upper indices $[n]$ and $[n+1]$ denote the quantities at the previous and at the current time, t_n and t_{n+1}, respectively, while $\Delta t = t_{n+1} - t_n$ is the time increment.

A. Right angle cantilever

This example is taken from [15]. The geometry and loading data are presented in Fig. 3. The remaining data reads:

$$\begin{aligned}
&A_1 = A_2 = A_3 = A && EA = GA = 10^6 \\
&J_1 = J_2 = J_3 = J && EJ = GJ = 10^3 \\
&A\rho = 1 && \mathbf{J}_\rho = \mathrm{diag}\,[\ 20 \quad 10 \quad 10\ ]\,.
\end{aligned}$$

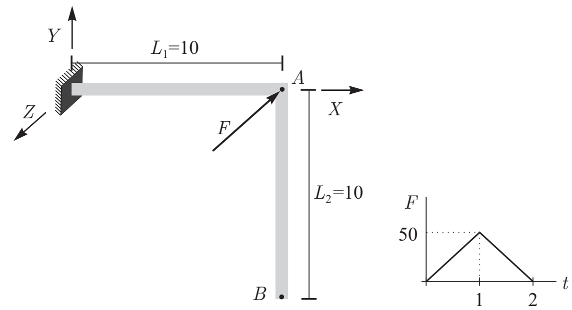

Figure 3. The right-angle cantilever beam subjected to out-of-plane loading.

The present results of the Newmark scheme-based method were obtained using the mesh consisting of 2×10 elements with three internal collocation points per element and the 6-point Gaussian integration rule.

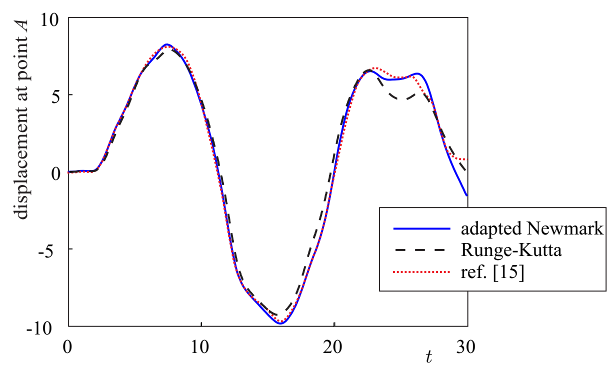

Figure 4. The right-angle cantilever: The right-angle comparison of displacements at point A.

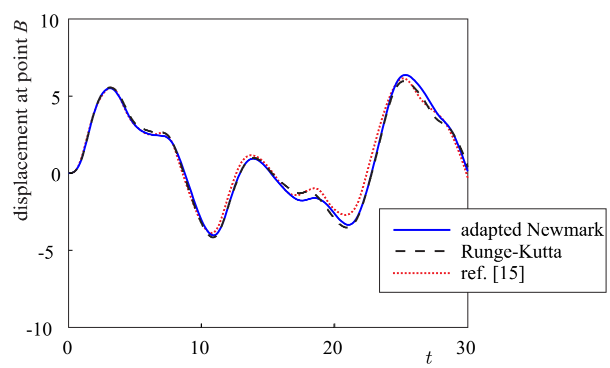

Figure 5. The right-angle cantilever: The right-angle comparison of displacements at point B.

On the whole time interval, $[0, 30]$, we used the same time step as Simo and Vu-Quoc [15]: $\Delta t = 0.25$. The results based on Runge-Kutta method were obtained for the mesh of 2×12 elements with two internal collocation points per element and the 4-point Gaussian integration rule. In contrast to Newmark scheme, the time step is not fixed and varies with respect to the prescribed local error tolerance, taken to be $\varepsilon = 10^{-5}$.

After the loading is removed at $t = 2$, the cantilever continues to vibrate freely, undergoing bending, torsion, axial deformations and large rotations. As observed from Fig. 4 and Fig. 5, the displacements are in a good agreement with [15], particularly in the time interval $[0, 15]$. With time differences between different time integrators become more evident.

VIII. Conclusion

Novel rotational-quaternion based approaches in finite-element methods for analysis of spatial frame structures under static and dynamic loads has been presented. The quaternion algebra was employed for the derivation of continuous equations of dynamic equilibrium with a special consideration of the unit norm constraint of rotational quaternion. Several approaches in discretization of the system of governing equation in terms of quaternions and several solution approaches are possible. The most suitable are the ones that are fully in accord with the nature of three-dimensional rotations and their quaternion representation. When properly treated the quaternions were found to be a computationally efficient, and robust tool for describing incremental and iterative rotations in non-linear beams.

References

[1] S. S. Antman, "Kirchhoffs problem for nonlinearly elastic rods," Q. Appl. Math., vol. 32, no. 3, 1974, pp. 221–240.

[2] E. Reissner, "On finite deformations of space-curved beams," Z. Angew. Math. Phys., vol. 32, no. 6, 1981, pp. 734–744.

[3] J. C. Simo, "A finite strain beam formulation - the three-dimensional dynamic problem. Part I." Comput. Meth. Appl. Mech. Eng., vol. 49, no. 1, 1985, pp. 55–70.

[4] J. Argyris, "An excursion into large rotations," Comput. Meth. Appl. Mech. Eng., vol. 32, no. 1-3, 1982, pp. 85–155.

[5] M. Borri and C. L. Bottasso, "An intrinsic beam model-based on a helicoidal approximation .1. formulation," Int. J. Numer. Methods Eng., vol. 37, no. 13, 1994, pp. 2267–2289.

[6] G. Jelenic and M. A. Crisfield, "Geometrically exact 3D beam theory: implementation of a strain-invariant finite element for statics and dynamics," Comput. Meth. Appl. Mech. Eng., vol. 171, no. 1-2, 1999, pp. 141–171.

[7] P. Betsch and P. Steinmann, "Frame-indifferent beam finite elements based upon the geometrically exact beam theory," Int. J. Numer. Methods Eng., vol. 54, no. 12, 2002, pp. 1775–1788.

[8] H. Lang, J. Linn, and M. Arnold, "Multi-body dynamics simulation of geometrically exact Cosserat rods," Multibody Syst. Dyn., vol. 25, no. 3, 2011, pp. 285–312.

[9] H. Lang and M. Arnold, "Numerical aspects in the dynamic simulation of geometrically exact rods," Appl. Numer. Math., vol. 62, no. 10, SI, 2012, pp. 1411–1427.

[10] E. Zupan, M. Saje, and D. Zupan, "The quaternion-based three-dimensional beam theory," Comput. Meth. Appl. Mech. Eng., vol. 198, no. 49-52, 2009, pp. 3944–3956.

[11] ——, "Quaternion-based dynamics of geometrically nonlinear spatial beams using the Runge-Kutta method," Finite Elem. Anal. Des., vol. 54, 2012, pp. 48–60.

[12] ——, "Dynamics of spatial beams in quaternion description based on the Newmark integration scheme," Comput. Mech., vol. 51, no. 1, 2013, pp. 47–64.

[13] ——, "On a virtual work consistent three-dimensional ReissnerSimo beam formulation using the quaternion algebra," Acta Mechanica, vol. in press, 2013.

[14] K. J. Bathe and S. Bolourchi, "Large displacement analysis of 3-dimensional beam structures," Int. J. Numer. Methods Eng., vol. 14, no. 7, 1979, pp. 961–986.

[15] J. C. Simo and L. Vu-Quoc, "On the dynamics in space of rods undergoing large motions - a geometrically exact approach," Comput. Meth. Appl. Mech. Eng., vol. 66, no. 2, 1988, pp. 125–161.