RESEARCH ARTICLE



Nonunit quaternion parametrization of a Petrov–Galerkin Cosserat rod finite element

Jonas Harsch 💿 | Simon R. Eugster 💿

Institute for Nonlinear Mechanics, University of Stuttgart, Stuttgart, Germany

Correspondence

Jonas Harsch, Institute for Nonlinear Mechanics, University of Stuttgart, D-70569 Stuttgart, Germany. Email: harsch@inm.uni-stuttgart.de

Abstract

The application of the Petrov–Galerkin projection method in Cosserat rod finite element formulations offers significant advantages in simplifying the expressions within the discrete virtual work functionals. Moreover, it enables a straight-forward and systematic exchange of the ansatz functions, specifically for centerline positions and cross-section orientations. In this concise communication, we present a total Lagrangian finite element formulation for Cosserat rods that attempts to minimize the number of required theoretical concepts. The chosen discretization preserves objectivity and allows for large displacements/rotations and for large strains. The orientation parametrization with nonunit quaternions results in a singularity-free formulation.

1 | INTRODUCTION

This article complements the two papers [1, 2] on Petrov–Galerkin rod finite element formulations for Cosserat rods. The cross-section orientations are parameterized using nonunit quaternions instead of total rotation vectors, which for dynamics require additionally the concept of the complement rotation vector for a singularity-free parametrization. To keep the formulation as simple as possible, we opt for the \mathbb{R}^{12} -interpolation for the ansatz functions, see Refs. [2–4].

The paper is structured as follows. In Section 2, the Cosserat rod theory is recapitulated very briefly; mainly to introduce all quantities required for the further finite element formulation. For those interested in additional comments as well as a thorough introduction and explanation of the chosen notation, we recommend reading Refs. [1, 2]. The Petrov–Galerkin finite element formulation in terms of nodal nonunit quaternions is presented in Section 3. The last section on numerical experiments investigates the static analysis of a helical spring in line with Marino [5]. Additionally, the Wilberforce example from Harsch et al. [6] with a helical spring with three coils is discussed.

2 | COSSERAT ROD THEORY

Let $\xi \in \mathcal{J} = [0, 1] \subset \mathbb{R}$ be the centerline parameter and let *t* denote time. The motion of a Cosserat rod is captured by a time-dependent centerline curve represented in an inertial *I*-basis $_{I}\mathbf{r}_{OP} = _{I}\mathbf{r}_{OP}(\xi, t) \in \mathbb{R}^{3}$ augmented by the crosssection orientations $\mathbf{A}_{IK} = \mathbf{A}_{IK}(\xi, t) \in SO(3) = \{\mathbf{A} \in \mathbb{R}^{3\times 3} | \mathbf{A}^{T}\mathbf{A} = \mathbf{1}_{3\times 3} \land \det(\mathbf{A}) = 1\}$. The subscripts *O* and *P* in the centerline curve refer to the origin and the centerline point, respectively. The cross-section orientation \mathbf{A}_{IK} can also be

© 2023 The Authors. Proceedings in Applied Mathematics & Mechanics published by Wiley-VCH GmbH.

This is an open access article under the terms of the Creative Commons Attribution License, which permits use, distribution and reproduction in any medium, provided the original work is properly cited.

The derivatives with respect to time *t* and centerline parameter ξ are denoted by (•) and (•), ξ , respectively. The variation of a function is indicated by $\delta(\bullet)$. With this, we can introduce the centerline velocity $_{I}\mathbf{v}_{P} = (_{I}\mathbf{r}_{OP})^{\circ}$ and the virtual displacement $_{I}\delta\mathbf{r}_{P} = \delta(_{I}\mathbf{r}_{OP})$. The angular velocity of the cross-section-fixed *K*-basis relative to the inertial *I*-basis, in components with respect to the *K*-basis, is defined by $_{K}\omega_{IK} := j^{-1}(\mathbf{A}_{IK}^{T}(\mathbf{A}_{IK}))$, where $j : \mathbb{R}^{3} \to \mathfrak{so}(3) = \{\mathbf{B} \in \mathbb{R}^{3\times 3} | \mathbf{B}^{T} = -\mathbf{B}\}$ is the linear and bijective map such that $\widetilde{\omega}\mathbf{r} = j(\omega)\mathbf{r} = \omega \times \mathbf{r}$ for all $\omega, \mathbf{r} \in \mathbb{R}^{3}$. Analogously, the virtual rotations and the scaled curvature are defined as $_{K}\delta\phi_{IK} := j^{-1}(\mathbf{A}_{IK}^{T}\delta(\mathbf{A}_{IK}))$ and $_{K}\bar{\mathbf{x}}_{IK} := j^{-1}(\mathbf{A}_{IK}^{T}(\mathbf{A}_{IK}),\xi)$, respectively. For the reference centerline curve $_{I}\mathbf{r}_{OP}^{0}$, the length of the rod's tangent vector is $J = \|_{I}\mathbf{r}_{OP}^{0},\xi\|$. Thus, for a given centerline parameter ξ , the reference arc length increment is $ds = Jd\xi$. The derivative with respect to the reference arc length *s* of a function $\mathbf{f} = \mathbf{f}(\xi, t) \in \mathbb{R}^{3}$ can then be defined as $\mathbf{f}_{s}(\xi, t) := \mathbf{f}_{\xi}(\xi, t)/J(\xi)$. The objective strain measures of a Cosserat rod are the curvature $_{K}\kappa_{IK} = _{K}\bar{\mathbf{x}}_{IK}/J$, which measures torsion and bending, together with the measures for dilatation and shear strains contained in $_{K}\gamma = _{K}\bar{\gamma}/J$ determined by $_{K}\bar{\gamma} := (\mathbf{A}_{IK})^{\Gamma}_{I}\mathbf{r}_{OP}\xi$.

The internal virtual work of a Cosserat rod is defined as

$$\delta W^{\text{int}} := -\int_{\mathcal{J}} \left\{ (_{I} \delta \mathbf{r}_{P,\xi})^{\mathrm{T}} \mathbf{A}_{IKK} \mathbf{n} + (_{K} \delta \boldsymbol{\phi}_{IK,\xi})^{\mathrm{T}} _{K} \mathbf{m} - (_{K} \delta \boldsymbol{\phi}_{IK})^{\mathrm{T}} [_{K} \bar{\boldsymbol{\gamma}} \times_{K} \mathbf{n} + _{K} \bar{\boldsymbol{\kappa}}_{IK} \times_{K} \mathbf{m}] \right\} \mathrm{d}\xi , \qquad (1)$$

where $_{K}\mathbf{n}$ and $_{K}\mathbf{m}$ denote the resultant contact forces and moments, respectively. For hyperelastic material models with a strain energy density with respect to the reference arc length $W = W(_{K}\boldsymbol{\gamma},_{K}\boldsymbol{\kappa}_{IK};\boldsymbol{\xi})$, they can be determined by the constitutive relations $_{K}\mathbf{n} = (\partial W/\partial_{K}\boldsymbol{\gamma})^{T}$ and $_{K}\mathbf{m} = (\partial W/\partial_{K}\boldsymbol{\kappa}_{IK})^{T}$.

Assume that the line distributed external forces $_{I}\mathbf{b} = _{I}\mathbf{b}(\xi, t) \in \mathbb{R}^{3}$ and moments $_{K}\mathbf{c} = _{K}\mathbf{c}(\xi, t) \in \mathbb{R}^{3}$ to be given as densities with respect to the reference arc length. Moreover, for $i \in \{0, 1\}$, point forces $_{I}\mathbf{b}_{i} = _{I}\mathbf{b}_{i}(t) \in \mathbb{R}^{3}$ and point moments $_{K}\mathbf{c}_{i} = _{K}\mathbf{c}_{i}(t) \in \mathbb{R}^{3}$ can be applied to the rod's boundaries at $\xi_{0} = 0$ and $\xi_{1} = 1$. The corresponding external virtual work functional is defined as

$$\delta W^{\text{ext}} := \int_{\mathcal{J}} \left\{ (_{I} \delta \mathbf{r}_{P})^{\mathrm{T}}{}_{I} \mathbf{b} + (_{K} \delta \boldsymbol{\phi}_{IK})^{\mathrm{T}}{}_{K} \mathbf{c} \right\} J \mathrm{d}\xi + \sum_{i=0}^{1} \left[(_{I} \delta \mathbf{r}_{P})^{\mathrm{T}}{}_{I} \mathbf{b}_{i} + (_{K} \delta \boldsymbol{\phi}_{IK})^{\mathrm{T}}{}_{K} \mathbf{c}_{i} \right]_{\xi_{i}}.$$
(2)

In case, ${}_{I}\mathbf{r}_{OP}$ is the line of centroids, the inertial virtual work functional of the Cosserat rod can be written as

$$\delta W^{\mathrm{dyn}} := -\int_{\mathcal{J}} \left\{ ({}_{I}\delta \mathbf{r}_{P})^{\mathrm{T}} A_{\rho_{0}} ({}_{I}\mathbf{v}_{P})^{\cdot} + ({}_{K}\delta \boldsymbol{\phi}_{IK})^{\mathrm{T}} ({}_{K}\mathbf{I}_{\rho_{0}} ({}_{K}\boldsymbol{\omega}_{IK})^{\cdot} + {}_{K}\boldsymbol{\omega}_{IK} \times {}_{K}\mathbf{I}_{\rho_{0}K}\boldsymbol{\omega}_{IK}) \right\} J \mathrm{d}\xi , \qquad (3)$$

where A_{ρ_0} is the cross-section mass density and ${}_{K}\mathbf{I}_{\rho_0}$ the constant cross-section inertia tensor represented in the cross-section-fixed *K*-basis.

3 | PETROV-GALERKIN FINITE ELEMENT FORMULATION

The rod's parameter space \mathcal{J} is divided into $n_{\rm el}$ linearly spaced element intervals $\mathcal{J}^e = [\xi^e, \xi^{e+1})$ via $\mathcal{J} = \bigcup_{\substack{e=0\\e=0}}^{n_{\rm el}-1} \mathcal{J}^e$. For a *p*th-order finite element, the closure of each of the intervals \mathcal{J}^e contains p + 1 evenly spaced points $\xi_i^e \in \operatorname{cl}(\mathcal{J}^e) = [\xi^e, \xi^{e+1}]$ with $i \in \{0, ..., p\}$ such that $\xi_0^e = \xi^e < \xi_1^e < \cdots < \xi_p^e = \xi^{e+1}$. Note, for $e \in \{0, ..., n_{\rm el} - 2\}$, the points $\xi_p^e = \xi_0^{e+1}$ denote the same point ξ^{e+1} , which is the boundary point of the adjacent element intervals. It is convenient to use both indexations in the following. For a given element interval $\mathcal{J}^e = [\xi^e, \xi^{e+1}]$, the *p*th-order Lagrange basis function and derivative of node $i \in \{0, ..., p\}$ are

$$N_{i}^{p,e}(\xi) = \prod_{\substack{0 \le j \le p \\ j \ne i}} \frac{\xi - \xi_{j}^{e}}{\xi_{i}^{e} - \xi_{j}^{e}} \quad \text{and} \quad N_{i,\xi}^{p,e}(\xi) = N_{i}^{p,e}(\xi) \sum_{\substack{k=0 \\ k \ne i}}^{p} \frac{1}{\xi - \xi_{k}^{e}}, \tag{4}$$

where ξ_i^e, ξ_j^e , and ξ_k^e are the points contained in the set $\{\xi_0^e = \xi^e, \xi_1^e, \dots, \xi_p^e = \xi^{e+1}\}$.

The centerline curve $_{I}\mathbf{r}_{OP}$ and the cross-section orientations \mathbf{A}_{IK} are approximated by interpolating nodal centerline points $_{I}\mathbf{r}_{OP_{i}^{e}}(t) \in \mathbb{R}^{3}$ and nodal transformation matrices $\mathbf{A}_{IK_{i}^{e}}(t) \in SO(3)$. For each node $i \in \{0, ..., p\}$ within element $e \in \{0, ..., n_{el} - 1\}$, it will hold that $_{I}\mathbf{r}_{OP_{i}^{e}}(t) = _{I}\mathbf{r}_{OP}(\xi_{i}^{e}, t)$ and $\mathbf{A}_{IK_{i}^{e}}(t) = \mathbf{A}_{IK}(\xi_{i}^{e}, t)$. In contrast to Refs. [1, 2], the nodal transformation matrices

$$\mathbf{A}_{IK_i^e} = \mathbf{A}(\mathbf{P}_i^e) = \mathbf{1}_{3\times 3} + 2\left((\widetilde{\mathbf{p}}_i^e)^2 + p_{0,i}^e \widetilde{\mathbf{p}}_i^e\right) / \|\mathbf{P}_i^e\|^2$$
(5)

are parametrized by nodal nonunit quaternions $\mathbf{P}_{i}^{e}(t) = (p_{0,i}^{e}(t), \mathbf{p}_{i}^{e}(t)) \in \mathbb{R}^{4}$ with the scalar part $p_{0,i}^{e}(t) \in \mathbb{R}$ and the vectorial part $\mathbf{p}_{i}^{e}(t) \in \mathbb{R}^{3}$, see Rucker [7]. Note that Equation (5) is formulated in such a way to return orthogonal matrices also for nonunit quaternions.

Accordingly, the $N = (pn_{el} + 1)$ nodal generalized position coordinates $\mathbf{q}_i^e(t) = (_I \mathbf{r}_{OP_i^e}, \mathbf{P}_i^e)(t) \in \mathbb{R}^7$ are given by the nodal centerline points $_I \mathbf{r}_{OP_i^e}$ and the nodal nonunit quaternions \mathbf{P}_i^e resulting in $n_{\mathbf{q}} = 7N$ positional degrees of freedom for the discretized rod. The nodal quantities can be assembled in the global tuple of generalized position coordinates $\mathbf{q}(t) = (\mathbf{q}_0^0, \dots, \mathbf{q}_{p-1}^0, \dots, \mathbf{q}_0^{e_1-1}, \dots, \mathbf{q}_0^{n_{el}-1}, \mathbf{q}_p^{n_{el}-1})(t) \in \mathbb{R}^{n_{\mathbf{q}}}$. Note, for $e \in \{0, \dots, n_{el} - 2\}$, the coordinates $\mathbf{q}_p^e = \mathbf{q}_0^{e+1}$ refer to the same nodal coordinates. Introducing an appropriate Boolean connectivity matrix $\mathbf{C}_e \in \mathbb{R}^{7(p+1) \times n_{\mathbf{q}}}$, the element generalized position coordinates $\mathbf{q}^e(t) = (\mathbf{q}_0^e, \dots, \mathbf{q}_p^e)(t) \in \mathbb{R}^{7(p+1)}$ can be extracted from \mathbf{q} via $\mathbf{q}^e = \mathbf{C}_e \mathbf{q}$. Note that during a numerical implementation, it is advisable to slice arrays instead of multiply them with Boolean matrices.

In the sense of Refs. [3, 4], both the nodal centerline points and the cross-section orientations are interpolated by *p*thorder Lagrangian polynomials. Using the characteristic function $\chi_{\mathcal{J}^e} : \mathcal{J} \to \{0, 1\}$, which is one for $\xi \in \mathcal{J}^e = [\xi^e, \xi^{e+1})$ and zero elsewhere, together with the *p*th-order Lagrange basis functions (4), the ansatz functions for centerline and cross-section orientations are

$${}_{I}\mathbf{r}_{OP}(\xi,\mathbf{q}) = \sum_{e=0}^{n_{\rm el}-1} \chi_{\mathcal{J}^{e}}(\xi) \sum_{i=0}^{p} N_{i}^{p,e}(\xi)_{I}\mathbf{r}_{OP_{i}^{e}} \quad \text{and} \quad \mathbf{A}_{IK}(\xi,\mathbf{q}) = \sum_{e=0}^{n_{\rm el}-1} \chi_{\mathcal{J}^{e}}(\xi) \sum_{i=0}^{p} N_{i}^{p,e}(\xi) \mathbf{A}(\mathbf{P}_{i}^{e}).$$
(6)

The discretized version of the curvature strain is computed as

$${}_{K}\boldsymbol{\kappa}_{IK} = j^{-1} \left(\text{Skw}(\mathbf{A}_{IK}^{T} \mathbf{A}_{IK,\xi}) \right) / J, \qquad (7)$$

where the map $\text{Skw}(\mathbf{M}) = \frac{1}{2}(\mathbf{M} - \mathbf{M}^{T}) \in \mathfrak{so}(3)$ extracts the skew-symmetric part of the matrix $\mathbf{M} \in \mathbb{R}^{3\times 3}$. Hence, the curvature can efficiently be computed using $j^{-1}(\text{Skw}(\mathbf{M})) = \frac{1}{2}(M_{32} - M_{23}, M_{13} - M_{31}, M_{21} - M_{12})$.

At the same *N* nodes as for the nodal generalized position coordinates, we introduce the nodal generalized virtual displacements $\delta \mathbf{s}_i^e(t) = (_I \delta \mathbf{r}_{P_i^e}, _{K_i^e} \delta \phi_{IK_i^e})(t) \in \mathbb{R}^6$ given by the nodal virtual centerline displacement $_I \delta \mathbf{r}_{P_i^e}(t) \in \mathbb{R}^3$ and the nodal virtual rotation $_{K_i^e} \delta \phi_{IK_i^e}(t) \in \mathbb{R}^3$. In analogy to the generalized virtual displacements, we also introduce the nodal generalized velocities $\mathbf{u}_i^e(t) = (_I \mathbf{v}_{P_i^e}, _{K_i^e} \boldsymbol{\omega}_{IK_i^e})(t) \in \mathbb{R}^6$ given by the nodal centerline velocity $_I \mathbf{v}_{P_i^e}(t) \in \mathbb{R}^3$ and the nodal angular velocity $_{K_i^e} \boldsymbol{\omega}_{IK_i^e}(t) \in \mathbb{R}^3$. Similar to the generalized position coordinates \mathbf{q} , the nodal generalized virtual displacements and velocities are assembled in the global tuple of generalized virtual displacements $\delta \mathbf{s}(t) \in \mathbb{R}^{n_u}$ and velocities $\mathbf{u}(t) \in \mathbb{R}^{n_u}$. In contrast to the nodal position coordinates, there are only six nodal generalized virtual displacements or velocity degrees of freedom for the discretized rod.

Consequently, we require a new Boolean connectivity matrix $\mathbf{C}_{\mathbf{u},e} \in \mathbb{R}^{6(p+1)\times n_{\mathbf{u}}}$, which extracts the element generalized virtual displacements $\delta \mathbf{s}^{e}(t) = (\delta \mathbf{s}_{0}^{e}, ..., \delta \mathbf{s}_{p}^{e})(t) \in \mathbb{R}^{6(p+1)}$ and velocities $\mathbf{u}^{e}(t) = (\mathbf{u}_{0}^{e}, ..., \mathbf{u}_{p}^{e})(t) \in \mathbb{R}^{6(p+1)}$ from the global quantities via $\delta \mathbf{s}^{e} = \mathbf{C}_{\mathbf{u},e} \delta \mathbf{s}$ and $\mathbf{u}^{e} = \mathbf{C}_{\mathbf{u},e} \mathbf{u}$. By further introducing the Boolean connectivity matrices $\mathbf{C}_{\mathbf{r},i} \in \mathbb{R}^{3\times 6(p+1)}$, the nodal virtual centerline displacements ${}_{I}\delta \mathbf{r}_{P_{i}^{e}}$ and centerline velocities ${}_{I}\mathbf{v}_{P_{i}^{e}}$ can be extracted from the element generalized virtual displacements $\delta \mathbf{s}^{e}$ and velocities \mathbf{u}^{e} via ${}_{I}\delta \mathbf{r}_{P_{i}^{e}} = \mathbf{C}_{\mathbf{r},i}\delta \mathbf{s}^{e}$ and ${}_{I}\mathbf{v}_{P_{i}^{e}} = \mathbf{C}_{\mathbf{r},i}\mathbf{u}^{e}$, respectively. Identical extraction operations hold for the nodal virtual rotations ${}_{K_{i}^{e}}\delta \phi_{IK_{i}^{e}} = \mathbf{C}_{\phi,i}\delta \mathbf{s}^{e}$ and angular velocities ${}_{K_{i}^{e}}\omega_{IK_{i}^{e}} = \mathbf{C}_{\phi,i}\mathbf{u}^{e}$, where $\mathbf{C}_{\phi,i} \in \mathbb{R}^{3\times 6(p+1)}$. The test functions are then given by interpolating the nodal generalized virtual displacements by *p*th-order Lagrangian

basis functions (4) in agreement with

$${}_{I}\delta\mathbf{r}_{P}(\xi,\delta\mathbf{s}) = \sum_{e=0}^{n_{\rm el}-1} \chi_{\mathcal{J}^{e}}(\xi) \sum_{i=0}^{p} N_{i}^{p,e}(\xi)_{I}\delta\mathbf{r}_{P_{i}^{e}} \quad \text{and} \quad {}_{K}\delta\boldsymbol{\phi}_{IK}(\xi,\delta\mathbf{s}) = \sum_{e=0}^{n_{\rm el}-1} \chi_{\mathcal{J}^{e}}(\xi) \sum_{i=0}^{p} N_{i}^{p,e}(\xi)_{K_{i}^{e}}\delta\boldsymbol{\phi}_{IK_{i}^{e}}.$$
(8)

Note that the interpolation of the virtual rotations must be understood in the sense of a Petrov–Galerkin projection, where the virtual rotations are not obtained from a consistent variation of the ansatz functions (6).

To obtain a constant and symmetric mass matrix in the discretized formulation, see Equation (13) below, the velocities are considered as independent fields and are interpolated with the same interpolation as the virtual displacements and rotations as

$${}_{I}\mathbf{v}_{P}(\xi,\mathbf{u}) = \sum_{e=0}^{n_{el}-1} \chi_{\mathcal{J}^{e}}(\xi) \sum_{i=0}^{p} N_{i}^{p,e}(\xi)_{I}\mathbf{v}_{P_{i}^{e}} \quad \text{and} \quad {}_{K}\boldsymbol{\omega}_{IK}(\xi,\mathbf{u}) = \sum_{e=0}^{n_{el}-1} \chi_{\mathcal{J}^{e}}(\xi) \sum_{i=0}^{p} N_{i}^{p,e}(\xi)_{K_{i}^{e}}\boldsymbol{\omega}_{IK_{i}^{e}}.$$
(9)

The independent introduction of velocity fields (9) demands an additional relation defining the coupling between position coordinates **q** and velocity coordinates **u**. This coupling is given by the nodal kinematic differential equations

$$\dot{\mathbf{q}}_{i}^{e} = \begin{pmatrix} I^{\dot{\mathbf{r}}_{OP_{i}^{e}}} \\ \dot{\mathbf{p}}_{i}^{e} \end{pmatrix} = \begin{pmatrix} \mathbf{1}_{3\times3} & \mathbf{0}_{3\times3} \\ \mathbf{0}_{4\times3} & \mathbf{Q}(\mathbf{P}_{i}^{e}) \end{pmatrix} \begin{pmatrix} I^{\mathbf{V}_{P_{i}^{e}}} \\ K_{i}^{e} \boldsymbol{\omega}_{IK_{i}^{e}} \end{pmatrix} = \mathbf{F}(\mathbf{q}_{i}^{e})\mathbf{u}_{i}^{e}, \quad \text{where } \mathbf{Q}(\mathbf{P}) = \frac{1}{2} \begin{pmatrix} -\mathbf{p}^{\mathrm{T}} \\ p_{0}\mathbf{1}_{3\times3} + \widetilde{\mathbf{p}} \end{pmatrix}, \quad (10)$$

compare [7]. The nodal kinematic equations (10) can easily be assembled to a global kinematic differential equation of the form $\dot{\mathbf{q}} = \mathbf{B}(\mathbf{q})\mathbf{u}$. Note that the kinematic differential equation is linear in \mathbf{q} too. This allows to write the relation also in the form $\dot{\mathbf{q}} = \mathbf{D}(\mathbf{u})\mathbf{q}$, see Rucker [7] for more details.

Inserting the test functions (8) together with the corresponding approximations for centerline, cross-section orientations (6), and strain measures into Equation (1), the continuous internal virtual work is approximated by $\delta W^{\text{int}}(\mathbf{q}; \delta \mathbf{s}) = \delta \mathbf{s}^{\text{T}} \mathbf{f}^{\text{int}}(\mathbf{q})$, where the internal generalized forces are computed element-wise by

$$\mathbf{f}^{\text{int}}(\mathbf{q}) = \sum_{e=0}^{n_{el}-1} \mathbf{C}_{\mathbf{u},e}^{\mathrm{T}} \mathbf{f}_{e}^{\text{int}}(\mathbf{C}_{e}\mathbf{q}),$$

$$\mathbf{f}_{e}^{\text{int}}(\mathbf{q}^{e}) = -\int_{\mathcal{J}^{e}} \sum_{i=0}^{p} \left\{ N_{i,\xi}^{p,e} \mathbf{C}_{\mathbf{r},i}^{\mathrm{T}} \mathbf{A}_{IKK} \mathbf{n} + N_{i,\xi}^{p,e} \mathbf{C}_{\phi,iK}^{\mathrm{T}} \mathbf{m} - N_{i}^{p,e} \mathbf{C}_{\phi,i(K}^{\mathrm{T}} \mathbf{\tilde{\gamma}} \times_{K} \mathbf{n} + _{K} \bar{\kappa}_{IK} \times_{K} \mathbf{m}) \right\} \mathrm{d}\xi.$$

$$(11)$$

Similarly, the external virtual work (2) is discretized by $\delta W^{\text{ext}}(t, \mathbf{q}; \delta \mathbf{s}) = \delta \mathbf{s}^{\text{T}} \mathbf{f}^{\text{ext}}(t, \mathbf{q})$ with

$$\mathbf{f}^{\text{ext}}(t,\mathbf{q}) = \sum_{e=0}^{n_{\text{el}}-1} \mathbf{C}_{\mathbf{u},e}^{\text{T}} \mathbf{f}_{e}^{\text{ext}}(t,\mathbf{C}_{e}\mathbf{q}) + \mathbf{C}_{\mathbf{u},0}^{\text{T}} \Big[\mathbf{C}_{\mathbf{r},0I}^{\text{T}} \mathbf{b}_{0} + \mathbf{C}_{\phi,0K}^{\text{T}} \mathbf{c}_{0} \Big]_{\xi=0} + \mathbf{C}_{\mathbf{u},n_{\text{el}}-1}^{\text{T}} \Big[\mathbf{C}_{\mathbf{r},pI}^{\text{T}} \mathbf{b}_{1} + \mathbf{C}_{\phi,pK}^{\text{T}} \mathbf{c}_{1} \Big]_{\xi=1},$$

$$\mathbf{f}_{e}^{\text{ext}}(t,\mathbf{q}^{e}) = \int_{\mathcal{J}^{e}} \sum_{i=0}^{p} \Big\{ N_{i}^{p,e} \mathbf{C}_{\mathbf{r},iI}^{\text{T}} \mathbf{b} + N_{i}^{p,e} \mathbf{C}_{\phi,iK}^{\text{T}} \mathbf{c} \Big\} J \mathrm{d}\xi.$$
(12)

Finally, inserting Equations (8) and (9) into the inertial virtual work functional (3) yields the discrete counterpart $\delta W^{\text{dyn}}(\mathbf{u}; \delta \mathbf{s}) = -\delta \mathbf{s}^{\text{T}}(\mathbf{M}\dot{\mathbf{u}} + \mathbf{f}^{\text{gyr}}(\mathbf{u}))$, where we have introduced the symmetric and constant mass matrix

$$\mathbf{M} = \sum_{e=0}^{n_{\rm el}-1} \mathbf{C}_{\mathbf{u},e}^{\rm T} \mathbf{M}_{e} \mathbf{C}_{\mathbf{u},e}, \quad \mathbf{M}_{e} = \int_{\mathcal{J}^{e}} \sum_{i=0}^{p} \sum_{k=0}^{p} N_{i}^{p,e} N_{k}^{p,e} \Big\{ A_{\rho_{0}} \mathbf{C}_{\mathbf{r},i}^{\rm T} \mathbf{C}_{\mathbf{r},k} + \mathbf{C}_{\boldsymbol{\phi},iK}^{\rm T} \mathbf{I}_{\rho_{0}} \mathbf{C}_{\boldsymbol{\phi},k} \Big\} J d\xi , \qquad (13)$$

and the gyroscopic forces

$$\mathbf{f}^{\text{gyr}}(\mathbf{u}) = \sum_{e=0}^{n_{\text{el}}-1} \mathbf{C}_{\mathbf{u},e}^{\text{T}} \mathbf{f}_{e}^{\text{gyr}}(\mathbf{C}_{\mathbf{u},e}\mathbf{u}), \quad \mathbf{f}_{e}^{\text{gyr}}(\mathbf{u}^{e}) = \int_{\mathcal{J}^{e}} \sum_{i=0}^{p} N_{i}^{p,e} \Big\{ \mathbf{C}_{\phi,i}^{\text{T}}({}_{K}\boldsymbol{\omega}_{IK} \times {}_{K}\mathbf{I}_{\rho_{0}K}\boldsymbol{\omega}_{IK}) \Big\} J \mathrm{d}\boldsymbol{\xi} \,. \tag{14}$$

Element integrals of the form $\int_{\mathcal{J}^e} f(\xi) d\xi$ arising in the discretized external and gyroscopic forces, as well as in the mass matrix, are subsequently computed using a Gauss–Legendre quadrature rule with ceil[$(p + 1)^2/2$] quadrature points. To alleviate locking, the internal generalized forces (11) are integrated by a reduced *p*-point quadrature rule.

Applying the principle of virtual work, which requires the total virtual work functional to vanish, we readily obtain the system dynamics in the form

$$\dot{\mathbf{q}} = \mathbf{B}(\mathbf{q})\mathbf{u},$$

$$\dot{\mathbf{u}} = \mathbf{M}^{-1} \left(\mathbf{f}^{\text{gyr}}(\mathbf{u}) + \mathbf{f}^{\text{int}}(\mathbf{q}) + \mathbf{f}^{\text{ext}}(t, \mathbf{q}) \right),$$
(15)

where the two lines correspond to the global kinematic differential equation and the equations of motion, respectively. Even though deviations from unit length of \mathbf{P}_i^e do not affect the kinematic differential equation, to avoid numerical issues due to quaternion magnitudes near zero or floating point overflow, the nodal quaternions are normalized after each timestep, that is, $\mathbf{P}_i^e = \mathbf{P}_i^e / ||\mathbf{P}_i||$. For static problems, the $n_u = 6N$ nonlinear generalized force equilibrium equations

$$\mathbf{0} = \mathbf{f}^{\text{int}}(\mathbf{q}) + \mathbf{f}^{\text{ext}}(\mathbf{q}) \tag{16}$$

must be augmented by the N constraint equations

$$\mathbf{0} = \mathbf{g}(\mathbf{q}) = (\|\mathbf{P}_0^0\|^2 - 1, \dots, \|\mathbf{P}_p^{n_{el}-1}\|^2 - 1)$$
(17)

to ensure solvability.

4 | NUMERICAL EXPERIMENTS

In the following, the quadratic strain energy density

$$W(_{K}\boldsymbol{\gamma},_{K}\boldsymbol{\kappa}_{IK};\boldsymbol{\xi}) = \frac{1}{2} (_{K}\boldsymbol{\gamma} - _{K}\boldsymbol{\gamma}^{0})^{\mathrm{T}} \mathbf{K}_{\boldsymbol{\gamma}} (_{K}\boldsymbol{\gamma} - _{K}\boldsymbol{\gamma}^{0}) + \frac{1}{2} (_{K}\boldsymbol{\kappa}_{IK} - _{K}\boldsymbol{\kappa}_{IK}^{0})^{\mathrm{T}} \mathbf{K}_{\boldsymbol{\kappa}} (_{K}\boldsymbol{\kappa}_{IK} - _{K}\boldsymbol{\kappa}_{IK}^{0})$$
(18)

is used. The superscript 0 refers to the evaluation in the rod's reference configuration. Moreover, $\mathbf{K}_{\gamma} = \text{diag}(EA, GA, GA)$ and $\mathbf{K}_{\kappa} = \text{diag}(G(I_y + I_z), EI_y, EI_z)$ denote the diagonal elasticity matrices with constant coefficients given by Saint-Venant's relations from linear elasticity. Therein, *E* and *G*, respectively denote the Young's and shear modulus. The cross-sectional surface is denoted *A* and I_y , I_z are the respective second moments of area.

4.1 | Helical spring

Following Marino [5], we investigate the elongation of an initially curved helical rod due to an applied external force at its tip, pointing in positive \mathbf{e}_z^I -direction. The rod has a Young's modulus $E = 10^{11}$ N/m² and Poisson's ratio $\nu = 0.2$, that is, a shear modulus $G = E/2(1 + \nu) = 41.7 \cdot 10^9$ N/m². It has an undeformed shape of a perfect helix with $n_c = 10$ coils, coil radius R = 10 mm, wire diameter d = 1 mm, and unloaded pitch k = 5 mm, that is, a total height of h = 50 mm.

In the simulation, the spring was discretized using 75 elements of the presented finite element formulation with p = 2. Reduced integration was performed with 2 quadrature points, while 5 points were used for all other integrals. The rod's curved initial configuration was obtained by solving the following minimization problem. Let $\xi_j = \frac{j}{m-1} \in [0,1]$ for $j \in \{0,1,...,m-1\}$ denote the *m* linearly spaced evaluation points of the reference helix curve

$${}_{I}\mathbf{r}(\xi) = R \begin{pmatrix} \sin\varphi(\xi) \\ -\cos\varphi(\xi) \\ c\varphi(\xi) \end{pmatrix}, \quad \text{with} \quad c = \frac{k}{2\pi R} \quad \text{and} \quad \varphi(\xi) = 2\pi n_{c}\xi.$$
(19)

Hence, the evaluation of the reference curve (19) at all ξ_j 's leads to *m* target centerline points ${}_{I}\mathbf{r}_j = {}_{I}\mathbf{r}(\xi_j)$. Similarly, the corresponding cross-section orientations are given by evaluating the Serret–Frenet basis $\mathbf{A}_{IK_j} = ({}_{I}\mathbf{e}_{x}^{K_j} {}_{I}\mathbf{e}_{y}^{K_j} {}_{I}\mathbf{e}_{z}^{K_j})$ with



FIGURE 1 Force-displacement diagram and deformed configurations of the helical spring.

 $_{I}\mathbf{e}_{x}^{K_{j}} = _{I}\mathbf{r}_{\xi}(\xi_{j})/\|_{I}\mathbf{r}_{\xi}(\xi_{j})\|, _{I}\mathbf{e}_{y}^{K_{j}} = _{I}\mathbf{r}_{\xi\xi}(\xi_{j})/\|_{I}\mathbf{r}_{\xi\xi}(\xi_{j})\|, \text{ and } \mathbf{e}_{z}^{K_{j}} = _{I}\mathbf{e}_{x}^{K_{j}} \times _{I}\mathbf{e}_{y}^{K_{j}}$ for the individual ξ_{j} 's. Following Harsch et al. [1], the centerline positions and cross-section orientations can be assembled in the Euclidean transformations

$$\mathbf{H}_{j} = \begin{pmatrix} \mathbf{A}_{IK_{j}} & {}^{I}\mathbf{r}_{j} \\ \mathbf{0}_{1\times3} & 1 \end{pmatrix} \text{ and } \mathbf{H}(\xi_{j}) = \begin{pmatrix} \mathbf{A}_{IK}(\xi_{j}) & {}^{I}\mathbf{r}_{OP}(\xi_{j}) \\ \mathbf{0}_{1\times3} & 1 \end{pmatrix}, \text{ with } \mathbf{H}_{j}^{-1} = \begin{pmatrix} \mathbf{A}_{IK_{j}}^{T} & -\mathbf{A}_{IK_{j}}^{T} {}^{I}\mathbf{r}_{j} \\ \mathbf{0}_{1\times3} & 1 \end{pmatrix}.$$
 (20)

Using the $S\!E(3)$ -logarithm map $\text{Log}_{S\!E(3)}$ introduced in Harsch et al. [1], the optimal initial generalized position coordinates \mathbf{q}_0 results from the nonlinear least squares problem

$$\mathbf{q}_{0} = \operatorname*{argmin}_{\mathbf{q} \in \mathbb{R}^{n_{\mathbf{q}}}} K(\mathbf{q}), \quad \text{with} \quad K(\mathbf{q}) = \frac{1}{2} \sum_{j=0}^{m-1} \|\boldsymbol{\theta}_{j}(\mathbf{q})\|^{2} \quad \text{and} \quad \boldsymbol{\theta}_{j}(\mathbf{q}) = \operatorname{Log}_{SE(3)} \left(\mathbf{H}_{j}^{-1} \mathbf{H}(\xi_{j})\right), \tag{21}$$

in terms of the metric of relative twists. The minimization problem (21) can efficiently be solved using a Levenberg– Marquardt algorithm. The unity constraints of the nodal quaternions (17) can be incorporated into the optimization problem as equality constraints, albeit at the expense of employing a complex constrained nonlinear least squares solver. To simplify the process, we initially solved the unconstrained minimization problem and subsequently applied a projection step to normalize all nodal quaternions.

Starting from \mathbf{q}_0 , the maximal force of 100 N was applied within 500 linearly spaced force increments. During each iteration, the nonlinear equations (16) and (17) were solved up to an absolute error of 10^{-8} . As can be seen in Figure 1, the helical spring initially elongates proportional to the applied load. This is in line with classical helical spring theory [8], which assumes a linear force–displacement relation with linear equivalent stiffness $Gd^4/(64n_cR^3) \approx 65.1$ N/m. When the elongation exceeds a certain value (approx. 10 N), the linear theory does not longer agree with the numerically obtained nonlinear solution. This observation was also made by Marino [5] and can be explained as follows. The helical spring unwinds gradually and approaches slowly a straight line with an altered linear stiffness *EA*. For comparison, we also solved the problem with the two-node *SE*(3)-interpolation strategy proposed in Harsch et al. [1], using the same number of unknowns. As depicted in Figure 1, the results are in line with the proposed quaternion formulation.

4.2 | Wilberforce pendulum

More than 100 years ago, Lionel Robert Wilberforce did investigations *On the Vibrations of a Loaded Spiral Spring* [9]. The experimental setup can be described as follows. While one end of a helical spring is clamped, at the other end, a cylindrical bob is attached, see Figure 2. When the cylinder in the gravitational field is displaced vertically, it starts oscillating up and



FIGURE 2 Vertical position *z* of the cylinder's center of mass and rotation angle α corresponding to the first Euler angle with sequence "*zyx*" over time. Snapshots of the Wilberforce pendulum are attached to the corresponding time instants.

down. Due to the coupling of bending and torsion of the deformed spring, an additional torsional oscillation around the vertical axis of the cylinder is induced. When the cylinder's moment of inertia is properly adjusted, a beat phenomenon can be observed. In that case, the envelope of the vertical and torsional oscillations possess an almost perfect phase shift of $\pi/2$, that is, the maximal amplitude of the vertical oscillations coincides with a zero torsional amplitude and vice versa.

To have a benchmark example that can be reproduced with reasonably computational effort, we introduce here a Wilberforce pendulum consisting of a spring with three coils modeled as a precurved rod. The rod has the properties of steel with mass density $\rho_0 = 7850 \text{ kg/m}^3$, shear modulus $G = 81 \cdot 10^9 \text{ N/m}^2$, and Poisson's ratio $\nu = 0.23$, that is, a Young's modulus $E = 2G(1 + \nu) = 199 \cdot 10^9 \text{ N/m}^2$. The undeformed shape is given by a perfect helix with $n_c = 3$ coils, coil radius R = 16 mm, wire diameter d = 1 mm, and an unloaded pitch of k = 1 mm. The bob is modeled as a cylindrical rigid body with radius r = 23 mm and height h = 36 mm also having the mass density of steel.

In the simulations, the rod was discretized using 18 elements of the presented Cosserat rod finite element with p = 2. Gravitational forces for the rod were neglected. Again, reduced integration was performed with 2 quadrature points, while for all other integrals 5 points were used. The bob was parameterized by the inertial position of the center of mass $_{I}\mathbf{r}_{OS}$ together with a nonunit quaternion **P** for the orientation. The bob was subjected to gravity with gravity constant $g = 9.81 \text{ m/s}^2$. For the governing equations describing such a parameterized rigid body under the influence of gravity, we refer to model 4 in Sailer et al. [10]. Cylinder and rod were rigidly connected by perfect bilateral constraints [11]. Again, the optimal helical initial configuration \mathbf{q}_0 was found by solving the minimization problem (21). The system was initialized at rest with initial velocity $\mathbf{u}_0 = \mathbf{0}$. The resulting differential algebraic equations were solved using a first-order generalized-alpha method [12] for constrained mechanical systems of differential index 3, similar to the implementation found in Arnold and Brüls [13]. A constant step-size $\Delta t = 5 \cdot 10^{-3}$ s was chosen and the governing equations were solved up to a final time of $t_1 = 8$ s. Since the example includes high-frequency oscillations, we chose a spectral radius at infinity of $\rho_{\infty} = 0.8$. The internal Newton–Raphson method satisfied a tolerance of 10^{-8} with respect to the maximum absolute error. In Figure 2, the vertical position and the torsional angle of the rigid cylinder are plotted clearly showing the beat phenomenon of the Wilberforce pendulum.

5 | CONCLUSIONS

This brief communication presents a total Lagrangian Petrov–Galerkin finite element formulation for Cosserat rods. A singularity-free parametrization of the rod's orientations is given in terms of nonunit quaternions. To keep the formulation

as simple as possible, we have opted for the \mathbb{R}^{12} -interpolation strategy, which was independently introduced by Betsch and Steinmann [3] and Romero and Armero [4].

Despite this choice, the versatility of the applied Petrov–Galerkin method enables to apply diverse interpolation strategies. Therefore, an $\mathbb{R}^3 \times SO(3)$ - or *SE*(3)-interpolation strategy can be seamlessly incorporated into the formulation, without changing the discrete virtual work contributions nor the parametrization, see Refs. [1, 2].

ACKNOWLEDGMENTS

Open access funding enabled and organized by Projekt DEAL.

ORCID

Jonas Harsch https://orcid.org/0000-0003-1065-2216 Simon R. Eugster https://orcid.org/0000-0002-4562-1287

REFERENCES

- 1. Harsch, J., Sailer, S., & Eugster, S. R. (2023). A total Lagrangian, objective and intrinsically locking-free Petrov–Galerkin SE(3) Cosserat rod finite element formulation. *International Journal for Numerical Methods in Engineering*, *124*(13), 2965–2994.
- Eugster, S. R., & Harsch, J. (2023). A family of total Lagrangian Petrov-Galerkin Cosserat rod finite element formulations. GAMM-Mitteilungen, 46(2), e202300008.
- 3. Betsch, P., & Steinmann, P. (2002). Frame-indifferent beam finite elements based upon the geometrically exact beam theory. *International Journal for Numerical Methods in Engineering*, 54(12), 1775–1788.
- 4. Romero, I., & Armero, F. (2002). An objective finite element approximation of the kinematics of geometrically exact rods and its use in the formulation of an energy-momentum conserving scheme in dynamics. *International Journal for Numerical Methods in Engineering*, 54, 1683–1716.
- 5. Marino, E. (2017). Locking-free isogeometric collocation formulation for three-dimensional geometrically exact shear-deformable beams with arbitrary initial curvature. *Computer Methods in Applied Mechanics and Engineering*, *324*, 546–572.
- 6. Harsch, J., Capobianco, G., & Eugster, S. R. (2021). Finite element formulations for constrained spatial nonlinear beam theories. *Mathematics and Mechanics of Solids*, *26*(12), 1838–1863.
- 7. Rucker, C. (2018). Integrating rotations using non unit quaternions. *IEEE Robotics and Automation Letters*, 3(4), 2979–2986.
- 8. Berg, R. E., & Marshall, T. S. (1991). Wilberforce pendulum oscillations and normal modes. American Journal of Physics, 59(1), 32-38.
- 9. Wilberforce, L. R. (1894). On the vibrations of a loaded spiral spring. London, Edinburgh, and Dublin Philosophical Magazine and Journal of Science, 38(233), 386–392.
- 10. Sailer, S., Eugster, S. R., & Leine, R. I. (2020). The tippedisk: A tippetop without rotational symmetry. *Regular and Chaotic Dynamics*, 25(6), 553–580.
- 11. Géradin, M., & Cardona, A. (2001). Flexible multibody dynamics: A finite element approach. Wiley.
- 12. Jansen, K. E., Whiting, C. H., & Hulbert, G. M. (2000). A generalized-α method for integrating the filtered Navier–Stokes equations with a stabilized finite element method. *Computer Methods in Applied Mechanics and Engineering*, *190*(3), 305–319.
- Arnold, M., & Brüls, O. (2007). Convergence of the generalized-α scheme for constrained mechanical systems. *Multibody System Dynamics*, 18(2), 185–202.

How to cite this article: Harsch, J., & Eugster, S. R. (2023). Nonunit quaternion parametrization of a Petrov–Galerkin Cosserat rod finite element. *Proceedings in Applied Mathematics and Mechanics*, *23*, e202300172. https://doi.org/10.1002/pamm.202300172