



H. Lang, J. Linn

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Fraunhofer-Institut für Techno- und
Wirtschaftsmathematik ITWM
Fraunhofer-Platz 1

67663 Kaiserslautern
Germany

Telefon: 06 31/3 16 00-0
Telefax: 06 31/3 16 00-10 99
E-Mail: info@itwm.fraunhofer.de
Internet: www.itwm.fraunhofer.de

Vorwort

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Berichterstattung heißt hier Dokumentation des Transfers aktueller Ergebnisse aus mathematischer Forschungs- und Entwicklungsarbeit in industrielle Anwendungen und Softwareprodukte – und umgekehrt, denn Probleme der Praxis generieren neue interessante mathematische Fragestellungen.

A handwritten signature in black ink, appearing to read 'Dieter Prätzels-Wolters'.

Prof. Dr. Dieter Prätzels-Wolters
Institutsleiter

Kaiserslautern, im Juni 2001

Lagrangian field theory in space and time for geometrically exact Cosserat rods

HOLGER LANG[†], JOACHIM LINN[†]

[†] Fraunhofer Institut für Techno- und Wirtschaftsmathematik,
Fraunhofer Platz 1, 67663 Kaiserslautern, Germany
holger.lang@itwm.fraunhofer.de, joachim.linn@itwm.fraunhofer.de

Abstract

In this article, we derive the balance of linear and angular momentum equations for geometrically exact Cosserat rods from a two dimensional Lagrangian field approach in space and time. As we use a full quaternion description for the rotatory part of the balance equations, they constitute a system of nonlinear hyperbolic partial differential algebraic equations. We prove their equivalence to the classical Euclidean frame description.

Keywords. Cosserat rods, Geometrically exact rods, Small strains, Large deformations, Deformable bodies, Lagrangian field theory, Calculus of variations, Partial differential algebraic equations.

MSC Classification: 53Z05, 74K10, 72S20, 74B15, 74D05, 49S05, 35Q72.

Contents

1	Introduction	1
2	The Cosserat rod model	3
2.1	The kinematics	3
2.2	The internal energy densities	5
2.2.1	Potential energy densities	5
2.2.2	Dissipation energy densities	7
2.2.3	Kinetic energy densities	8
2.3	The frame and quaternion evolution differential equations	10
2.4	The internal forces and moments	11
2.5	The balance equations	11
3	Main theorems	14
A	Hamilton quaternion algebra	16
B	Lagrange field theory in two dimensions	18

1 Introduction

The *Cosserat rod model* is well known for the geometrically exact simulation of deformable/flexible slender one dimensional structures in space (statics) or space-time (quasi-statics or dynamics). A Cosserat rod can be considered as the geometrically nonlinear generalisation of a Timoshenko rod. In contrast to a Kirchhoff rod, which in turn can be considered as a geometrically nonlinear generalisation of a Euler-Bernoulli rod, a Cosserat rod allows to model not only *bending* (= flexure) and *torsion* (= twist) – these are ‘soft’ degrees of freedom –, but as well *extension* (= stretching) and *shearing* – these are ‘hard’ degrees of freedom. In this paper we consider the full dynamical problem for Cosserat rods in space and time.

The aim of this article is to derive the dynamical equations of motion from a *two* dimensional Lagrangian variational principle on a space-time domain. This is an interesting alternative, equivalent to [22], but much more elegant approach to derive the Newtonian balance of linear and

angular momentum equations, like it is for classical Lagrange Mechanics of point masses [8, 11]. Recently, a new discretisation approach has been developed by the authors that will be the topic of subsequent papers. In [17, 18], we present such a numerical model of a Cosserat rod, based on finite differences/quotients from discrete differential geometry, which is completely free even of square roots and trigonometry and which needs only the four basic arithmetic operations – additions, subtractions, multiplications and divisions. This article can be understood as a preparation in the sense that it provides the continuum equations in an appropriate ‘quaternion language’. We always assume that the considered quantities are sufficiently smooth.

The structure of this paper

In section 2, we describe the Cosserat exact rod model in the continuum, where we specify its reduced kinematics, its strain measures and its internal energy densities. We directly formulate the rotational degrees of freedom in terms of unit quaternions, in a similar way as already proposed by [9, 14] for the more special case of the inextensible Kirchhoff rod model. Quaternions in the three-dimensional subgroup

$$\mathbb{S}^3 = \partial B_1^{\mathbb{H}}(0) = \{p \in \mathbb{H} : \|p\|^2 = \bar{p}p = p\bar{p} = 1\} \subset \mathbb{H} \quad (1)$$

are one of several ways – each with its pros and cons – to describe non commutative, spatial rotations in

$$SO(3) = \{Q \in \mathbb{R}^{3 \times 3} : QQ^T = Q^T Q = \mathcal{I}, \det Q = 1\}. \quad (2)$$

Quaternions are so-to-say the analogue to complex numbers in the one-dimensional subgroup $\mathbb{S}^1 = \partial B_1^{\mathbb{C}}(0) = \{z \in \mathbb{C} : \|z\|^2 = \bar{z}z = z\bar{z} = 1\} \subset \mathbb{C}$, which describe commutative plane rotations in $SO(2) = \{Q \in \mathbb{R}^{2 \times 2} : QQ^T = Q^T Q = \mathcal{I}, \det Q = 1\}$. A pro for the choice of quaternions is the absence of singularities such as the ‘gimbal locking’ effect [12, 16, 21], which is an important practical aspect for the numerical modeling of arbitrary large rotations. A con is the need to keep them at unit length during numerical computations.

We finally present the governing partial differential equations for the Cosserat rod both in the classical ‘ $SO(3)$ language’ and in ‘quaternion language’. The equivalence of both descriptions is proven.

In section 3, we derive the equilibrium equations for Cosserat rods directly in ‘quaternion language’. In [22], they are derived from the full three-dimensional theory of elasticity [4, 6] by substitution of the reduced kinematics of the Cosserat rod. Here, we give a variational formulation directly in quaternion description. The calculus of variations yields the balance equations as the Euler-Lagrange equations resulting from the assumed stationarity of an action functional. In addition to [22], we include a simple internal viscoelastic friction damping model that is motivated by the works [1, 2, 3]. Since both the classical $SO(3)$ description and the quaternion description are equivalent, this approach yields another derivation of the classical balance equations for Cosserat rods.

Appendix A provides the main tools and identities from the Hamilton quaternion algebra, which are needed to follow the main sections of this article. For more detailed expositions concerning their algebraic properties, we refer to [10]. The connection to rotations is explained thoroughly in [12, 16]. See [5] for an overview of other possibilities to parametrise the manifold $SO(3)$ such as rotation vectors, Rodriguez parameters, Euler or Cardan angles. There, pros and cons of these parametrisations are discussed as well.

Appendix B summarises the classical Lagrangian field theory/variational calculus for several unknowns in two dimensions. For further details, the reader is referred to [8].

2 The Cosserat rod model

In this section we present the reduced kinematics of a Cosserat rod, its energy densities and its internal forces resp. moments, which are corresponding one-to-one to the Cosserat strain resp. curvature measures. We consider both a *purely linear elastic* and a simple *linear viscoelastic* constitutive material model, with the tacit overall assumption that locally the stresses and strains remain sufficiently small, whereas globally the deformations may become arbitrarily large.

We end up with the initial boundary value problems for the Cosserat rod in ‘quaternion language’ (41), which is the elastic case, and (42), which is the viscoelastic case. It is the aim of the subsequent section 3 to derive these systems of partial equations from the alternative classical Lagrangian field approach of appendix B.

2.1 The kinematics

We start with the kinematics of a Cosserat rod, which is completely determined by a vector field $x = x(s, t)$, the *centerline*, and a *unit quaternion field* $p = p(s, t)$, which in turn uniquely determines a frame field $R \circ p$ that is attached to the centerline. Always in this article, $s \in [0, L]$ denotes the arc length parameter of the rod in the undeformed state, $t \in [0, T]$ denotes the time. $L > 0$ is the total arc length of the undeformed rod, $T > 0$ is a fixed point in time. The dash $'$ and the dot $\dot{}$ always denote the partial derivatives with respect to space s and time t respectively, this is

$$' = \frac{\partial}{\partial s}, \quad \dot{} = \frac{\partial}{\partial t}.$$

The *centerline*

$$x : [0, L] \times [0, T] \rightarrow \Im(\mathbb{H}) = \mathbb{R}^3, \quad (s, t) \mapsto x(s, t) \quad (3)$$

of the Cosserat rod gives the positions of the centroids of mass of the cross sections. The latter are assumed as plane and rigid in the model during deformation.

The *unit quaternion field*

$$p : [0, L] \times [0, T] \rightarrow \mathbb{S}^3 = \partial B_1(0) \hookrightarrow \mathbb{H}, \quad (s, t) \mapsto p(s, t) \quad (4)$$

uniquely determines its attached *frame field*

$$R \circ p : [0, L] \times [0, T] \xrightarrow{p} \mathbb{S}^3 \xrightarrow{R} SO(3), \quad (s, t) \mapsto R(p(s, t)).$$

Here $\mathbb{H}$ is the four dimensional Hamilton quaternion algebra, see appendix A, and $\mathbb{S}^3$ as in (1) is the three dimensional unit sphere, embedded in $\mathbb{H} = \mathbb{R}^4$. We identify $\mathbb{R}^3$ with the imaginary part $\Im(\mathbb{H})$ of $\mathbb{H}$. Further, $SO(3) = SO(3, \mathbb{R}^3)$ as in (2) is the Lie group of special orthonormal rotations in three dimensional Euclidean space.

For a quaternion $p = p_0 + \hat{p} = (p_0; p_1, p_2, p_3) \in \mathbb{H}$, the frame $R(p) \in SO(3)$ is given by the *Euler map*

$$R : \mathbb{H} \rightarrow \mathbb{R}SO(3), \quad p \mapsto R(p) = (d^1(p) | d^2(p) | d^3(p)). \quad (5)$$

The three columns of R are the so-called *directors* – or the *moving base vectors*. The first two of them,

$$d^1(p) = \begin{pmatrix} p_0^2 + p_1^2 - p_2^2 - p_3^2 \\ 2(p_1p_2 + p_0p_3) \\ 2(p_1p_3 - p_0p_2) \end{pmatrix}, \quad d^2(p) = \begin{pmatrix} 2(p_1p_2 - p_0p_3) \\ p_0^2 - p_1^2 + p_2^2 - p_3^2 \\ 2(p_2p_3 + p_0p_1) \end{pmatrix}, \quad (6)$$

are spanning the rigid cross section of the rod. The third one,

$$d^3(p) = \begin{pmatrix} 2(p_1p_3 + p_0p_2) \\ 2(p_2p_3 - p_0p_1) \\ p_0^2 - p_1^2 - p_2^2 + p_3^2 \end{pmatrix}, \quad (7)$$

is kept close to the tangent $\partial_s x$ of the centerline by shearing forces. We have $R(\lambda p) = \lambda^2 R(p)$ for each $\lambda \in \mathbb{R}$ and $p \in \mathbb{H}$, so R maps the quaternion unit sphere $\mathbb{S}^3$ into $SO(3)$,

$$R : \mathbb{S}^3 \rightarrow SO(3). \quad (8)$$

We have $R(-p) = R(p)$ for each $p \in \mathbb{H}$, which implies that a quaternion p and its antipode $-p$ describe the same rotation. Furthermore, it is well known that for each rotation $Q \in SO(3)$ there exist exactly two quaternions p and q such that $R(p) = R(q) = Q$. They are necessarily antipodes $p = -q$. Articles [15, 23, 25] provide an algorithm that computes these p and $q = -p$, given Q . That way, $\mathbb{S}^3$ covers the manifold $SO(3)$ exactly two times [10, 12], and the restriction (8) is ‘twice onto’. Further, we have

$$R(p)v = pv\bar{p}, \quad R(p)^T v = \bar{p}vp \quad \text{for } p \in \mathbb{H}, v \in \mathfrak{S}(\mathbb{H}) = \mathbb{R}^3, \quad (9)$$

especially

$$d^\nu(p) = pe^\nu \bar{p} = R(p)e^\nu \quad (10)$$

for each of the Euclidean base vectors $e^1 = i$, $e^2 = j$ and $e^3 = k$ of $\mathbb{R}^3 = \mathfrak{S}(\mathbb{H})$, which are fixed in space. Note that $\bar{p} = p^{-1}$ and $d^3(p) = d^1(p) \times d^2(p)$ for $\|p\|^2 = 1$.

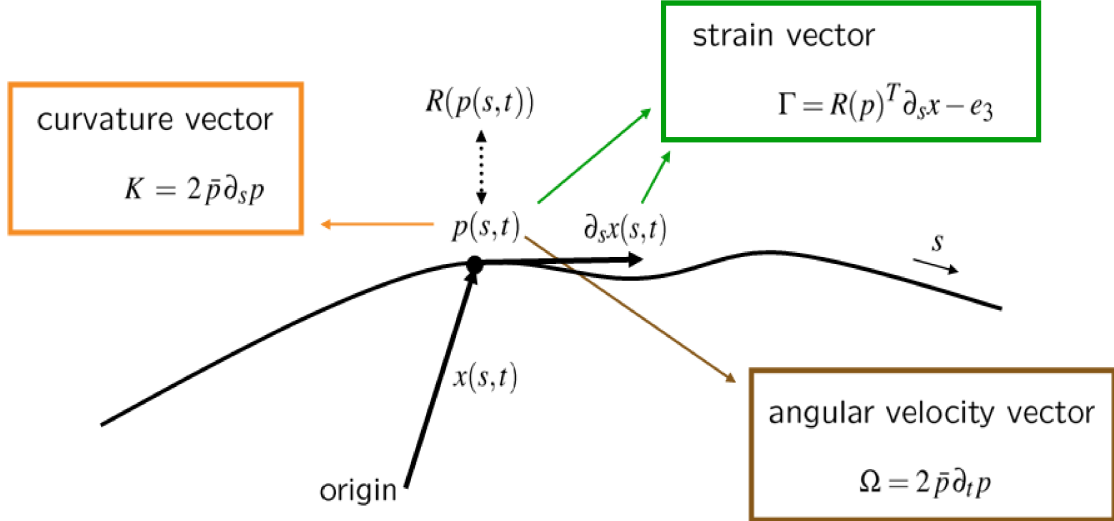


Figure. The kinematics of a Cosserat rod

Any point of the deformed rod in space-time (s, t) can be addressed – this means its kinematic is completely described – by the mapping

$$\varphi : [0, L] \times [0, T] \times \mathcal{A} \rightarrow \mathbb{R}^3, \quad (s, t, \xi) \mapsto x(s, t) + \xi_1 d^1(p(s, t)) + \xi_2 d^2(p(s, t)),$$

where $\xi = (\xi_1, \xi_2) \in \mathcal{A}$ with a plane domain $\mathcal{A} \subset \mathbb{R}^2$ are the coordinates in the rigid and plane cross section, spanned by d^1 and d^2 . The third director $d^3 = d^1 \times d^2$ is the cross section normal.

We continue with a further remark on the Euler map R . For each $p \in \mathbb{H}$, we can write $R(p)$ in the closed-form expression

$$R(p) = (2p_0^2 - \|p\|^2)\mathcal{I} + 2\hat{p} \otimes \hat{p} + 2p_0 \mathcal{E}(\hat{p}) \quad (11)$$

with the *alternating skew tensor*

$$\mathcal{E} : \mathbb{R}^3 = \mathfrak{S}(\mathbb{H}) \rightarrow so(3), \quad \mathcal{E}(\hat{p}) = \begin{pmatrix} 0 & -p_3 & +p_2 \\ +p_3 & 0 & -p_1 \\ -p_2 & +p_1 & 0 \end{pmatrix}, \quad (12)$$

which identifies skew tensors $\mathcal{E}(\hat{p})$ in $so(3)$ with their corresponding axial vectors $\hat{p}$ in $\mathbb{R}^3 = \Im(\mathbb{H})$ in the usual way via

$$\mathcal{E}(\hat{p})v = \hat{p} \times v \quad \text{for } v \in \Im(\mathbb{H}) = \mathbb{R}^3.$$

Here

$$so(3) = \{\omega \in \mathbb{R}^{3 \times 3} : \omega^T = -\omega\}$$

is the Lie algebra of $SO(3)$ at the identity $\mathcal{I} = R(1)$ and consists of all skew tensors of three dimensional Euclidean space.

For a quaternion $p \in \mathbb{S}^3 \setminus \{\pm 1\}$, we can write

$$p = \cos(\phi/2) + \sin(\phi/2)q$$

with a unique purely imaginary unit quaternion $q \in \Im(\mathbb{H}) \cap \mathbb{S}^3$ and a unique angle $0 < \phi < 2\pi$. So in Euclidean space,

$$R(p)v = \cos(\phi)v + \sin(\phi)q \times v + (1 - \cos(\phi))\langle q, v \rangle q \quad \text{for } v \in \Im(\mathbb{H}) = \mathbb{R}^3$$

is exactly the rotation of v about the axis $\mathbb{R}q$ with the angle ϕ , see [12, 10]. In classical differential geometry, the pair $(x(\cdot, t), (R \circ p)(\cdot, t))$ for each fixed point $t \in [0, T]$ in time constitutes a so-called ‘framed curve’.

2.2 The internal energy densities

In order to express the energy densities for a Cosserat rod, it is necessary that an *assumption* on the *constitutive material behaviour* is made. For the conservative *elastic* forces and moments, we assume locally small strains Γ resp. curvatures K , so that the corresponding internal conservative forces F^Γ resp. internal moments M^K can be derived as gradients of a potential energy density, which is quadratic in the strains and curvatures. As a consequence, the elastic forces F^Γ resp. moments M^K are linearly proportional to the strains Γ resp. curvatures K , see section 2.4 and [22]. This is a special case of a hyperelastic material behaviour [3].

In a similar fashion – in order to model internal friction – we choose a dissipation ‘potential’ that is quadratic in the strain rates $\dot{\Gamma}$ resp. curvature rates $\dot{K}$. Consequently, the corresponding internal dissipative forces $F^{\dot{\Gamma}}$ resp. moments $M^{\dot{K}}$ are linearly proportional to $\dot{\Gamma}$ resp. $\dot{K}$. This corresponds to the simplest form of *viscoelastic* material behaviour [1, 2, 3].

For the Lagrangian variational calculus of appendix B, we need energy *densities* $\mathcal{U}$. By ‘density’, we always mean density w. r. t. the arc length parameter s , so that the line integral $\int_0^L \mathcal{U} ds$ along the rod yields physical *energy*. The integral $\int_0^T \int_0^L \mathcal{U} ds dt$ then yields physical *action*.

Throughout this paper, we use the *material* description for the strain Γ (and its rate $\dot{\Gamma}$), the curvature K (and its rate $\dot{K}$) and the angular velocity Ω . In remark 2.3, we explain how to compute the real physical, *spatial* quantities.

2.2.1 Potential energy densities

The total potential energy density $\mathcal{V}$ is additively decomposed into *extensional* and *shearing* energy density $\mathcal{V}_{SE}$ and *bending* and *torsion* energy density $\mathcal{V}_{BT}$,

$$\mathcal{V} = \mathcal{V}_{SE} + \mathcal{V}_{BT}. \quad (13)$$

Sometimes in literature the synonyms ‘flexure’ for bending, ‘stretching’ for extension and ‘twist’ for torsion are used.

By ‘potential’ energy density we exclusively mean the *internal* potential elastic energy density. Additional conservative forces – such as gravitational force – or moments can be simply added as external forces $\hat{F}$ resp. moments $\hat{M}$ to the balance equations on the right hand side.

The **potential extensional** and **shearing energy density** is

$$\mathcal{V}_{SE} = \frac{1}{2} \Gamma^T C^\Gamma \Gamma, \quad C^\Gamma = \left(\begin{array}{cc|c} GA_1 & 0 & 0 \\ 0 & GA_2 & 0 \\ \hline 0 & 0 & EA \end{array} \right), \quad (14)$$

where the triple of components of the *material strain vector* w.r.t. the coordinate system (e^1, e^2, e^3) is given by

$$\Gamma = R(p)^T \partial_s x - e^3 = \bar{p}(\partial_s x) p - e^3. \quad (15)$$

We briefly call Γ the *strain (vector)*. Obviously, it is purely imaginary, i.e. an element of $\mathbb{R}^3 = \Im(\mathbb{H})$. Γ_1 resp. Γ_2 are the strains corresponding to *shearing* in local 1- resp. 2-direction. Γ_3 is the strain corresponding to *extension* in local 3-direction. $E > 0$ is Young's modulus and $G > 0$ is the shear modulus of the material, $A = \iint_{\mathcal{A}} d(\xi_1, \xi_2)$ is the area of the rigid cross section. The numbers $A_1 = \kappa_1 A$ and $A_2 = \kappa_2 A$ with some Timoshenko shear correction factors $0 < \kappa_1, \kappa_2 \leq 1$ denote some effective cross section areas for shearing in 1- resp. 2-direction. Locally, as small strains are assumed, the Cosserat rod behaves as a linear Timoshenko rod. For further details of the shear correction factors of different cross section shapes we refer to [7].

The **potential bending** and **torsion energy density** for the Cosserat rod is

$$\mathcal{V}_{BT} = \frac{1}{2} K^T C^K K, \quad C^K = \left(\begin{array}{cc|c} EI_1 & 0 & 0 \\ 0 & EI_2 & 0 \\ \hline 0 & 0 & GJ \end{array} \right), \quad (16)$$

where the triple of components of the *material curvature vector* (or the *material 'Darboux vector'* in [24]) w.r.t. the coordinate system (e^1, e^2, e^3) are given by

$$\frac{1}{2} K = \bar{p} \partial_s p. \quad (17)$$

We briefly use the short hand nomenclature *curvature (vector)* for K . For the single components, the reader should use formula (58) of the appendix. If p is a unit quaternion, or – more generally – a quaternion of constant length, it holds that $K = (0; K_1, K_2, K_3)^T = \Im(K)$ is purely imaginary, since $\Re(K) = p_0 \partial_s p_0 + \langle \hat{p}, \partial_s \hat{p} \rangle = \langle p, \partial_s p \rangle = \partial_s \|p\|^2 / 2 = 0$. The first two components K_1 resp. K_2 are the curvatures corresponding to *bending* in the local 1- resp 2-direction. K_3 is the curvature corresponding to *torsion* in the local 3-direction. $I_1 = \int_{\mathcal{A}} \xi_2^2 d(\xi_1, \xi_2)$ resp. $I_2 = \int_{\mathcal{A}} \xi_1^2 d(\xi_1, \xi_2)$ are the geometric moments of inertia of the cross section $\mathcal{A}$ in the 1- resp. 2-direction, $J = I_1 + I_2$ its polar moment. If the cross section is symmetric, then we have $I = I_1 = I_2$ and $J = 2I$. But $I_1 \neq I_2$ is allowed, the model is able to cover as well the case of non symmetric cross sections. In lemma 2.4, we show that the quaternion evolution (17) for the curvature is equivalent to the frame evolution $\mathcal{E}(K) = R^T \partial_s R$, where $R = R \circ p$.

Remark 2.1 (Pre-deformed rods) We give a short remark on *pre-tension*, *pre-shearing*, *pre-bending* and *pre-twist*. If the rod is pre-stretched, pre-sheared, pre-bent and/or pre-twisted, the potential energy densities (14) or (16) can be simply replaced by

$$\mathcal{V}_{SE} = \frac{1}{2} (\Gamma - \Gamma^0)^T C^\Gamma (\Gamma - \Gamma^0), \quad \mathcal{V}_{BT} = \frac{1}{2} (K - K^0)^T C^K (K - K^0). \quad (18)$$

Here the functions $\Gamma^0 = \Gamma^0(s)$ resp. $K^0 = K^0(s)$ are a-priori given pre-strains resp. pre-curvatures over the interval $[0, L]$, see [22]. For notational convenience, we assume in this article that $\Gamma^0 \equiv K^0 \equiv 0$. The inclusion of pre-strains or pre-curvatures does not harm the principal ideas of this article. $\square$

It is well known that the Cosserat *strain measures*, i.e. the strain Γ and the curvature K are frame indifferent. [We emphasise that the vocabulary 'strain measure' corresponds to *both* Γ and K .] We give a very short proof of that fact in quaternion notation.

Lemma 2.2 (Frame indifference) *The Cosserat material curvature $2K = \bar{p}\partial_s p$ in (17) and the Cosserat material strain $\Gamma = \bar{p}(\partial_s x)p - e^3$ in (15) are frame indifferent.*

Proof: If we superimpose a finite rotation $q \in \mathbb{S}^3$, which is independent of s and t , the associated material curvature K^* , which is obtained by replacing $p(s, t)$ by $qp(s, t)$, becomes

$$K^* = 2(\bar{q}\bar{p})\partial_s(qp) = 2\bar{p}\bar{q}q\partial_s p = 2\bar{p}\partial_s p = K,$$

since $\bar{q}q = \|q\|^2 = 1$. The components of the forward rotated tangents w.r.t. the global basis (e^1, e^2, e^3) are given by $\partial_s(qx(s, t)\bar{q})$. Therefore the associated material strain Γ^* , which is obtained by forward rotation of the whole system by q , satisfies

$$\Gamma^* = \bar{q}\bar{p}(q\partial_s x\bar{q})(qp) - e^3 = \bar{p}\bar{q}q\partial_s x\bar{q}qp - e^3 = \Gamma,$$

again, since q is a unit quaternion. ■

Likewise, as the situation for K and Ω is completely symmetric, it is seen that the material angular velocity Ω is frame indifferent.

2.2.2 Dissipation energy densities

For the choice of our dissipation potential, we follow the works [1, 2, 3] and choose friction forces resp. moments that are proportional to the strain rates resp. curvature rates. Concerning these damping parameters, we note that they are macroscopic and phenomenological, they are supposed to model not only pure material damping, but also miscellaneous damping mechanisms.

The total dissipation energy density $\mathcal{D}$ additively consists of dissipative *extensional* and *shearing* energy density $\mathcal{D}_{SE}$ and dissipative *bending* and *torsion* energy density $\mathcal{D}_{BT}$,

$$\mathcal{D} = \mathcal{D}_{SE} + \mathcal{D}_{BT}. \quad (19)$$

The **dissipative extensional** and **shearing energy density** is defined as

$$\mathcal{D}_{SE} = \dot{\Gamma}^T C \dot{\Gamma}, \quad C^{\dot{\Gamma}} = \left(\begin{array}{cc|c} r_1^{\dot{\Gamma}} & 0 & 0 \\ 0 & r_2^{\dot{\Gamma}} & 0 \\ \hline 0 & 0 & r_3^{\dot{\Gamma}} \end{array} \right), \quad (20)$$

where the triple of components of the *material strain rate vector* w.r.t. the coordinate system (e^1, e^2, e^3) are the time derivatives of (15), i. e.

$$\dot{\Gamma} = \dot{R}(p)^T \partial_s x + R(p)^T \partial_s \dot{x} = \dot{\bar{p}}(\partial_s x)p + \bar{p}(\partial_s \dot{x})p + \bar{p}(\partial_s x)\dot{p}.$$

$\dot{\Gamma}$ is simply called the *strain rate (vector)*. The nonnegative constants $r_1^{\dot{\Gamma}}$, $r_2^{\dot{\Gamma}}$ and $r_3^{\dot{\Gamma}}$ denote some effective viscoelastic material parameters for extension and shearing.

The **dissipative bending** and **torsion energy density** is defined as

$$\mathcal{D}_{BT} = \dot{K}^T C^{\dot{K}} \dot{K}, \quad C^{\dot{K}} = \left(\begin{array}{cc|c} r_1^{\dot{K}} & 0 & 0 \\ 0 & r_2^{\dot{K}} & 0 \\ \hline 0 & 0 & r_3^{\dot{K}} \end{array} \right), \quad (21)$$

where the triple of components of the *material curvature rate vector* w.r.t. the coordinate system (e^1, e^2, e^3) are given by the time derivative of (17), i. e.

$$\frac{1}{2}\dot{K} = \dot{\bar{p}}\partial_s p + \bar{p}\partial_s \dot{p}.$$

$\dot{K}$ is simply referred to as the *curvature rate (vector)*. For the single components, see again (58) and note that the dot $\dot{}$ and the bar $\bar{}$ ‘commute’. If p is a unit quaternion, it holds that $\Re(\dot{K}) = 0$, $\dot{K} = \Im(\dot{K})$, since $\Re(K) = 0$, $\Im(K) = K$. The nonnegative constants r_1^K , r_2^K and r_3^K denote some effective viscoelastic material parameters for bending and torsion.

The reader may ask, why we do not include a factor of one half in front of the dissipative terms. This is simply a matter of taste. The authors find it more convenient e.g. to write the balance equations for a linear harmonic oscillator in the form $m\ddot{q} + 2r\dot{q} + kq = 0$, resulting as the Euler-Lagrange equations with the energies $\mathcal{V} = kq^2/2$, $\mathcal{D} = \dot{q}^2$ and $\mathcal{T} = m\dot{q}^2/2$. It simplifies the analytic expressions for the eigenvalues, for example.

2.2.3 Kinetic energy densities

The total kinetic energy density $\mathcal{T}$ additively splits into *translatory* $\mathcal{T}_T$ and *rotatory* $\mathcal{T}_R$ kinetic energy density,

$$\mathcal{T} = \mathcal{T}_T + \mathcal{T}_R. \quad (22)$$

The **translatory** and **rotatory kinetic energy densities** are given by

$$T_T = \frac{\varrho A}{2} \|\dot{x}\|^2, \quad T_R = \frac{\varrho}{2} \Omega^T I \Omega, \quad I = \left(\begin{array}{cc|c} I_1 & 0 & 0 \\ 0 & I_2 & 0 \\ 0 & 0 & J \end{array} \right), \quad (23)$$

where the triple of components of the *material angular velocity vector* (or the *material ‘vorticity vector’* in [22]) w. r. t. the coordinate system (e^1, e^2, e^3) is

$$\frac{1}{2} \Omega = \bar{p} \partial_t p. \quad (24)$$

We will use the simple terminology *angular velocity (vector)* for Ω . For the single components, see again (58). A is the cross section area, $\varrho > 0$ the density of the rod. Like for the curvature K , if p is a unit quaternion, the angular velocity Ω satisfies $\Omega = \Im(\Omega) = (0; \Omega_1, \Omega_2, \Omega_3)^T$, since the real part $\Omega_0 = \Re(\Omega) = p_0 \partial_t p_0 + \langle \hat{p}, \partial_t \hat{p} \rangle = \langle p, \partial_t p \rangle = 0$ vanishes. In lemma 2.4, we show that the quaternion evolution (24) is equivalent to the frame evolution $\mathcal{E}(\Omega) = R^T \partial_t R$, where $R = R \circ p$. It equivalently holds that

$$\frac{\varrho}{2} \Omega^T I \Omega = \frac{\varrho}{2} \dot{p}^T \mu(p) \dot{p} \quad (25)$$

with the p dependent *quaternion mass matrix*

$$\mu(p) = 4 \left(\begin{array}{ccc|ccc} I_1 p_1^2 + I_2 p_2^2 + I_3 p_3^2 & I_{32} p_2 p_3 - I_{10} p_0 p_1 & I_{13} p_1 p_3 - I_{20} p_0 p_2 & I_{21} p_1 p_2 - I_{30} p_0 p_3 \\ I_{32} p_2 p_3 - I_{10} p_0 p_1 & I_1 p_0^2 + I_2 p_3^2 + I_3 p_2^2 & I_{21} p_0 p_3 - I_{31} p_1 p_2 & I_{13} p_0 p_2 - I_{21} p_1 p_3 \\ I_{13} p_1 p_3 - I_{20} p_0 p_2 & I_{21} p_0 p_3 - I_{31} p_1 p_2 & I_2 p_0^2 + I_1 p_3^2 + I_3 p_1^2 & I_{32} p_0 p_1 - I_{12} p_2 p_3 \\ I_{21} p_1 p_2 - I_{30} p_0 p_3 & I_{13} p_0 p_2 - I_{21} p_1 p_3 & I_{32} p_0 p_1 - I_{12} p_2 p_3 & I_3 p_0^2 + I_1 p_2^2 + I_2 p_1^2 \end{array} \right),$$

where we have set $I_{kl} = I_l - I_k$ for $k, l = 1, 2, 3$, for abbreviation. The mass matrix satisfies the symmetry property $\mu(-p) = \mu(p)$, which is a consequence of the fact that both p and $-p$ describe the same rotation $R(p) = R(-p)$, see (5). The kernel of $\mu(p)$ is given by $\ker \mu(p) = \mathbb{R}p$, its image is $\text{im } \mu(p) = \{p\}^\perp$, consequently we have $\text{rk } \mu(p) = 3$. $\mu(p)$ is positively semidefinite with one singular dimension in direction p . The factor 4 in front of the mass matrix is simply the square of the factor 2 in the angular velocity (24). To derive identity (25), it is convenient to use the ‘quaternion matrix’ $\mathcal{Q}(p)$ from (63). We replace

$$I = \left(\begin{array}{c|ccc} 0 & 0 & 0 & 0 \\ 0 & I_1 & 0 & 0 \\ 0 & 0 & I_2 & 0 \\ 0 & 0 & 0 & J \end{array} \right), \quad J = I_3 = I_1 + I_2 \quad (26)$$

for the quaternion inertia tensor in (23). Then we find with $\Omega = 2\bar{p}\dot{p}$ that

$$\frac{1}{2} \Omega^T I \Omega = 2(\bar{p}\dot{p})^T I (\bar{p}\dot{p}) = 2(\mathcal{Q}(p)^T \dot{p})^T I (\mathcal{Q}(p)^T \dot{p}) = \frac{1}{2} \dot{p}^T [4\mathcal{Q}(p) I \mathcal{Q}(p)^T] \dot{p} = \frac{1}{2} \dot{p}^T \mu(p) \dot{p},$$

yielding the closed form expression

$$\mu(p) = 4\mathcal{Q}(p)I\mathcal{Q}(p)^T, \quad \mu(p)q = 4pI\bar{p}q, \quad \text{where } q \in \mathbb{H}, \quad (27)$$

for the quaternion mass. Clearly, all this can be computed component by component, but here the quaternion matrix $\mathcal{Q}(p)$ is very practical. With (27) and $2\Omega = \bar{p}\dot{p} = \mathcal{Q}(p)^T\dot{p}$ we can conclude that $\mu(p)\dot{p} = 4\mathcal{Q}(p)I\mathcal{Q}(p)^T\dot{p} = 2pI\Omega$ is $2p$ times the angular momentum $I\Omega$. In a similar fashion, one can show

$$\frac{1}{2} \frac{\partial}{\partial p} (\dot{p}^T \mu(p) \dot{p}) = - \frac{\partial}{\partial p} (\mu(p) \dot{p}) \dot{p} = 4\mathcal{Q}(\dot{p})I\mathcal{Q}(\dot{p})^T p. \quad (28)$$

Consequently,

$$\frac{1}{2} \frac{\partial}{\partial p} (\dot{p}^T \mu(p) \dot{p}) - \frac{\partial}{\partial p} (\mu(p) \dot{p}) \dot{p} = 8\mathcal{Q}(\dot{p})I\mathcal{Q}(\dot{p})^T p = 8\dot{p}I\bar{p}p, \quad (29)$$

see as well [21]. The quaternion mass $\mu(p)$ is ‘almost’ regular in the following sense. If we formally define the ‘*tangential inverse*’ quaternion mass by

$$\mu(p)^{-1} = \frac{1}{4}\mathcal{Q}(p)I^{-1}\mathcal{Q}(p)^T, \quad I^{-1} = \left(\begin{array}{c|ccc} 0 & 0 & 0 & 0 \\ 0 & I_1^{-1} & 0 & 0 \\ 0 & 0 & I_2^{-1} & 0 \\ 0 & 0 & 0 & J^{-1} \end{array} \right), \quad (30)$$

we quickly find

$$\mu(p)\mu(p)^{-1} = \mathcal{I} - p \otimes p. \quad (31)$$

This means that $\mu(p)$ and $\mu(p)^{-1}$ invert each other ‘up to’ a tensor product $p \otimes p$. The tangential inverse mass is as well symmetric and positively semidefinite, and it as well annihilates p , this means we have $\mu(p)^{-1}p = 0$, $\ker \mu(p)^{-1} = \mathbb{R}p$, $\text{im } \mu(p)^{-1} = \{p\}^\perp$ and $\text{rk } \mu(p)^{-1} = 3$.

In order to see, why the nomenclature ‘tangential inverse’ is justified, we consider the action of (31) on an arbitrary quaternion $q \in \mathbb{H}$. We have $(\mathcal{I} - p \otimes p)q = q - \langle p, q \rangle p$, this means that $\mu(p)\mu(p)^{-1}q$ is exactly the projection of q onto the tangential space $T_p\mathbb{S}^3 = \{\pi \in \mathbb{H} : \langle p, \pi \rangle = 0\} = \{p\}^\perp$ of $\mathbb{S}^3$ at p .

Remark 2.3 (Material and spatial description) Before we continue, we give a short remark on *material* and *spatial* quantities and components. Throughout this whole article, we use the *material* description – i.e. we work with the *material* strains, *material* curvature and *material* angular velocities, etc. – for the Cosserat rod. It should be noted that from a spatial quantity (the real physical one), the corresponding material quantity is defined by a pull back via $R^T = R^{-1}$, for details see [22]. Now, if we formally write

$$\Gamma = \sum_{\nu=1,2,3} \Gamma_\nu e^\nu, \quad K = \sum_{\nu=1,2,3} K_\nu e^\nu, \quad \Omega = \sum_{\nu=1,2,3} \Omega_\nu e^\nu,$$

this means that the components γ_ν of the *spatial strain vector*, k_ν of the *spatial curvature vector* and ω_ν of the *spatial angular velocity vector* w.r.t. (e^1, e^2, e^3) are collected in the triples

$$\gamma = R\Gamma = \sum_{\nu=1,2,3} \Gamma_\nu d^\nu, \quad k = RK = \sum_{\nu=1,2,3} K_\nu d^\nu, \quad \omega = R\Omega = \sum_{\nu=1,2,3} \Omega_\nu d^\nu.$$

respectively. [The components of the *spatial strain rate* $\dot{\gamma}$ and the *spatial curvature rate* $\dot{k}$ then can be easily derived by differentiation w.r.t. time.] As a consequence, it follows that the components of any material quantity w.r.t. the fixed coordinate system (e^1, e^2, e^3) are *equal* to the components of the corresponding spatial counterpart w.r.t. the cross section fixed (= moving frame) coordinate system (d^1, d^2, d^3) . With the aid of (9) and (10), it is seen that

$$\gamma = p\Gamma\bar{p} = \partial_s x - d^3, \quad k = pK\bar{p} = 2(\partial_s p)\bar{p}, \quad \omega = p\Omega\bar{p} = 2(\partial_t p)\bar{p}.$$

If this all seems nebulous to the reader, see the detailed expositions in [22, 23]. For further explanations of the *pull back* ‘ R^T .’ and the *push forward* ‘ R .’ operations, we refer to [4]. $\square$

2.3 The frame and quaternion evolution differential equations

Via the isomorphism $\mathcal{E}$ in (12), skew tensors in the Lie algebra $so(3)$ can be identified in a one-to-one fashion with their corresponding axial vectors in $\mathbb{R}^3 = \Im(\mathbb{H})$. With the aid of $\mathcal{E}$, the differential equations (17) resp. (24) can be equivalently written as

$$R^T \partial_s R = \begin{pmatrix} 0 & -K_3 & +K_2 \\ +K_3 & 0 & -K_1 \\ -K_2 & +K_1 & 0 \end{pmatrix} = \mathcal{E}(K), \quad R^T \partial_t R = \begin{pmatrix} 0 & -\Omega_3 & +\Omega_2 \\ +\Omega_3 & 0 & -\Omega_1 \\ -\Omega_2 & +\Omega_1 & 0 \end{pmatrix} = \mathcal{E}(\Omega).$$

In components, this is

$$K_1 = \langle d^2, \partial_s d^3 \rangle = -\langle d^3, \partial_s d^2 \rangle, \quad K_2 = \langle d^3, \partial_s d^1 \rangle = -\langle d^1, \partial_s d^3 \rangle, \quad K_3 = \langle d^1, \partial_s d^2 \rangle = -\langle d^2, \partial_s d^1 \rangle$$

resp.

$$\Omega_1 = \langle d^2, \partial_t d^3 \rangle = -\langle d^3, \partial_t d^2 \rangle, \quad \Omega_2 = \langle d^3, \partial_t d^1 \rangle = -\langle d^1, \partial_t d^3 \rangle, \quad \Omega_3 = \langle d^1, \partial_t d^2 \rangle = -\langle d^2, \partial_t d^1 \rangle.$$

We write it down more precisely. Given the curvature vector K , we have the ordinary differential evolution equation for R in space s ,

$$R(p(s, t))^T \frac{\partial}{\partial s} R(p(s, t)) = 2\mathcal{E}(\bar{p}(s, t) \partial_s p(s, t)) = \mathcal{E}(K(s, t)). \quad (32)$$

Given the angular velocity vector Ω , we have the ordinary differential evolution equation for R in time t ,

$$R(p(s, t))^T \frac{\partial}{\partial t} R(p(s, t)) = 2\mathcal{E}(\bar{p}(s, t) \partial_t p(s, t)) = \mathcal{E}(\Omega(s, t)). \quad (33)$$

Both equations correspond to the Cosserat unit quaternion field $p = p(s, t)$ of the form (4) and $R = R \circ p$. One way, to prove these two evolution equations is component by component with the fundamental Jacobians

$$\frac{1}{2} \frac{\partial d^1(p)}{\partial p} = \begin{pmatrix} p_0 & p_1 & -p_2 & -p_3 \\ p_3 & p_2 & p_1 & p_0 \\ -p_2 & p_3 & -p_0 & p_1 \end{pmatrix}, \quad \frac{1}{2} \frac{\partial d^2(p)}{\partial p} = \begin{pmatrix} -p_3 & p_2 & p_1 & -p_0 \\ p_0 & -p_1 & p_2 & -p_3 \\ p_1 & p_0 & p_3 & p_2 \end{pmatrix} \quad (34)$$

$$\frac{1}{2} \frac{\partial d^3(p)}{\partial p} = \begin{pmatrix} p_2 & p_3 & p_0 & p_1 \\ -p_1 & -p_0 & p_3 & p_2 \\ p_0 & -p_1 & -p_2 & p_3 \end{pmatrix} \quad (35)$$

of the director vectors $d^\nu = d^\nu(p)$ in (6), (7) and the chain rule $\partial_t d^\nu = (\partial_p d^\nu)(\partial_t p)$ resp. $\partial_s d^\nu = (\partial_p d^\nu)(\partial_s p)$. This is carried out in [24] for example. An alternative would be to use expression (11), which is rather lengthy and prone to errors. Thus, we give a much easier and more elegant proof now here.

Lemma 2.4 (Equivalence of the frame and quaternion evolution equations) *The differential equations (17) and (33) for the curvature K resp. (24) and (32) for the angular velocity Ω are equivalent.*

Proof: It is sufficient to prove the equivalence of (24) and (32). We compute with an arbitrary, but fixed, vector $v \in \Im(\mathbb{H})$, $R = R \circ p$, (57) and the fact that $\bar{v} = -v$,

$$\begin{aligned} \mathcal{E}(2\bar{p}\dot{p})v &= 2\bar{p}\dot{p} \times v = 2\Im(\bar{p}\dot{p} \times v - \langle \bar{p}\dot{p}, v \rangle) = 2\Im(\bar{p}\dot{p}v) = \bar{p}\dot{p}v - \overline{\bar{p}\dot{p}v} = \bar{p}\dot{p}v + \overline{\dot{p}\bar{p}v} \\ &= \bar{p}\dot{p}v + v\dot{\bar{p}}p = \bar{p}(\dot{p}v\bar{p} + p\dot{v}\bar{p})p = \bar{p}\partial_t(pv\bar{p})p = \bar{p}\partial_t(Rv)p = \bar{p}(\dot{R}v)p \\ &= R^T \dot{R}v. \end{aligned}$$

Now, if $R^T \dot{R} = \mathcal{E}(\Omega)$, then it follows that $\Omega = 2\bar{p}\dot{p}$, as v can be chosen arbitrarily. The converse is clear as well. ■

It is not hard to see that for the spatial curvature $k = RK$, the equivalent evolutions $k = 2(\partial_s p)\bar{p}$ resp. $\mathcal{E}(k) = (\partial_s R)R^T$ hold. Likewise, the spatial angular velocity $\omega = R\Omega$ satisfies the equivalent evolutions $\omega = 2(\partial_t p)\bar{p}$ resp. $\mathcal{E}(\omega) = (\partial_t R)R^T$. Here always $R = R \circ p$. Similarly, an analogous assertion to lemma 2.2 holds for k and γ .

Remark 2.5 (Symmetry) The quaternion differential equations (17) in s for K and (24) in t for Ω are completely symmetric for the continuum model. From the two dimensional point of view, it is consequently very natural to treat both K (resp. the bending and torsion energy density $\mathcal{V}_{BT}$) and Ω (resp. the rotatory kinetic energy density $\mathcal{T}_R$) in exactly the same way, i.e. in a fully symmetric fashion. This means, we could write $\mathcal{V}_{BT} = \frac{1}{2}(p')^T N(p)p'$ with p dependent 4×4 symmetric, positively semidefinite ‘curvature mass’ matrix $N(p) = 4Q(p)C^K Q(p)^T$ with C^K in (16) replaced by $\text{diag}(0; C^K)$, similarly as we replaced I in (23) by $\text{diag}(0; I)$ in section 2.2.3 in the rotatory energy. Or vice versa.

However, in numerical Multibody Dynamics, the evolution (17) is discretised in *space* with finite differences/quotients or finite elements, whereas the evolution (24) is solved ‘continuously’ in *time* with the aid of appropriate time integrators. The dynamical problem is hyperbolic, and the static problem is elliptic for fixed $t \in [0, T]$. This is why we slightly prefer the asymmetric approach here, see as well [17, 18]. Clearly for numerical simulations, simultaneous discretisations on a two dimensional (s, t) -grid should as well be feasible. $\square$

2.4 The internal forces and moments

First we have a look at the purely **elastic** case. As the potential energy densities $\mathcal{V}$ are assumed to be quadratic and positively definite in the strain measures, the conservative *elastic internal forces* F^Γ resp. *moments* M^K are related in a linear and one-to-one constitutive manner to the strains Γ resp. curvatures K . This is

$$F^\Gamma = C^\Gamma \Gamma = \frac{1}{2} \frac{\partial}{\partial \Gamma} (\Gamma^T C^\Gamma \Gamma), \quad M^K = C^K K = \frac{1}{2} \frac{\partial}{\partial K} (K^T C^K K). \quad (36)$$

Likewise for the **viscoelastic** case, since we assume the dissipation energy densities $\mathcal{D}$ to be quadratic and positively definite in the strain rates, the non-conservative *dissipative internal forces* $F^{\dot{\Gamma}}$ resp. *moments* $M^{\dot{K}}$ are related linearly and one-to-one to the strain resp. curvature rates. More precisely,

$$F^{\dot{\Gamma}} = 2C^{\dot{\Gamma}} \dot{\Gamma} = \frac{\partial}{\partial \dot{\Gamma}} (\dot{\Gamma}^T C^{\dot{\Gamma}} \dot{\Gamma}), \quad M^{\dot{K}} = 2C^{\dot{K}} \dot{K} = \frac{\partial}{\partial \dot{K}} (\dot{K}^T C^{\dot{K}} \dot{K}). \quad (37)$$

Then the *total internal forces* F resp. *moments* M are given by

$$F = F^\Gamma + F^{\dot{\Gamma}} = C^\Gamma \Gamma + 2C^{\dot{\Gamma}} \dot{\Gamma} \quad \text{resp.} \quad M = M^K + M^{\dot{K}} = C^K K + 2C^{\dot{K}} \dot{K}.$$

Here the Hookean-like matrices C^Γ , C^K are from (14), (16) and the matrices $C^{\dot{\Gamma}}$, $C^{\dot{K}}$ are from (20), (21). Clearly, other forms of constitutive assumptions could replace (36) and (37).

2.5 The balance equations

If we introduce the *spatial strains* $\gamma = R\Gamma$, the *spatial curvatures* $k = RK$, the *spatial angular velocities* $\omega = R\Omega$, the *spatial internal forces* $f = RF$, the *spatial internal moments* $m = RM$, the *spatial inertia tensor* $i = RIR^T$, each received by a push forward operation via R from the corresponding material ones, it was shown in [22] that the Cosserat rod, for prescribed *exterior spatial force densities* $\hat{f} = \hat{f}(s, t)$ and *exterior spatial moment densities* $\hat{m} = \hat{m}(s, t)$, satisfies the following geometrically nonlinear partial differential equations on the rectangular domain $[0, L] \times [0, T]$ in the (s, t) -plane.

- Balance equations (Spatial description)

$$\begin{cases} \varrho A \ddot{x} &= \partial_s f + \hat{f} \\ \varrho(i\dot{\omega} + \omega \times i\omega) &= \partial_s m + \partial_s x \times f + \hat{m} \end{cases} \quad (38)$$

By definition of the material and spatial quantities as presented in the preceding sections, it is not hard to see that – with pulled back *material exterior force densities* $\hat{F} = R^T \hat{f}$ and *material exterior moment densities* $\hat{M} = R^T \hat{m}$ – the system (38) can be equivalently written as follows.

- Balance equations (Material description)

$$\begin{cases} \varrho A \ddot{x} &= \partial_s(RF) + R\hat{F} \\ \varrho R(I\dot{\Omega} + \Omega \times I\Omega) &= \partial_s(RM) + \partial_s x \times (RF) + R\hat{M} \end{cases} \quad (39)$$

For the transformation from spatial to material description, the reader should note that the components of a *spatial* quantity γ , k , ω , f , m , i in the *moving* coordinate system (d^1, d^2, d^3) are identical to the components of the corresponding *material* quantity Γ , K , Ω , F , M , I , measured in the *fixed* coordinate system (e^1, e^2, e^3) . So, as an example, it holds $\Gamma = \sum_\nu \Gamma_\nu e^\nu$, if and only if $\gamma = \sum_\nu \Gamma_\nu d^\nu$, since $d^\nu = R e^\nu = p e^\nu \bar{p}$, see (10) and remark 2.3.

For our purposes, we prefer the following equivalent quaternion description of (38) or (39), which consists a system of nonlinear hyperbolic *partial differential algebraic equations*.

- Balance equations (Quaternion language)

$$\begin{cases} \varrho A \ddot{x} &= \partial_s(pF\bar{p}) + p\hat{F}\bar{p} \\ \varrho(\ddot{p} - \langle p, \ddot{p} \rangle p) &= 2\mu(p)^{-1} \{ 4\varrho \dot{p} I \dot{p} p + (\partial_s p)M + \partial_s(pM) + (\partial_s x)pF + p\hat{M} \} \\ 0 &= \|p\|^2 - 1 \end{cases} \quad (40)$$

Together with appropriate initial and boundary conditions, we receive the *initial boundary value problem*, which has to be solved.

With the **elastic** constitutive assumptions (36), the quaternion description (40) can be completed in the following form.

$$\boxed{\begin{cases} \varrho A \ddot{x} &= \partial_s(pF\bar{p}) + p\hat{F}\bar{p} \\ \varrho(\ddot{p} - \langle p, \ddot{p} \rangle p) &= 2\mu(p)^{-1} \{ 4\varrho \dot{p} I \dot{p} p + (\partial_s p)M + \partial_s(pM) + (\partial_s x)pF + p\hat{M} \} \\ 0 &= \|p\|^2 - 1 \\ F &= C^T \Gamma \\ M &= C^K K \end{cases}} \quad (41)$$

Likewise, with the **viscoelastic** constitutive assumptions in (37), the system (40) can be augmented as follows.

$$\boxed{\begin{cases} \varrho A \ddot{x} &= \partial_s(pF\bar{p}) + p\hat{F}\bar{p} \\ \varrho(\ddot{p} - \langle p, \ddot{p} \rangle p) &= 2\mu(p)^{-1} \{ 4\varrho \dot{p} I \dot{p} p + (\partial_s p)M + \partial_s(pM) + (\partial_s x)pF + p\hat{M} \} \\ 0 &= \|p\|^2 - 1 \\ F &= C^T \Gamma + 2C^T \dot{\Gamma} \\ M &= C^K K + 2C^K \dot{K} \end{cases}} \quad (42)$$

In (40), (41), (42) the balance of (material) *linear momentum* equation – the first each – is completely identical to the corresponding one in the frame description (39). The second relations each represent the balance of (material) *angular momentum* equation and correspond to the second relation in the frame description (39). They describe the *tangential acceleration* of the quaternion field p . The *normal acceleration* of the quaternion field $\langle p, \ddot{p} \rangle = -\|\dot{p}\|^2$ can be obtained by differentiation of the unity constraint $\|p\|^2 = 1$ twice w. r. t. time.

Proposition 2.6 (Equivalence of descriptions) *Let $R = R \circ p$ with p from (4) and R from (5). Then the Euclidean descriptions (38), (39) and the quaternion description (40) are equivalent.*

Proof: Since $RF = pF\bar{p}$ according to (9), there is nothing left to prove for the balance of linear momentum. For the balance of angular momentum, we carry out the derivative w.r.t. s at the right hand side of (39), multiply with R^T from the left and use the identity $R^T(v \times w) = R^T v \times R^T w$ for $v, w \in \Im(\mathbb{H}) = \mathbb{R}^3$. We then obtain

$$\begin{aligned} \varrho(I\dot{\Omega} + \Omega \times I\Omega) &= R^T[(\partial_s R)M + R\partial_s M + (\partial_s x) \times (RF) + R\hat{M}] \\ &= R^T(\partial_s R)M + \partial_s M + (R^T \partial_s x) \times F + \hat{M}. \end{aligned} \quad (43)$$

Using (9) and the frame differential equation (33), we find that the right hand side of (43) is equal to

$$\begin{aligned} K \times M + \partial_s M + \bar{p}(\partial_s x)p \times F + \hat{M} &= KM + \langle K, M \rangle + \partial_s M + \bar{p}(\partial_s x)pF + \langle \bar{p}(\partial_s x)p, F \rangle + \hat{M} \\ &= 2\bar{p}(\partial_s p)M + \partial_s M + \bar{p}(\partial_s x)pF + \hat{M} + \eta_r, \end{aligned}$$

where (57) for the quaternion product of two purely imaginary quaternions has been applied and $\eta_r = \langle K, M \rangle + \langle \bar{p}(\partial_s x)p, F \rangle$ collects purely real summands of the right hand side. From (24) it follows that

$$\frac{1}{2}\dot{\Omega} = \bar{p}\ddot{p} + \|\dot{p}\|^2, \quad (44)$$

so that we can conclude – according to the closed form expression for the quaternion mass matrix (27) – that

$$I\dot{\Omega} = 2I\bar{p}\ddot{p} = \frac{1}{2}\bar{p}\mu(p)\ddot{p}.$$

The real quantity $\|\dot{p}\|^2$ is annihilated by the quaternion inertia tensor I , which carries a zero at its ‘real’ position, see (26). Similarly,

$$\Omega \times I\Omega = \Omega(I\Omega) + \langle \Omega, I\Omega \rangle = 4\bar{p}\dot{p}I\bar{p}\dot{p} + \eta_l = -4\bar{p}\dot{p}I\bar{p}\dot{p} + \eta_l,$$

since $\langle p, \dot{p} \rangle = \Re(\bar{p}\dot{p}) = 0$, where as well $\eta_l = \langle \Omega, I\Omega \rangle$ collects purely real summands. Thus, left-multiplication of (43) with $2p$ yields

$$\begin{aligned} \varrho(\mu(p)\ddot{p} - 8\dot{p}I\bar{p}\dot{p} + 2\eta_l p) &= \varrho(4pI\bar{p}\ddot{p} - 8\dot{p}I\bar{p}\dot{p} + 2\eta_l p) \\ &= 4(\partial_s p)M + 2p\partial_s M + 2(\partial_s x)pF + 2p\hat{M} + 2\eta_r p \\ &= 2(\partial_s p)M + 2\partial_s(pM) + 2(\partial_s x)pF + 2p\hat{M} + 2\eta_r p. \end{aligned} \quad (45)$$

Now left-multiplication with the tangential inverse mass $\mu(p)^{-1}$ and $p \in \ker \mu(p)^{-1}$, together with property (31), yields

$$\varrho(\mathcal{I} - p \otimes p)\ddot{p} = \mu(p)^{-1}(8\varrho\dot{p}I\bar{p}\dot{p} + 2(\partial_s p)M + 2\partial_s(pM) + 2(\partial_s x)pF + 2p\hat{M}).$$

With $(p \otimes p)\ddot{p} = \langle p, \ddot{p} \rangle p$, the assertion (40) finally follows. It remains to show that the converse is also true. Left multiplication of (40) with $\mu(p)^{-1}$ yields

$$\varrho\mu(p)\ddot{p} = q - \langle p, q \rangle p, \quad q = 8\varrho\dot{p}I\bar{p}\dot{p} + 4(\partial_s p)M + 2p\partial_s M + 2(\partial_s x)pF + 2p\hat{M}$$

because of $p \in \ker \mu(p)$ and (31). Left-multiplication with $\bar{p}/2$ yields

$$\begin{aligned} \varrho(I\dot{\Omega} + \Omega \times I\Omega - \langle \Omega, I\Omega \rangle) &= \frac{\varrho}{2}\bar{p}\mu(p)\ddot{p} = \frac{1}{2}\bar{p}q - \frac{1}{2}\langle p, q \rangle \\ &= 2\bar{p}(\partial_s p)M + \partial_s M + \bar{p}(\partial_s x)pF + \hat{M} + \eta, \end{aligned}$$

where $\eta = -\langle K, M \rangle - \langle \bar{p}(\partial_s x)p, F \rangle + \langle p, q \rangle/2$ again collects purely real summands. Taking the imaginary part $\Im(\cdot)$ on both sides and computing backwards as in the first part of the proof gives the final result (39). Thus the desired equivalence is proven. $\blacksquare$

3 Main theorems

In this section, we present the main theorems of this paper, where we derive the balance of linear and angular momentum relations for the Cosserat rod from the stationarity of two dimensional action functionals.

Like in standard classical Lagrangian rigid body mechanics [11], where the stationarity $\delta \int \mathcal{L} dt = 0$ with a Lagrangian that only depends on q , $\dot{q}$, λ and t , leads to ordinary differential algebraic equations in t for the rigid bodies, here the stationarity $\delta \iint \mathcal{L} ds dt = 0$ with a Lagrangian that depends on q , q' , $\dot{q}$, λ and t , leads to partial differential algebraic equations in space s and time t for the translatory and rotatory unknowns x and p . These are equivalent to the balance of linear and angular momentum equations (41) in the elastic case resp. (42) in the viscoelastic case.

For notational simplicity, we assume that no external force densities $\hat{F}$ and no external moment densities $\hat{M}$ are present.

Theorem 3.1 (Derivation from Lagrange field theory, Elastic case)

With the Lagrangian $\mathcal{L} = \mathcal{T} - \mathcal{V} - g^T \lambda$, where the potential energy density $\mathcal{V}$ from (13), the kinetic energy density $\mathcal{T}$ from (23) and the constraint density $g = g(p) = (\|p\|^2 - 1)/2$, the two dimensional (s, t) -variational principle

$$\delta \int_0^T \int_0^L \mathcal{L} ds dt = 0$$

yields

$$\left\{ \begin{array}{l} \varrho A \ddot{x} = \partial_s(pF\bar{p}) \\ \varrho \mu(p)\ddot{p} + \lambda p = 2x'pF + \partial_s(2pM) + 2p'M + \varrho \left[\frac{1}{2} \partial_p(\dot{p}^T \mu(p)\dot{p}) - \partial_p(\mu(p)\dot{p})\dot{p} \right] \\ 0 = \|p\|^2 - 1 \end{array} \right. , \quad (46)$$

where the forces and moments are

$$F = F^\Gamma = C^\Gamma \Gamma, \quad M = M^K = C^K K. \quad (47)$$

Proof: We apply the two dimensional variational calculus in the variables s and t from appendix B with

$$q = (x, p), \quad q' = (x', p') = (\partial_s x, \partial_s p), \quad \dot{q} = (\dot{x}, \dot{p}) = (\partial_t x, \partial_t p)$$

and $(s, t) \in U$. Here U denotes the rectangular space-time domain $U = [0, L] \times [0, T] \subset \mathbb{R}^2$. It holds that $\mathcal{V}_{SE} = \mathcal{V}_{SE}(p, x')$ due to (14), $\mathcal{V}_{BT} = \mathcal{V}_{BT}(p, p')$ due to (16) and $\mathcal{T}_T = \mathcal{T}_T(\dot{x})$, $\mathcal{T}_R = \mathcal{T}_R(p, \dot{p})$ due to (23). Thus

$$\mathcal{L} = \mathcal{L}(p, x', p', \dot{x}, \dot{p}, \lambda), \quad \mathcal{V} = \mathcal{V}(p, x', p'), \quad \mathcal{T} = \mathcal{T}(p, \dot{x}, \dot{p}), \quad g = g(p).$$

We have to compute the partial derivatives of the strain measures w. r. t. the generalised coordinates,

$$\frac{\partial \Gamma}{\partial x'} = R(p)^T, \quad \frac{\partial \Gamma}{\partial p} = -2x'p, \quad \frac{\partial K}{\partial p'} = 2\mathcal{Q}(p)^T, \quad \frac{\partial K}{\partial p} = 2\hat{\mathcal{Q}}(p')C, \quad (48)$$

where the quaternion identity (65) is helpful. Here $C = \text{diag}(1; -1, -1, -1)$ denotes the ‘conjugator’. With the calculus rule $\partial_q(v^T A v)/2 = (\partial v/\partial q)^T A v$ for constant symmetric matrices A and vectors $v = v(q)$, we derive

$$\frac{\partial \mathcal{V}_{SE}}{\partial x'} = p(C^\Gamma \Gamma)\bar{p}, \quad \frac{\partial \mathcal{V}_{SE}}{\partial p} = -2x'pC^\Gamma \Gamma, \quad \frac{\partial \mathcal{V}_{BT}}{\partial p'} = 2pC^K K, \quad \frac{\partial \mathcal{V}_{BT}}{\partial p} = -2p'C^K K. \quad (49)$$

Here the quaternion matrices $\mathcal{Q}$, $\hat{\mathcal{Q}}$ and $\mathcal{F}$ of section A are helpful. The remaining partial derivatives of the potential energy densities $\mathcal{V}$ vanish. Further for the kinetic energies $\mathcal{T}$, we find

$$\frac{d}{dt} \left(\frac{\partial \mathcal{T}}{\partial \dot{x}} \right) = \varrho A \ddot{x}, \quad \frac{d}{dp} \left(\frac{\partial \mathcal{T}}{\partial \dot{p}} \right) = \varrho \mu(p)\ddot{p} + \varrho \frac{\partial}{\partial p} (\mu(p)\dot{p})\dot{p}, \quad \frac{\partial \mathcal{T}}{\partial p} = \frac{\varrho}{2} \frac{\partial}{\partial p} (\dot{p}^T \mu(p)\dot{p}).$$

So, plugging things together, the Euler-Lagrange equations (71) and (72) yield the assertion (46) and (47). $\blacksquare$

By left-multiplication of the quaternion differential equation in (46) with $\mu(p)^{-1}$ the constraint force λp is eliminated, and together with (31) and (29) as in the proof of proposition 2.6, it is shown that (46) with (47) is equivalent to (41). The Lagrange multiplier λ can be computed by left-multiplication of (46) with p^T , the fact that $p^T \mu(p) = (\mu(p)^T p)^T = (\mu(p)p)^T = 0$ and $p^T p = \langle p, p \rangle = \|p\|^2 = 1$. It turns out that $\lambda = 2\langle \Omega, I\Omega \rangle = 4\mathcal{T}_R$, cf. as well [21].

An alternative way to solve (46) for $\ddot{p}$ and λ is close to the *index reduction* method [19] in modern Multibody Dynamics. The constraint for the quaternion field on *position level* is $g(p) = (\|p\|^2 - 1)/2$. Taking the total partial derivative w. r. t. time yields the constraint on *velocity level* $G(p)\dot{p} = \langle p, \dot{p} \rangle = 0$, which expresses the fact that the quaternion velocity must always be tangential to $\mathbb{S}^3$. Here $G(p) = \partial g(p)/\partial p = p$ is the constraint gradient. Differentiating once more w. r. t. time yields the constraint on *acceleration level* $G(p)\ddot{p} = \langle p, \ddot{p} \rangle = -\|\dot{p}\|^2$, which exactly yields the radial acceleration that is necessary to keep the quaternion on its spherical orbit. Thus, from the analytical – not at all from the numerical! – point of view, the last couple in (46) can be equivalently rewritten as

$$\left(\begin{array}{c|c} \frac{\partial \mu(p)}{\partial p^T} & p \\ \hline & 0 \end{array} \right) \begin{pmatrix} \ddot{p} \\ \lambda \end{pmatrix} = \begin{pmatrix} \ddots \\ -\|\dot{p}\|^2 \end{pmatrix}, \quad (50)$$

if the position constraint is replaced by the acceleration constraint. Now the 5×5 mass-constraint matrix at the left-hand side in (50) is regular, has full rank and its inverse can be explicitly calculated as

$$\left(\begin{array}{c|c} \frac{\partial \mu(p)}{\partial p^T} & p \\ \hline & 0 \end{array} \right)^{-1} = \left(\begin{array}{c|c} \frac{1}{\partial} \mu(p)^{-1} & p \\ \hline & 0 \end{array} \right). \quad (51)$$

The equivalence of (46), (47) with (41) can thus be proved with (51) and the acceleration constraint $\langle p, \ddot{p} \rangle = -\|\dot{p}\|^2$ in an alternative fashion.

Theorem 3.2 (Derivation from Lagrange field theory, Viscoelastic case)

With the Lagrangian $\mathcal{L} = \mathcal{T} - \mathcal{V} - g^T \lambda$, where the potential energy density $\mathcal{V}$ from (13), the kinetic energy density $\mathcal{T}$ from (23) and the constraint density $g = g(p) = (\|p\|^2 - 1)/2$, the two dimensional (s, t) -variational principle

$$\delta \int_0^T \int_0^L \mathcal{L} \, ds \, dt - \int_0^T \int_0^L \frac{\partial \mathcal{D}}{\partial \dot{q}} \delta q \, ds \, dt - \int_0^T \int_0^L \frac{\partial \mathcal{D}}{\partial \dot{q}'} \delta q' \, ds \, dt = 0$$

with the dissipation energy density $\mathcal{D}$ from (19), yields (46) where the forces and moments are given by

$$F = C^\Gamma \Gamma + 2C^{\dot{\Gamma}} \dot{\Gamma}, \quad M = C^K K + 2C^{\dot{K}} \dot{K}. \quad (52)$$

Proof: Again, we apply the results of appendix B. From $\Gamma = \Gamma(p, x')$ in (15) and $K = K(p, p')$ in (17), we conclude with the chain rule that

$$\dot{\Gamma} = \frac{\partial \Gamma}{\partial p} \dot{p} + \frac{\partial \Gamma}{\partial x'} \dot{x}', \quad \dot{K} = \frac{\partial K}{\partial p} \dot{p} + \frac{\partial K}{\partial p'} \dot{p}',$$

so that – note that the strain and curvature gradients do not depend on $\dot{x}$, $\dot{x}'$, $\dot{p}$, $\dot{p}'$ – we have the following ‘truncation rule’ for the dot $\dot{}$, namely

$$\frac{\partial \dot{\Gamma}}{\partial \dot{p}} = \frac{\partial \Gamma}{\partial p}, \quad \frac{\partial \dot{\Gamma}}{\partial \dot{x}'} = \frac{\partial \Gamma}{\partial x'}, \quad \frac{\partial \dot{K}}{\partial \dot{p}} = \frac{\partial K}{\partial p}, \quad \frac{\partial \dot{K}}{\partial \dot{p}'} = \frac{\partial K}{\partial p'}.$$

The right hand side gradients therein are already known from (48). By the way: This is a special case of a very general feature of any strain measures, derived from some generalised coordinates,

see remark 3.3 below. So we obtain – completely analogously to (49) –

$$\frac{1}{2} \frac{\partial \mathcal{D}_{SE}}{\partial \dot{x}'} = p(C^{\dot{\Gamma}} \dot{\Gamma}) \bar{p}, \quad \frac{1}{2} \frac{\partial \mathcal{D}_{SE}}{\partial \dot{p}} = -2x' p C^{\dot{\Gamma}} \dot{\Gamma}, \quad \frac{1}{2} \frac{\partial \mathcal{D}_{BT}}{\partial \dot{p}'} = 2p C^{\dot{K}} \dot{K}, \quad \frac{1}{2} \frac{\partial \mathcal{D}_{BT}}{\partial \dot{p}} = -2p' C^{\dot{K}} \dot{K}.$$

Finally, plugging all the pieces together, the Euler-Lagrange equations (74) and (72) yield the assertion (46) with (52). $\blacksquare$

As above for the elastic case, it can be shown that system (46) with the viscoelastic forces and moments (52) is equivalent to (42).

Remark 3.3 (A truncation rule) We end with a general remark on strain measures, potential and dissipation energy densities. Let some strain measure components ξ_n be given by *any* smooth enough — linear or nonlinear — mappings

$$\xi_n = \phi_n(q, q', t). \quad (53)$$

For the Cosserat rod model, these ξ_n are the strain components Γ_ν or the curvature components K_ν , $n = \nu$, with the nonlinear transformations (15) resp. (17). Taking the time derivative, we find with the chain rule

$$\dot{\xi}_n = \sum_k \frac{\partial \phi_n}{\partial q_k}(q, q', t) \dot{q}_k + \sum_k \frac{\partial \phi_n}{\partial q'_k}(q, q', t) \dot{q}'_k + \frac{\partial \phi_n}{\partial t}(q, q', t),$$

from which the ‘dot truncation’ rule

$$\frac{\partial \dot{\xi}_n}{\partial \dot{q}_\kappa} = \frac{\partial \phi_n}{\partial q_\kappa} = \frac{\partial \xi_n}{\partial q_\kappa}, \quad \frac{\partial \dot{\xi}_n}{\partial \dot{q}'_\kappa} = \frac{\partial \phi_n}{\partial q'_\kappa} = \frac{\partial \xi_n}{\partial q'_\kappa} \quad (54)$$

follows. The reader should note that this rule holds without any restrictions on the mappings ϕ_n in (53). It is a very convenient tool for a general framework in Multibody Dynamics to derive the forces, Jacobians and Hessians corresponding to a convex potential (in the strain measures) and a consistent convex dissipation potential (in the strain measure rates). See as well [17, 18] for the quadratic case. $\square$

A Hamilton quaternion algebra

Hamilton’s quaternion algebra, which we denote by $\mathbb{H} = \mathfrak{R}(\mathbb{H}) \oplus \mathfrak{I}(\mathbb{H})$, is a real division algebra, a skew field and a vector space, the latter isomorphic to $\mathbb{R}^4 = \mathbb{R} \oplus \mathbb{R}^3$. For details, have a look into the ‘book of numbers’ [10]. We write down a quaternion $p \in \mathbb{H}$ as

$$p = \mathfrak{R}(p) + \mathfrak{I}(p) = p_0 + \hat{p} = (p_0; p_1, p_2, p_3)^T = p_0 + p_1 i + p_2 j + p_3 k,$$

where the imaginary units, classically denoted by $i \simeq e^1$, $j \simeq e^2$, $k \simeq e^3$, satisfying

$$i^2 = -1, \quad j^2 = -1, \quad k^2 = -1, \quad ij = k, \quad jk = i, \quad ki = j, \quad (55)$$

build up the basis of the imaginary space $\mathfrak{I}(\mathbb{H}) = \mathbb{R}^3$. Clearly, $1 \simeq e^0$ is the basis of the real line $\mathfrak{R}(\mathbb{H}) = \mathbb{R}$. The three components of the imaginary part of p are conveniently denoted by $p_1 = \mathfrak{I}_1(p)$, $p_2 = \mathfrak{I}_2(p)$ and $p_3 = \mathfrak{I}_3(p)$ as well. For two quaternions $p, q \in \mathbb{H}$, the product $pq \in \mathbb{H}$ is defined by – or follows from the basic definitions (55) –

$$pq = p_0 q_0 - \langle \hat{p}, \hat{q} \rangle + p_0 \hat{q} + q_0 \hat{p} + \hat{p} \times \hat{q} \quad (p, q \in \mathbb{H}). \quad (56)$$

In single components, this is

$$\mathfrak{R}(pq) = p_0 q_0 - \langle \hat{p}, \hat{q} \rangle = p_0 q_0 - p_1 q_1 - p_2 q_2 - p_3 q_3$$

and

$$\Im(pq) = p_0\hat{q} + q_0\hat{p} + \hat{p} \times \hat{q} = p_0 \begin{pmatrix} q_1 \\ q_2 \\ q_3 \end{pmatrix} + q_0 \begin{pmatrix} p_1 \\ p_2 \\ p_3 \end{pmatrix} + \begin{pmatrix} p_2q_3 - p_3q_2 \\ p_3q_1 - p_1q_3 \\ p_1q_2 - p_2q_1 \end{pmatrix}.$$

Here $\langle \cdot, \cdot \rangle$ is the inner (scalar), $\times$ is the outer (cross) product in $\Im(\mathbb{H}) = \mathbb{R}^3$. It is convenient to denote the imaginary (= vector) part of a quaternion q by the hat symbol $\hat{q} = \Im(q)$. We point out the special case of (56), where for two purely imaginary quaternions (= vectors) $\hat{p}$ and $\hat{q}$

$$\hat{p}\hat{q} = -\langle \hat{p}, \hat{q} \rangle + \hat{p} \times \hat{q} \quad (\hat{p}, \hat{q} \in \mathbb{H}). \quad (57)$$

For a quaternion $p = p_0 + \hat{p} = (p_0; p_1, p_2, p_3) \in \mathbb{H}$, the conjugate $\bar{p}$ is given by $\bar{p} = p_0 - \hat{p} = (p_0; -p_1, -p_2, -p_3)^T$, the Euclidean norm $\|p\|$ by $\|p\| = \sqrt{p\bar{p}} = \sqrt{\bar{p}p} = \sqrt{\langle p, p \rangle}$, the multiplicative inverse p^{-1} by $p^{-1} = \bar{p}/\|p\|^2$. Conjugation obviously satisfies $\overline{pq} = \bar{q}\bar{p}$ for $p, q \in \mathbb{H}$.

For the special purposes of this paper, the following identities are useful, especially for the Cosserat material curvature K or the Cosserat material angular velocity Ω ,

$$\bar{p}q = p_0q_0 + \langle \hat{p}, \hat{q} \rangle + p_0\hat{q} - q_0\hat{p} - \hat{p} \times \hat{q} \quad (p, q \in \mathbb{H}). \quad (58)$$

In components, these identities are written

$$\Re(\bar{p}q) = p_0q_0 + \langle \hat{p}, \hat{q} \rangle = \langle p, q \rangle = p_0q_0 + p_1q_1 + p_2q_2 + p_3q_3 \quad (59)$$

and

$$\Im(\bar{p}q) = p_0\hat{q} - q_0\hat{p} - \hat{p} \times \hat{q} = p_0 \begin{pmatrix} q_1 \\ q_2 \\ q_3 \end{pmatrix} - q_0 \begin{pmatrix} p_1 \\ p_2 \\ p_3 \end{pmatrix} - \begin{pmatrix} p_2q_3 - p_3q_2 \\ p_3q_1 - p_1q_3 \\ p_1q_2 - p_2q_1 \end{pmatrix}. \quad (60)$$

Similar relations hold for $p\bar{q}$ and $\Im(p\bar{q})$. We have $\Re(p\bar{q}) = \Re(p\bar{q}) = \langle p, q \rangle$. For two quaternions $p, q \in \mathbb{H}$, it holds that

$$\mathcal{F}(p) = \frac{\partial}{\partial q} \Im(\bar{p}q), \quad \mathcal{F}(q) = -\frac{\partial}{\partial p} \Im(\bar{p}q) \quad (61)$$

with the fundamental matrix

$$\mathcal{F}(p) = \left(\begin{array}{c|ccc} -p_1 & p_0 & p_3 & -p_2 \\ -p_2 & -p_3 & p_0 & p_1 \\ -p_3 & p_2 & -p_1 & p_0 \end{array} \right) = \left(\begin{array}{c|c} -\hat{p} & p_0\mathcal{I} - \mathcal{E}(\hat{p}) \end{array} \right) \quad (62)$$

for $p \in \mathbb{H}$. The ‘quaternion matrix’, see [13, 21] for example,

$$\mathcal{Q}(p) = \left(\begin{array}{c|ccc} p_0 & -p_1 & -p_2 & -p_3 \\ p_1 & p_0 & -p_3 & p_2 \\ p_2 & p_3 & p_0 & -p_1 \\ p_3 & -p_2 & p_1 & p_0 \end{array} \right) = \left(\begin{array}{c|c} p_0 & -\hat{p} \\ \hat{p} & p_0\mathcal{I} + \mathcal{E}(\hat{p}) \end{array} \right) = (p \mid \mathcal{F}(p)^T), \quad (63)$$

which satisfies $\mathcal{Q}(p)\mathcal{Q}(p)^T = \mathcal{Q}^T(p)\mathcal{Q}(p) = \|p\|^2 I$, allows to express left-multiplication with p in $\mathbb{H}$ as left multiplication with $\mathcal{Q}(p)$. Left-multiplication with the conjugate $\bar{q}$ is nothing else but left-multiplication with the transpose $\mathcal{Q}(p)^T$. Likewise,

$$\hat{\mathcal{Q}}(p) = \left(\begin{array}{c|ccc} p_0 & -p_1 & -p_2 & -p_3 \\ p_1 & p_0 & p_3 & -p_2 \\ p_2 & -p_3 & p_0 & p_1 \\ p_3 & p_2 & -p_1 & p_0 \end{array} \right) = \left(\begin{array}{c|c} p_0 & -\hat{p} \\ \hat{p} & p_0\mathcal{I} - \mathcal{E}(\hat{p}) \end{array} \right) \quad (64)$$

makes right-multiplication with p in matrix-vector notation easily possible. Summarising, this means

$$pq = \mathcal{Q}(p)q, \quad \bar{p}q = \mathcal{Q}(p)^T q, \quad pq = \hat{\mathcal{Q}}(q)p, \quad p\bar{q} = \hat{\mathcal{Q}}(q)^T p$$

for all $p, q \in \mathbb{H}$. It clearly holds $\mathcal{Q}(p)\hat{\mathcal{Q}}(p)^T = \hat{\mathcal{Q}}(p)^T\mathcal{Q}(p) = \text{diag}(1, R(p))$ because of (9). Likewise, left-multiplication pv for purely imaginary quaternions (= vectors) v can be expressed as $pv = \mathcal{F}(p)^T v$. We further note the useful identity

$$\frac{1}{2} \left(\left(\frac{\partial d^1}{\partial p} \right)^T v \mid \left(\frac{\partial d^2}{\partial p} \right)^T v \mid \left(\frac{\partial d^3}{\partial p} \right)^T v \right) f = -vpf \quad (p \in \mathbb{H}, v, f \in \mathfrak{S}(\mathbb{H})) \quad (65)$$

for purely imaginary quaternions (= vectors) v and f . The 3×4 matrices $\partial_p d^\nu(p)$ are the fundamental Jacobians (34), (35) of the directors $d^\nu(p)$ in (6) and (7).

The reader should always note that we use the langles $\langle \cdot, \cdot \rangle$ for both the scalar products in $\mathfrak{S}(\mathbb{H}) = \mathbb{R}^3$ and $\mathbb{H} = \mathbb{R}^4$, depending on the context. This means

$$\langle v, w \rangle = \sum_{\nu=1,2,3} v_\nu w_\nu, \quad \langle p, q \rangle = \sum_{\nu=0,1,2,3} p_\nu q_\nu, \quad \langle \hat{p}, \hat{q} \rangle = \sum_{\nu=1,2,3} p_\nu q_\nu$$

for quaternions $p, q \in \mathbb{H}$ and purely imaginary quaternions (= vectors) $v, w, \hat{p}, \hat{q} \in \mathfrak{S}(\mathbb{H}) = \mathbb{R}^3$. For $p, q \in \mathbb{H}$, the dyadic product is defined by $p \otimes q = pq^T$, in components $(p \otimes q)_{\mu\nu} = p_\mu q_\nu$ for $\mu, \nu = 0, \dots, 3$.

B Lagrange field theory in two dimensions

In this section, we recapitulate the main results from classical Lagrange field theory and variational calculus in two dimensions for arbitrary many unknown functions. The first dimension is the ‘space’ s , the second one is the ‘time’ t . To this end, we combine the ideas of sections 2 and 4 of [8], chapter IV, §3.

Let N denote a natural number, $U \subset \mathbb{R}^2$ a domain with sufficiently smooth boundary ∂U , e.g. piecewise continuously differentiable. Let further a *Lagrange density*

$$\mathcal{L} : U \times \mathbb{R} \times \mathbb{R}^N \times \mathbb{R}^N \times \mathbb{R}^N \rightarrow \mathbb{R}, \quad ((s, t), \lambda, q, q', \dot{q}) \mapsto \mathcal{L}((s, t), \lambda, q, q', \dot{q}) \quad (66)$$

be given. For example, $\mathcal{L}$ may be of the form

$$\mathcal{L}((s, t), \lambda, q, q', \dot{q}) = \mathcal{T}((s, t), q, \dot{q}) - \mathcal{V}((s, t), q, q') - g((s, t), q)^T \lambda \quad (67)$$

with a *potential energy density* $\mathcal{V} : U \times \mathbb{R}^N \times \mathbb{R}^N \rightarrow \mathbb{R}$, a *kinetic energy density* $\mathcal{T} : U \times \mathbb{R}^N \times \mathbb{R}^N \rightarrow \mathbb{R}$ and a *constraint density* $g : U \times \mathbb{R}^N \rightarrow \mathbb{R}$. We consider the *action functional*

$$\mathcal{S}[\lambda, q] = \iint_U \mathcal{L}((s, t), \lambda(s, t), q(s, t), q'(s, t), \dot{q}(s, t)) \, d(s, t)$$

for twice continuously differentiable functions $q : U \rightarrow \mathbb{R}^N$ and continuous functions $\lambda : U \rightarrow \mathbb{R}$. As usual, ∂_s is denoted by a dash ' and ∂_t is denoted by a dot '. We look for a critical point (λ, q) of $\mathcal{S}$, which makes the functional $\mathcal{S}$ stationary,

$$\delta \mathcal{S} = \delta \iint_U \mathcal{L}((s, t), \lambda, q, q', \dot{q}) \, d(s, t) = 0 \quad (68)$$

among all smooth enough variations $(\delta \lambda, \delta q)$ that are vanishing on the boundary ∂U . Then necessarily all the directional derivatives

$$\left. \frac{\partial}{\partial \epsilon_n} \Phi(\epsilon_0, \dots, \epsilon_N) \right|_{\epsilon=0}$$

where

$$\Phi(\epsilon_0, \dots, \epsilon_N) = \mathcal{S}[\lambda^\epsilon, q_1^\epsilon, \dots, q_N^\epsilon], \quad \lambda^\epsilon = \lambda + \epsilon_0 \delta \lambda, \quad q_n^\epsilon = q + \epsilon_n \delta q_n$$

for each $n = 0, \dots, N$ and each such admissible variation $(\delta\lambda, \delta q)$ must vanish. For $n = 1, \dots, N$, differentiation under the integral yields

$$\begin{aligned} \frac{\partial}{\partial \epsilon_n} \Phi(\epsilon) &= \iint_U \frac{\partial}{\partial \epsilon_n} \left\{ \mathcal{L}((s, t), \lambda^\epsilon, q_1^\epsilon, \dots, q_N^\epsilon, \partial_s q_1^\epsilon, \dots, \partial_s q_N^\epsilon, \partial_t q_1^\epsilon, \dots, \partial_t q_N^\epsilon) \right\} d(s, t) \\ &= \iint_U \left\{ \frac{\partial \mathcal{L}}{\partial q_n}((s, t), \lambda^\epsilon, q_\nu^\epsilon, \partial_s q_\nu^\epsilon, \partial_t q_\nu^\epsilon) \delta q_n + \frac{\partial \mathcal{L}}{\partial q'_n}((s, t), \lambda^\epsilon, q_\nu^\epsilon, \partial_s q_\nu^\epsilon, \partial_t q_\nu^\epsilon) \delta q'_n \right. \\ &\quad \left. + \frac{\partial \mathcal{L}}{\partial \dot{q}_n}((s, t), \lambda^\epsilon, q_\nu^\epsilon, \partial_s q_\nu^\epsilon, \partial_t q_\nu^\epsilon) \delta \dot{q}_n \right\} d(s, t), \end{aligned}$$

where the chain rule has been applied. Letting $\epsilon = 0$, i.e. $\lambda^0 = \lambda$, $q_\nu^0 = q_\nu$, and integration by parts yields

$$\begin{aligned} \left. \frac{\partial}{\partial \epsilon_n} \Phi(\epsilon) \right|_{\epsilon=0} &= \iint_U \left\{ \frac{\partial \mathcal{L}}{\partial q_n}((s, t), \lambda, q_\nu, q'_\nu, \dot{q}_\nu) \delta q_n + \frac{\partial \mathcal{L}}{\partial q'_n}((s, t), \lambda, q_\nu, q'_\nu, \dot{q}_\nu) \delta q'_n \right. \\ &\quad \left. + \frac{\partial \mathcal{L}}{\partial \dot{q}_n}((s, t), \lambda, q_\nu, q'_\nu, \dot{q}_\nu) \delta \dot{q}_n \right\} d(s, t) \\ &= \iint_U \frac{\partial \mathcal{L}}{\partial q_n} \delta q_n d(s, t) + \int_{\partial U} \delta q_n \left\{ \frac{\partial \mathcal{L}}{\partial \dot{q}_n} dt - \frac{\partial \mathcal{L}}{\partial q'_n} ds \right\} \\ &\quad - \iint_U \delta q_n \left\{ \frac{\partial}{\partial s} \left(\frac{\partial \mathcal{L}}{\partial q'_n} \right) + \frac{\partial}{\partial t} \left(\frac{\partial \mathcal{L}}{\partial \dot{q}_n} \right) \right\} d(s, t) \\ &= \iint_U \delta q_n \left\{ \frac{\partial \mathcal{L}}{\partial q_n} - \frac{\partial}{\partial s} \left(\frac{\partial \mathcal{L}}{\partial q'_n} \right) - \frac{\partial}{\partial t} \left(\frac{\partial \mathcal{L}}{\partial \dot{q}_n} \right) \right\} d(s, t). \end{aligned}$$

The boundary line integral vanishes, as $\delta q_n = 0$ on ∂U . So, as the variations δq_n are arbitrary, with the aid of the *fundamental lemma of variational calculus*, the Euler-Lagrange equations

$$\frac{\partial}{\partial t} \left(\frac{\partial \mathcal{L}}{\partial \dot{q}} \right) = \frac{\partial \mathcal{L}}{\partial q} - \frac{\partial}{\partial s} \left(\frac{\partial \mathcal{L}}{\partial q'} \right) \quad (69)$$

follow component by component. For the special choice $\mathcal{L} = \mathcal{T} - \mathcal{V} - g^T \lambda$ from (67) of the Lagrangian function, the corresponding equations (69) become

$$\frac{\partial}{\partial t} \left(\frac{\partial \mathcal{T}}{\partial \dot{q}} \right) = \frac{\partial \mathcal{T}}{\partial q} - \frac{\partial \mathcal{V}}{\partial q} + \frac{\partial}{\partial s} \left(\frac{\partial \mathcal{V}}{\partial q'} \right) - \mathcal{G}^T \lambda, \quad (70)$$

where $\mathcal{G} = \partial g / \partial q$ denotes the constraint gradient. If further the kinetic energy density function $\mathcal{T}$ is of the form

$$\mathcal{T} = \mathcal{T}((s, t), q, \dot{q}) = \frac{1}{2} \dot{q}^T \mathcal{M}(q) \dot{q} + f(s, t)$$

with state q dependent symmetric positively semidefinite mass density matrix $q \mapsto \mathcal{M}(q) \in \mathbb{R}^{N \times N}$, carrying out the partial derivative $\partial / \partial t$, the Euler-Lagrange equations (70) become

$$\boxed{\mathcal{M} \ddot{q} + \frac{\partial}{\partial q} (\mathcal{M} \dot{q}) \dot{q} - \frac{1}{2} \frac{\partial}{\partial q} (\dot{q}^T \mathcal{M} \dot{q}) = - \frac{\partial \mathcal{V}}{\partial q} + \frac{\partial}{\partial s} \left(\frac{\partial \mathcal{V}}{\partial q'} \right) - \mathcal{G}^T \lambda.} \quad (71)$$

In a similar fashion for $n = 0$, since the Lagrangian does not depend on λ' and $\dot{\lambda}$, i.e. $\partial \mathcal{L} / \partial \lambda' = \partial \mathcal{L} / \partial \dot{\lambda} = 0$, we find $\partial \mathcal{L} / \partial \lambda = 0$, which results in

$$\boxed{g((s, t), q) = 0,} \quad (72)$$

which is nothing but the constraint equation. This was the non-dissipative case. We now turn to the dissipative one. If – in addition to the Lagrangian (66) – a *dissipation density*

$$\mathcal{D} : U \times \mathbb{R}^N \times \mathbb{R}^N \times \mathbb{R}^N \times \mathbb{R}^N \rightarrow \mathbb{R}, \quad ((s, t), q, q', \dot{q}, \dot{q}') \mapsto \mathcal{D}((s, t), q, q', \dot{q}, \dot{q}')$$

is given, then the variational principle

$$\delta \iint_U \mathcal{L} \, d(s, t) - \iint_U \frac{\partial \mathcal{D}}{\partial \dot{q}} \delta q \, d(s, t) - \iint_U \frac{\partial \mathcal{D}}{\partial \dot{q}'} \delta q' \, d(s, t) = 0 \quad (73)$$

yields the Euler-Lagrange equations

$$\mathcal{M}\ddot{q} + \frac{\partial}{\partial q}(\mathcal{M}\dot{q})\dot{q} - \frac{1}{2} \frac{\partial}{\partial q}(\dot{q}^T \mathcal{M}\dot{q}) = -\frac{\partial \mathcal{V}}{\partial q} - \frac{\partial \mathcal{D}}{\partial \dot{q}} + \frac{\partial}{\partial s} \left(\frac{\partial \mathcal{V}}{\partial q'} \right) + \frac{\partial}{\partial s} \left(\frac{\partial \mathcal{D}}{\partial \dot{q}'} \right) - g^T \lambda, \quad (74)$$

together with the constraint equation (72). This is proven in exactly the same way as above, where integration-by-parts is applied to the third integral in (73).

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