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Rigid body dynamics in terms of quaternions: Hamiltonian formulation and conserving numerical integration

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SUMMARY

In the present paper unit quaternions are used to describe the rotational motion of a rigid body. The unit-length constraint is enforced explicitly by means of an algebraic constraint. Correspondingly, the equations of motion assume the form of differential-algebraic equations (DAEs). A new route to the derivation of the mass matrix associated with the quaternion formulation is presented. In contrast to previous works, the newly proposed approach yields a non-singular mass matrix. Consequently, the passage to the Hamiltonian framework is made possible without the need to introduce undetermined inertia terms. The Hamiltonian form of the DAEs along with the notion of a discrete derivative make possible the design of a new quaternion-based energy–momentum scheme. Two numerical examples demonstrate the performance of the newly developed method. In this connection, comparison is made with a quaternion-based variational integrator, a director-based energy–momentum scheme, and a momentum conserving scheme relying on the discretization of the classical Euler's equations. Copyright © 2009 John Wiley & Sons, Ltd.

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1. INTRODUCTION

Unit quaternions (or Euler parameters) are known to be well suited for the singularity-free description of finite rotations. There are plenty of applications dealing with purely kinematic aspects. In contrast to that, the equations of motion for rigid bodies are rarely formulated in terms of unit quaternions. Notable exceptions are the pioneering works by Nikravesh, Haug and co-workers, see [1, 2] and the references cited therein. In these works (see also Wendlandt and Marsden [3, Section 5.1], O'Reilly and Varadi [4, Section 6] and Rabier and Rheinboldt [5]) the orientation

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of a single rigid body is specified by a quaternion, considered as a vector in 4-space subject to the unit-length constraint.

In the aforementioned works, the Lagrangian framework of mechanics is used to obtain the equations governing the rotational motion of the rigid body. In this connection, the quaternion form of the kinetic energy is commonly obtained from the standard expression in terms of the angular velocity vector and the classical inertia tensor. Consequently, the 4×4 mass matrix of the quaternion formulation is singular in general.

In the present work we newly propose an alternative approach, which starts from a formulation of rigid body dynamics in terms of the nine redundant components of the rotation matrix (see, e.g. Vallee *et al.* [6], Betsch and Steinmann [7] and Leimkuhler and Reich [8, Chapter 8]). The size-reduction from 9-space to 4-space yields in a natural way a non-singular mass matrix associated with the quaternion formulation.

The present approach makes possible the straightforward transition to the Hamiltonian form of the equations of motion in terms of quaternions. This is in contrast to previous works by Maciejewski [9] and Morton [10] (see also Arribas *et al.* [11] and Borri *et al.* [12, Section 5.2]), which require the introduction of an undetermined inertia term in order to set up the quaternion-based Hamiltonian formulation.

In the present work the quaternion-based Hamiltonian form of the equations of motion provides the starting point for the design of a new energy–momentum conserving time-stepping scheme. Energy–momentum schemes are well known for their advantageous numerical stability properties (see, for example, Gonzalez and Simo [13]). It is worth mentioning that the majority of previous works aiming at the design of conserving schemes for rigid body dynamics relies on the discretization of the classical Euler's equations (see, e.g. Simo and Wong [14], Lens *et al.* [15], Krysl [16] and Romero [17]).

The remainder of this paper is structured as follows. Section 2 outlines main properties of quaternions and their connection with finite rotations. Moreover, a convenient matrix representation of quaternion algebra is introduced. Section 3 deals with the rotational motion of a rigid body in terms of the nine redundant components of the rotation matrix. In Section 4 the 9×9 mass matrix corresponding to the formulation in terms of the rotation matrix is reduced to the 4×4 mass matrix associated with the quaternion formulation. In addition to that, the quaternion-based Hamiltonian equations of motion are derived and subsequently discretized. After the presentation of numerical examples in Section 5, conclusions are drawn in Section 6.

2. QUATERNIONS

In this section pertinent properties of quaternions are summarized. See Altmann [18] and Kuipers [19] for more background on the subject.

2.1. The skew field of quaternions

A quaternion can be regarded as a 4-tuple of real numbers consisting of a scalar part $q_0 \in \mathsf{R}$ and a vector part $\mathbf{q}\in\mathsf{R}^3$. The vector part may be written as $\mathbf{q}=q_i\mathbf{e}_i$, where $\{\mathbf{e}_i\}$, $i=1,2,3$, is the standard orthonormal basis in R^3. In the present work, a quaternion $\mathfrak{q}\in\mathsf{H}\simeq\mathsf{R}^4$ is denoted by

$$\mathfrak{q}=(q_0,\mathbf{q})$$

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The product of two quaternions $\mathbb{q}, \mathbb{p} \in \mathsf{H}$ is defined by

$$\mathbb{q} \circ \mathbb{p} = (q_0 p_0 - \mathbf{q} \cdot \mathbf{p}, q_0 \mathbf{p} + p_0 \mathbf{q} + \mathbf{q} \times \mathbf{p}) \tag{1}$$

where $\mathbf{q} \cdot \mathbf{p} = q_i p_i$ is the standard dot product. Owing to the presence of the cross product $\mathbf{q} \times \mathbf{p}$, the quaternion product is not commutative. The quaternions form a (non-abelian) group under multiplication with the identity element

$$\mathbb{e} = (1, \mathbf{0})$$

Introducing the conjugate quaternion

$$\overline{\mathbb{q}} = (q_0, -\mathbf{q})$$

one gets

$$\overline{\mathbb{q}} \circ \mathbb{q} = \mathbb{q} \circ \overline{\mathbb{q}} = (q_0^2 + \mathbf{q} \cdot \mathbf{q}, \mathbf{0})$$

It can be easily verified that

$$\overline{\mathbb{q} \circ \mathbb{p}} = \overline{\mathbb{p}} \circ \overline{\mathbb{q}}$$

The norm (or length) of a quaternion is defined by

$$|\mathbb{q}| = \sqrt{q_0^2 + \mathbf{q} \cdot \mathbf{q}} = \sqrt{\mathbb{q} \cdot \mathbb{q}}$$

Eventually, the inverse element can be shown to be

$$\mathbb{q}^{-1} = \frac{1}{|\mathbb{q}|^2} \overline{\mathbb{q}}$$

2.2. *Unit quaternions*

We next focus on quaternions of unit length, i.e. $|\mathbb{q}| = 1$ or $\mathbb{q} \circ \overline{\mathbb{q}} = (1, \mathbf{0})$. Unit quaternions form an orthogonal group called $\mathsf{Sp}(1)$, the symplectic group. Obviously, $\mathsf{Sp}(1) \simeq \mathsf{S}^3$, the unit sphere in R^4, defined by

$$\mathsf{S}^3 = \{\mathbb{q} \in \mathsf{R}^4 \mid |\mathbb{q}| = 1\}$$

Assume that the rotational motion of a rigid body is characterized by $\mathbb{q}(t) \in \mathsf{S}^3$, where t denotes the time. Differentiating the unit-length constraint $\mathbb{q} \cdot \mathbb{q} = 1$ with respect to time shows that admissible velocities $\dot{\mathbb{q}}$ are restricted to lie in the tangent space $T_{\mathbb{q}}\mathsf{S}^3$ at $\mathbb{q} \in \mathsf{S}^3$ given by

$$T_{\mathbb{q}}\mathsf{S}^3 = \{\mathbb{w} \in \mathsf{R}^4 \mid \mathbb{q} \cdot \mathbb{w} = 0\}$$

Alternatively, differentiating $\overline{\mathbb{q}} \circ \mathbb{q} = (1, \mathbf{0})$ with respect to time yields

$$\dot{\overline{\mathbb{q}}} \circ \mathbb{q} + \overline{\mathbb{q}} \circ \dot{\mathbb{q}} = (0, \mathbf{0}) \tag{2}$$

Since, for any $\mathbb{a}, \mathbb{b} \in \mathsf{H}$

$$\overline{\mathbb{a}} \circ \mathbb{b} + \overline{\mathbb{b}} \circ \mathbb{a} = (2\mathbb{a} \cdot \mathbb{b}, \mathbf{0})$$

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condition (2) is satisfied for $\dot{\mathbf{q}} \in T_{\mathbf{q}}\mathsf{S}^3$. Admissible velocities $\dot{\mathbf{q}} \in T_{\mathbf{q}}\mathsf{S}^3$ can be represented by introducing the vector space of skew-symplectic quaternions

$$\mathsf{sp}(1) = \{\mathbf{w} \in \mathsf{R}^4 \mid \mathbf{w} + \overline{\mathbf{w}} = (0, \mathbf{0})\}$$

In particular, $\mathsf{sp}(1)$ can be viewed as tangent space to $\mathsf{Sp}(1) \simeq \mathsf{S}^3$ at the identity (see Curtis [20, Chapter 3]). Moreover, $\mathsf{sp}(1)$ is the Lie algebra of $\mathsf{Sp}(1)$. Obviously, $\mathbf{w} \in \mathsf{sp}(1)$ coincides with the set of pure quaternions given by $\mathbf{w} = (0, \mathbf{w})$ for $\mathbf{w} \in \mathsf{R}^3$. Thus, $\mathsf{sp}(1)$ can be identified with R^3. In view of (2), we define $(0, \frac{1}{2}\mathbf{\Omega}) = \overline{\mathbf{q}} \circ \dot{\mathbf{q}} \in \mathsf{sp}(1)$, where $\mathbf{\Omega} \in \mathsf{R}^3$ is the convective angular velocity. Then velocities $\dot{\mathbf{q}} \in T_{\mathbf{q}}\mathsf{S}^3$ can be written in the form

$$\dot{\mathbf{q}} = \mathbf{q} \circ (0, \tfrac{1}{2}\mathbf{\Omega}) \tag{3}$$

Upon introduction of

$$(0, \tfrac{1}{2}\boldsymbol{\omega}) = \mathbf{q} \circ (0, \tfrac{1}{2}\mathbf{\Omega}) \circ \overline{\mathbf{q}}$$

admissible velocities $\dot{\mathbf{q}} \in T_{\mathbf{q}}\mathsf{S}^3$ may also be written as

$$\dot{\mathbf{q}} = (0, \tfrac{1}{2}\boldsymbol{\omega}) \circ \mathbf{q} \tag{4}$$

This is equivalent to $(0, \frac{1}{2}\boldsymbol{\omega}) = \dot{\mathbf{q}} \circ \overline{\mathbf{q}} \in \mathsf{sp}(1)$, where $\boldsymbol{\omega} \in \mathsf{R}^3$ is the spatial angular velocity.

2.3. *Exponential map on* S^3

We next introduce the exponential map $\exp_{\mathsf{S}^3} : \mathsf{sp}(1) \simeq \mathsf{R}^3 \to \mathsf{Sp}(1) \simeq \mathsf{S}^3$. By definition, the exponential map is given by the series

$$\exp_{\mathsf{S}^3}\left(\left(0, \frac{1}{2}\mathbf{w}\right)\right) = \sum_{k=0}^{\infty} \frac{(0, \frac{1}{2}\mathbf{w})^k}{k!} = \sum_{k=0}^{\infty} \left\{ \frac{(0, \frac{1}{2}\mathbf{w})^{2k}}{(2k)!} + \frac{(0, \frac{1}{2}\mathbf{w})^{2k+1}}{(2k+1)!} \right\} \tag{5}$$

It can be easily verified that

$$\begin{aligned}(0, \mathbf{w})^{2k} &= (-1)^k |\mathbf{w}|^{2k} (1, \mathbf{0})\\ (0, \mathbf{w})^{2k+1} &= (-1)^k |\mathbf{w}|^{2k} (0, \mathbf{w})\end{aligned}$$

so that (5) yields

$$\begin{aligned}\exp_{\mathsf{S}^3}\left(\left(0, \frac{1}{2}\mathbf{w}\right)\right) &= \sum_{k=0}^{\infty} \frac{(-1)^k |\frac{1}{2}\mathbf{w}|^{2k}}{(2k)!}(1, \mathbf{0}) + \frac{1}{|\mathbf{w}|}\sum_{k=0}^{\infty} \frac{(-1)^k |\frac{1}{2}\mathbf{w}|^{2k+1}}{(2k+1)!}(0, \mathbf{w})\\ &= \cos\left(\frac{1}{2}|\mathbf{w}|\right)(1, \mathbf{0}) + \frac{\sin(\frac{1}{2}|\mathbf{w}|)}{|\mathbf{w}|}(0, \mathbf{w})\end{aligned} \tag{6}$$

This representation is in line with Euler's theorem, which states that every rotation can be characterized by a rotation axis defined by a unit vector $\mathbf{w}/|\mathbf{w}|$ and a rotation angle $|\mathbf{w}|$. In this connection, the four components of a unit quaternion are often called Euler parameters.

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2.4. Connection between quaternions and rotation matrices

We next focus on the connection between S^3 and the special orthogonal group $\mathsf{SO}(3)$ consisting of 3×3 orthogonal matrices with unit determinant. Accordingly, for $\mathbf{R}\in\mathsf{SO}(3)$, $\mathbf{R}^{\mathrm{T}}\mathbf{R}=\mathbf{R}\mathbf{R}^{\mathrm{T}}=\mathbf{I}_3$ and $\det\mathbf{R}=1$. Differentiating $\mathbf{R}^{\mathrm{T}}\mathbf{R}=\mathbf{I}_3$ with respect to time yields

$$\dot{\mathbf{R}}^{\mathrm{T}}\mathbf{R}+\mathbf{R}^{\mathrm{T}}\dot{\mathbf{R}}=\mathbf{0}$$

Consequently, $\mathbf{R}^{\mathrm{T}}\dot{\mathbf{R}}$ belongs to the vector space of skew-symmetric matrices

$$\mathsf{so}(3)=\{\widehat{\mathbf{w}}:\mathsf{R}^3\rightarrow\mathsf{R}^3\,|\,\widehat{\mathbf{w}}+\widehat{\mathbf{w}}^{\mathrm{T}}=\mathbf{0}\}$$

In particular, $\mathsf{so}(3)$ is the Lie algebra of $\mathsf{SO}(3)$. Since $\widehat{\mathbf{w}}\mathbf{a}=\mathbf{w}\times\mathbf{a}$, for any $\mathbf{a}\in\mathsf{R}^3$, $\mathsf{so}(3)$ can be identified with R^3. Specifically, the skew-symmetric matrix corresponding to the axial vector $\mathbf{w}=w_i\mathbf{e}_i\in\mathsf{R}^3$ is given by

$$\widehat{\mathbf{w}}=\begin{bmatrix}0 & -w_3 & w_2\\ w_3 & 0 & -w_1\\ -w_2 & w_1 & 0\end{bmatrix}$$

Similar to $\exp_{\mathsf{S}^3}$ dealt with in Section 2.3, there exists a closed-form expression for the exponential map $\exp_{\mathsf{SO}(3)}:\mathsf{so}(3)\rightarrow\mathsf{SO}(3)$, given by the Rodrigues' formula

$$\exp_{\mathsf{SO}(3)}(\widehat{\mathbf{w}})=\mathbf{I}_3+\frac{\sin(|\mathbf{w}|)}{|\mathbf{w}|}\widehat{\mathbf{w}}+\frac{1-\cos(|\mathbf{w}|)}{|\mathbf{w}|^2}\widehat{\mathbf{w}}^2$$

It is well known that unit quaternions can be linked to rotation matrices via the mapping $\mathscr{R}:\mathsf{S}^3\rightarrow\mathsf{SO}(3)$ defined by

$$(0,\mathscr{R}(\mathbb{q})\mathbf{x})=\mathbb{q}\circ(0,\mathbf{x})\circ\overline{\mathbb{q}}\tag{7}$$

A straightforward calculation based on (1) yields the explicit representation

$$\mathscr{R}(\mathbb{q})=(q_0^2-\mathbf{q}\cdot\mathbf{q})\mathbf{I}_3+2\mathbf{q}\otimes\mathbf{q}+2q_0\widehat{\mathbf{q}}\tag{8}$$

The map $\mathscr{R}:\mathsf{S}^3\rightarrow\mathsf{SO}(3)$ in (8) is often called the Euler–Rodrigues parametrization (see, for example, Marsden and Ratiu [21, Chapter 9]). It can be easily verified that for given $\mathscr{R}\in\mathsf{SO}(3)$, (8) has two solutions $\mathbb{q}\in\mathsf{S}^3$ and $-\mathbb{q}\in\mathsf{S}^3$. Indeed, (8) represents a smooth 2–1 surjective map. Moreover, the map $\mathscr{R}:\mathsf{S}^3\rightarrow\mathsf{SO}(3)$ respects the group operations:

$$(0,\mathscr{R}(\mathbb{p}\circ\mathbb{q})\mathbf{x})=(\mathbb{p}\circ\mathbb{q})\circ(0,\mathbf{x})\circ\overline{\mathbb{p}\circ\mathbb{q}}=\mathbb{p}\circ(\mathbb{q}\circ(0,\mathbf{x})\circ\overline{\mathbb{q}})\circ\overline{\mathbb{p}}=(0,\mathscr{R}(\mathbb{p})\mathscr{R}(\mathbb{q})\mathbf{x})$$

Accordingly, $\mathscr{R}$ is a homomorphism of S^3 onto $\mathsf{SO}(3)$ (see Curtis [20, Chapter 5]). The differential $\mathrm{d}\mathscr{R}$ is an isomorphism of the Lie algebras $\mathsf{sp}(1)$ and $\mathsf{so}(3)$, both of which can be identified with R^3. To see this, consider a curve $\mathbb{q}(\varepsilon)\in\mathsf{S}^3$ with $\mathbb{q}(0)=(1,\mathbf{0})$ and tangent vector $\mathbb{q}'(0)=(0,\mathbf{w})\in\mathsf{sp}(1)$ to S^3 at the identity. The corresponding tangent vector to $\mathsf{SO}(3)$ at the identity is defined by

$$\mathrm{d}\mathscr{R}(\mathbb{q}'(0))=\mathscr{R}(\mathbb{q})'(0)$$

Evaluating the right-hand side of the above equation by making use of (8) yields

$$\mathrm{d}\mathscr{R}((0,\mathbf{w}))=2q_0(0)\widehat{\mathbf{q}}'(0)=2\widehat{\mathbf{w}}$$

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The fundamental relationships between unit quaternions and rotations are further illustrated with the commutative diagram

$$\begin{tikzcd} \mathsf{sp}(1) \arrow[r, "d\mathscr{R}"] \arrow[d, "\exp_{\mathsf{S}^3}"'] & \mathsf{so}(3) \arrow[d, "\exp_{\mathsf{SO}(3)}"] \\ \mathsf{S}^3 \arrow[r, "\mathscr{R}"'] & \mathsf{SO}(3) \end{tikzcd}$$

We finally remark that, similar to (3) and (4), the time derivative of $\mathbf{R}\in\mathsf{SO}(3)$ may be written in the form

$$\dot{\mathbf{R}}=\mathbf{R}\widehat{\boldsymbol{\Omega}}=\widehat{\boldsymbol{\omega}}\mathbf{R}$$

where, as before, $\boldsymbol{\Omega}$ and $\boldsymbol{\omega}$ denote the convective and the spatial angular velocity, respectively.

2.5. Matrix representation of quaternions

We next summarize a specific matrix representation of quaternions which, due to its convenience, is often used in practical applications. The reader is referred to Chou [22] and Kuipers [19] for further information about the matrix form of quaternions and their algebra. In the matrix representation, a quaternion $\mathbb{q}\in\mathsf{H}\simeq\mathsf{R}^4$ is regarded as a column matrix. Then the multiplication of two quaternions

$$\mathbb{c}=\mathbb{b}\circ\mathbb{a}$$

may alternatively be written in the matrix form

$$\mathbb{c}=\mathbf{Q}_l(\mathbb{b})\mathbb{a}=\mathbf{Q}_r(\mathbb{a})\mathbb{b} \tag{9}$$

With regard to the multiplication rule (1), the 4×4 matrices $\mathbf{Q}_l$ and $\mathbf{Q}_r$ are given by

$$\begin{aligned} \mathbf{Q}_l(\mathbb{q}) &= [\mathbb{q}\ \ \mathbf{G}(\mathbb{q})^{\mathrm{T}}]=q_0\mathbf{I}_4+\overset{+}{\mathbf{q}} \\ \mathbf{Q}_r(\mathbb{q}) &= [\mathbb{q}\ \ \mathbf{E}(\mathbb{q})^{\mathrm{T}}]=q_0\mathbf{I}_4+\overset{-}{\mathbf{q}} \end{aligned} \tag{10}$$

In this connection, the 3×4 matrices

$$\begin{aligned} \mathbf{E}(\mathbb{q}) &= [-\mathbf{q}\ \ q_0\mathbf{I}_3+\widehat{\mathbf{q}}] \\ \mathbf{G}(\mathbb{q}) &= [-\mathbf{q}\ \ q_0\mathbf{I}_3-\widehat{\mathbf{q}}] \end{aligned}$$

have been introduced along with the 4×4 skew-symmetric matrices

$$\begin{aligned} \overset{+}{\mathbf{q}} &= \begin{bmatrix} 0 & -\mathbf{q}^{\mathrm{T}} \\ \mathbf{q} & \widehat{\mathbf{q}} \end{bmatrix} \\ \overset{-}{\mathbf{q}} &= \begin{bmatrix} 0 & -\mathbf{q}^{\mathrm{T}} \\ \mathbf{q} & -\widehat{\mathbf{q}} \end{bmatrix} \end{aligned} \tag{11}$$

Appendix A contains a summary of useful algebraic relationships between the above-introduced matrices, which will be required in the sequel. Using the matrices in (10), the quaternion product

$$\mathbb{a}\circ\mathbb{x}\circ\mathbb{b}$$

can be written in the alternative form

$$\mathbf{Q}_l(\mathbb{a})\mathbf{Q}_r(\mathbb{b})\mathbb{x} = \mathbf{Q}_r(\mathbb{b})\mathbf{Q}_l(\mathbb{a})\mathbb{x}$$

In particular, for $\mathbb{q} \in \mathsf{S}^3 \subset \mathsf{R}^4$,

$$\mathbb{q} \circ \mathbb{x} \circ \overline{\mathbb{q}}$$

can be written as

$$\mathbf{Q}_l(\mathbb{q})\mathbf{Q}_r(\mathbb{q})^{\mathrm{T}}\mathbb{x} = \mathbf{Q}_r(\mathbb{q})^{\mathrm{T}}\mathbf{Q}_l(\mathbb{q})\mathbb{x} = \begin{bmatrix} 1 & \mathbf{0}^{\mathrm{T}} \\ \mathbf{0} & \mathbf{E}(\mathbb{q})\mathbf{G}(\mathbb{q})^{\mathrm{T}} \end{bmatrix} \begin{bmatrix} x_0 \\ \mathbf{x} \end{bmatrix}$$

where use has been made of (A4). Comparison with (7) shows that the map $\mathscr{R}: \mathsf{S}^3 \to \mathsf{SO}(3)$ can also be written in the matrix form

$$\mathscr{R}(\mathbb{q}) = \mathbf{E}(\mathbb{q})\mathbf{G}(\mathbb{q})^{\mathrm{T}} \tag{12}$$

Differentiating (12) with respect to time yields

$$\dot{\mathscr{R}} = \mathbf{E}(\dot{\mathbb{q}})\mathbf{G}(\mathbb{q})^{\mathrm{T}} + \mathbf{E}(\mathbb{q})\mathbf{G}(\dot{\mathbb{q}})^{\mathrm{T}}$$

or taking into account $(\mathrm{A}2)_3$,

$$\dot{\mathscr{R}} = 2\mathbf{E}(\mathbb{q})\mathbf{G}(\dot{\mathbb{q}})^{\mathrm{T}} = 2\mathbf{E}(\dot{\mathbb{q}})\mathbf{G}(\mathbb{q})^{\mathrm{T}} \tag{13}$$

Eventually, the matrix counterpart of (3) is given by

$$\dot{\mathbb{q}} = \mathbf{Q}_l(\mathbb{q}) \begin{bmatrix} 0 \\ \frac{1}{2}\mathbf{\Omega} \end{bmatrix} = \mathbf{Q}_r((0, \tfrac{1}{2}\mathbf{\Omega}))\mathbb{q}$$

or in view of (10),

$$\dot{\mathbb{q}} = \tfrac{1}{2}\mathbf{G}(\mathbb{q})^{\mathrm{T}}\mathbf{\Omega} = \tfrac{1}{2}\overset{-}{\mathbf{\Omega}}\mathbb{q}$$

Similarly, (4) can be written in the form

$$\dot{\mathbb{q}} = \tfrac{1}{2}\mathbf{E}(\mathbb{q})^{\mathrm{T}}\boldsymbol{\omega} = \tfrac{1}{2}\overset{+}{\boldsymbol{\omega}}\mathbb{q}$$

Eventually, it can be easily verified that

$$\begin{aligned} \mathbf{\Omega} &= 2\mathbf{G}(\mathbb{q})\dot{\mathbb{q}}, \quad \widehat{\mathbf{\Omega}} = 2\mathbf{G}(\mathbb{q})\mathbf{G}(\dot{\mathbb{q}})^{\mathrm{T}} \\ \boldsymbol{\omega} &= 2\mathbf{E}(\mathbb{q})\dot{\mathbb{q}}, \quad \widehat{\boldsymbol{\omega}} = 2\mathbf{E}(\dot{\mathbb{q}})\mathbf{E}(\mathbb{q})^{\mathrm{T}} \end{aligned} \tag{14}$$

for $(\mathbb{q}, \dot{\mathbb{q}}) \in T\mathsf{S}^3$.

3. RIGID BODY DYNAMICS IN TERMS OF DIRECTORS

We next outline a specific rigid body formulation, which provides the starting point for our subsequent developments. The rotational motion of a rigid body can be described by using the canonical embedding of $\mathsf{SO}(3)$ into R^9. That is, the nine components of the rotation matrix are employed as coordinates for the description of the orientation of a rigid body. Of course, the components of the rotation matrix are redundant due to six independent geometric constraints reflecting the orthogonality of the rotation matrix.

Consider a right-handed body frame $\{\mathbf{d}_i\}$, $\mathbf{d}_i(t)\in\mathsf{R}^3$ $(i=1,2,3)$, located at the center of mass of a rigid body. The rotational motion of the rigid body relative to an orthonormal reference frame $\{\mathbf{e}_i\}$ can be characterized by a rotation tensor

$$\mathbf{R}=\mathbf{d}_k\otimes\mathbf{e}_k \tag{15}$$

Expressing the rotation tensor with respect to the reference frame, i.e. $\mathbf{R}=R_{ij}\mathbf{e}_i\otimes\mathbf{e}_j$, yields the direction cosines $R_{ij}=\mathbf{e}_i\cdot\mathbf{d}_j$. Accordingly, the columns of the rotation matrix correspond to the directors $\mathbf{d}_j=R_{ij}\mathbf{e}_i$. The three directors may be arranged in the vector of coordinates $\mathbf{q}\in\mathsf{R}^9$, such that

$$\mathbf{q}=\begin{bmatrix}\mathbf{d}_1\\ \mathbf{d}_2\\ \mathbf{d}_3\end{bmatrix} \tag{16}$$

Orthogonality of the rotation matrix implies that the directors are mutually orthonormal, i.e. $\mathbf{d}_i\cdot\mathbf{d}_j=\delta_{ij}$, where δ_{ij} is the Kronecker delta. The last equation gives rise to six independent constraint equations $\Phi_i(\mathbf{q})=0$, with associated constraint functions $\Phi_i:\mathsf{R}^9\to\mathsf{R}$. These functions may be arranged in the vector-valued function of geometric constraints

$$\mathbf{\Phi}(\mathbf{q})=\begin{bmatrix}\frac{1}{2}[\mathbf{d}_1^{\mathrm{T}}\mathbf{d}_1-1]\\ \frac{1}{2}[\mathbf{d}_2^{\mathrm{T}}\mathbf{d}_2-1]\\ \frac{1}{2}[\mathbf{d}_3^{\mathrm{T}}\mathbf{d}_3-1]\\ \mathbf{d}_1^{\mathrm{T}}\mathbf{d}_2\\ \mathbf{d}_1^{\mathrm{T}}\mathbf{d}_3\\ \mathbf{d}_2^{\mathrm{T}}\mathbf{d}_3\end{bmatrix} \tag{17}$$

Let further $h:\mathsf{R}^9\to\mathsf{R}$ be defined by $h(\mathbf{q})=\mathbf{d}_1\cdot(\mathbf{d}_2\times\mathbf{d}_3)$. Concerning rotational motions of a rigid body, the corresponding configuration space may now be written in the form

$$\mathsf{Q}=\{\mathbf{q}\in\mathsf{R}^9\,|\,\Phi_i(\mathbf{q})=0,\ i=1,\ldots,6;\ h(\mathbf{q})=1\}\simeq\mathsf{SO}(3)$$

Obviously, the constraints also restrict possible velocities $\mathbf{v}=\dot{\mathbf{q}}$. In particular, (17) gives rise to six constraints on velocity level of the form

$$\frac{\mathrm{d}}{\mathrm{d}t}\Phi_i(\mathbf{q})=\nabla\Phi_i(\mathbf{q})\cdot\dot{\mathbf{q}}=0$$

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Accordingly, the velocity vectors $\mathbf{v}$ have to lie in the tangent space $T_{\mathbf{q}}Q$ at $\mathbf{q}\in Q$, given by

$$T_{\mathbf{q}}\mathsf{Q}=\{\mathbf{v}\in\mathsf{R}^9 \mid \nabla\Phi_i(\mathbf{q})\cdot\mathbf{v}=0,\ i=1,\ldots,6\}$$

Note that in the present case $\dot{\mathbf{q}}\in T_{\mathbf{q}}Q$ can be ensured by introducing the angular velocity vector $\boldsymbol{\omega}\in\mathsf{R}^3$ or, alternatively, its convective counterpart $\boldsymbol{\Omega}=\mathbf{R}^{\mathrm{T}}\boldsymbol{\omega}$, via

$$\dot{\mathbf{d}}_i=\boldsymbol{\omega}\times\mathbf{d}_i=\mathbf{R}(\boldsymbol{\Omega}\times\mathbf{e}_i)$$

For purely rotational motion, the kinetic energy of the rigid body assumes the form

$$T=\tfrac{1}{2}\dot{\mathbf{q}}^{\mathrm{T}}\mathbf{M}_9\dot{\mathbf{q}} \tag{18}$$

with the constant and non-singular 9×9 mass matrix

$$\mathbf{M}_9=\operatorname{diag}(\mathscr{E}_1\mathbf{1}_3,\mathscr{E}_2\mathbf{1}_3,\mathscr{E}_3\mathbf{1}_3) \tag{19}$$

Here, the $\mathscr{E}_i$'s are the principal values of the convective Euler tensor. Note that the Euler tensor $\mathscr{E}$ can be connected with the classical inertia tensor $\mathscr{J}$ through the relationship

$$\mathscr{J}=(\operatorname{tr}\mathscr{E})\mathbf{I}-\mathscr{E} \tag{20}$$

The rotational equations of motion pertaining to the rigid body under consideration can be obtained by applying Lagrange's equations in a straightforward way. To this end, consider the Lagrangian

$$L_\lambda(\mathbf{q},\dot{\mathbf{q}})=T(\dot{\mathbf{q}})-V_\lambda(\mathbf{q}) \quad \text{with } V_\lambda(\mathbf{q})=V(\mathbf{q})+\sum_{i=1}^{6}\lambda_i\Phi_i(\mathbf{q}) \tag{21}$$

For simplicity it has been assumed that the external forces can be derived from a potential function $V(\mathbf{q})$. Now Lagrange's equations may be written in the form

$$\begin{aligned}\frac{\mathrm{d}}{\mathrm{d}t}(\nabla_{\dot{\mathbf{q}}}L_\lambda(\mathbf{q},\dot{\mathbf{q}}))-\nabla_{\mathbf{q}}L_\lambda(\mathbf{q},\dot{\mathbf{q}})&=\mathbf{0}\\ \boldsymbol{\Phi}(\mathbf{q})&=\mathbf{0}\end{aligned} \tag{22}$$

Taking into account (21) and expression (18) for the kinetic energy, $(22)_1$ assumes the specific form

$$\mathbf{M}_9\ddot{\mathbf{q}}+\nabla V(\mathbf{q})+\sum_{i=1}^{6}\lambda_i\nabla\Phi_i(\mathbf{q})=\mathbf{0}$$

We finally remark that the angular momentum of the rigid body relative to its center of mass is given by

$$\mathbf{J}=\sum_{I=1}^{3}\mathscr{E}_I\mathbf{d}_I\times\dot{\mathbf{d}}_I \tag{23}$$

More details about the director-based formulation of rigid body dynamics outlined in this section can be found in Betsch and Steinmann [7] and Betsch and Leyendecker [23], see also the references cited therein.

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4. RIGID BODY DYNAMICS IN TERMS OF QUATERNIONS

We next aim at a rigid body formulation in terms of quaternions. This goal can be achieved by performing a size-reduction of the rigid body formulation outlined in the previous section. To this end, we reconsider the connection between the coordinates $\boldsymbol{\mathfrak{q}} \in \mathsf{S}^3 \subset \mathsf{R}^4$ and $\mathbf{q} \in \mathsf{Q} \subset \mathsf{R}^9$. With regard to (15) and (12) we get

$$\mathbf{d}_I = \mathscr{R}(\boldsymbol{\mathfrak{q}})\mathbf{e}_I = \mathbf{E}(\boldsymbol{\mathfrak{q}})\mathbf{G}(\boldsymbol{\mathfrak{q}})^{\mathrm{T}}\mathbf{e}_I = \mathbf{E}(\boldsymbol{\mathfrak{q}})\,\bar{\mathbf{e}}_I\,\boldsymbol{\mathfrak{q}} \tag{24}$$

where $(\mathrm{A}3)_2$ has been employed. Now, with regard to (16), we introduce the mapping $\mathbf{f}\colon \mathsf{S}^3 \to \mathsf{Q}$ such that

$$\mathbf{q} = \mathbf{f}(\boldsymbol{\mathfrak{q}}) = \mathbf{F}(\boldsymbol{\mathfrak{q}})\boldsymbol{\mathfrak{q}}$$

where the 9×4 matrix $\mathbf{F}(\boldsymbol{\mathfrak{q}})$ is given by

$$\mathbf{F}(\boldsymbol{\mathfrak{q}}) = \begin{bmatrix} \mathbf{E}(\boldsymbol{\mathfrak{q}})\,\bar{\mathbf{e}}_1 \\ \mathbf{E}(\boldsymbol{\mathfrak{q}})\,\bar{\mathbf{e}}_2 \\ \mathbf{E}(\boldsymbol{\mathfrak{q}})\,\bar{\mathbf{e}}_3 \end{bmatrix} \tag{25}$$

Differentiating (24) with respect to time yields

$$\dot{\mathbf{d}}_I = \frac{\mathrm{d}}{\mathrm{d}t}\mathscr{R}(\boldsymbol{\mathfrak{q}})\mathbf{e}_I = 2\mathbf{E}(\boldsymbol{\mathfrak{q}})\mathbf{G}(\dot{\boldsymbol{\mathfrak{q}}})^{\mathrm{T}}\mathbf{e}_I = 2\mathbf{E}(\boldsymbol{\mathfrak{q}})\,\bar{\mathbf{e}}_I\,\dot{\boldsymbol{\mathfrak{q}}} \tag{26}$$

where use has been made of (13). Thus

$$\dot{\mathbf{q}} = D\mathbf{f}(\boldsymbol{\mathfrak{q}})\dot{\boldsymbol{\mathfrak{q}}} \tag{27}$$

where the Jacobian $D\mathbf{f}(\boldsymbol{\mathfrak{q}})$ is given by

$$D\mathbf{f}(\boldsymbol{\mathfrak{q}}) = 2\mathbf{F}(\boldsymbol{\mathfrak{q}}) \tag{28}$$

Now the kinetic energy of the rigid body can be written in terms of quaternions. Inserting (27) into (18) yields

$$T(\boldsymbol{\mathfrak{q}}, \dot{\boldsymbol{\mathfrak{q}}}) = \tfrac{1}{2}\dot{\boldsymbol{\mathfrak{q}}}^{\mathrm{T}}\mathbf{M}_4(\boldsymbol{\mathfrak{q}})\dot{\boldsymbol{\mathfrak{q}}} \tag{29}$$

where the reduced 4×4 mass matrix $\mathbf{M}_4$ is given by

$$\mathbf{M}_4(\boldsymbol{\mathfrak{q}}) = D\mathbf{f}(\boldsymbol{\mathfrak{q}})^{\mathrm{T}}\mathbf{M}_9\,D\mathbf{f}(\boldsymbol{\mathfrak{q}})$$

Taking into account (28), (25) and (19), the last equation gives

$$\begin{aligned} \mathbf{M}_4(\boldsymbol{\mathfrak{q}}) &= 4\mathbf{F}(\boldsymbol{\mathfrak{q}})^{\mathrm{T}}\mathbf{M}_9\mathbf{F}(\boldsymbol{\mathfrak{q}}) = 4\sum_{I=1}^{3}\mathscr{E}_I\,\bar{\mathbf{e}}_I^{\mathrm{T}}\,\mathbf{E}(\boldsymbol{\mathfrak{q}})^{\mathrm{T}}\mathbf{E}(\boldsymbol{\mathfrak{q}})\,\bar{\mathbf{e}}_I = 4\sum_{I=1}^{3}\mathscr{E}_I\{-\bar{\mathbf{e}}_I\bar{\mathbf{e}}_I - \bar{\mathbf{e}}_I\,\boldsymbol{\mathfrak{q}}\otimes(\bar{\mathbf{e}}_I\,\boldsymbol{\mathfrak{q}})\} \\ &= 4\sum_{I=1}^{3}\mathscr{E}_I\{(\mathbf{e}_I\cdot\mathbf{e}_I)\mathbf{I}_4 - \mathbf{G}(\boldsymbol{\mathfrak{q}})^{\mathrm{T}}\mathbf{e}_I\otimes\mathbf{e}_I\mathbf{G}(\boldsymbol{\mathfrak{q}})\} = 4(\mathrm{tr}\,\mathscr{E})\mathbf{I}_4 - 4\mathbf{G}(\boldsymbol{\mathfrak{q}})^{\mathrm{T}}\mathscr{E}\mathbf{G}(\boldsymbol{\mathfrak{q}}) \end{aligned} \tag{30}$$

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where use has been made of $(A1)_3$, (A5) and $(A3)_2$. Alternatively, in the last equation one may employ the convective inertia tensor (20) instead of the convective Euler tensor. In that case one gets

$$\mathbf{M}_4(\mathbf{q}) = 2(\operatorname{tr}\mathscr{J})\mathbf{q}\otimes\mathbf{q} + 4\mathbf{G}(\mathbf{q})^{\mathrm{T}}\mathscr{J}\mathbf{G}(\mathbf{q}) \tag{31}$$

Yet another representation of the mass matrix $\mathbf{M}_4$ follows from (31) by introducing the extended convective inertia matrix

$$\mathscr{J}_4 = \begin{bmatrix} \mathscr{J}_0 & \mathbf{0}^{\mathrm{T}} \\ \mathbf{0} & \mathscr{J} \end{bmatrix}$$

where $\mathscr{J}_0 = \frac{1}{2}\operatorname{tr}\mathscr{J}$. Then (31) can be written in the alternative form

$$\mathbf{M}_4(\mathbf{q}) = 4\mathbf{Q}_l(\mathbf{q})\mathscr{J}_4\mathbf{Q}_l(\mathbf{q})^{\mathrm{T}} \tag{32}$$

The last representation of $\mathbf{M}_4$ is especially useful for calculating the inverse

$$\mathbf{M}_4(\mathbf{q})^{-1} = \tfrac{1}{4}\mathbf{Q}_l(\mathbf{q})\mathscr{J}_4^{-1}\mathbf{Q}_l(\mathbf{q})^{\mathrm{T}} \tag{33}$$

where use has been made of property $(A4)_1$ along with $\mathbf{q}\in \mathsf{S}^3$.

We next write the angular momentum (23) of the rigid body in terms of quaternions. For this purpose, we make use of the relationship

$$\widehat{\mathbf{d}}_I = -\mathbf{E}(\mathbf{q})\,\bar{\mathbf{e}}_I\,\mathbf{E}(\mathbf{q})^{\mathrm{T}} \tag{34}$$

which is verified in Appendix B. Now, expression (23) for the angular momentum can be rewritten in the form

$$\mathbf{J} = \sum_{I=1}^{3}\mathscr{E}_I\widehat{\mathbf{d}}_I\dot{\mathbf{d}}_I = 2\mathbf{E}(\mathbf{q})\sum_{I=1}^{3}\mathscr{E}_I\,\bar{\mathbf{e}}_I^{\mathrm{T}}\,\mathbf{E}(\mathbf{q})^{\mathrm{T}}\mathbf{E}(\mathbf{q})\,\bar{\mathbf{e}}_I\,\dot{\mathbf{q}}$$

where (26) and the skew-symmetry of $\bar{\mathbf{e}}_I$ have been taken into account. Incorporating the mass matrix (30) into the last equation, the angular momentum assumes the form

$$\mathbf{J} = \tfrac{1}{2}\mathbf{E}(\mathbf{q})\mathbf{M}_4(\mathbf{q})\dot{\mathbf{q}} \tag{35}$$

Remark 4.1
In contrast to the procedure outlined above, in previous works (see, e.g. [1–3, 5, 9, 10]) the deduction of the quaternion mass matrix relies on the classical inertia matrix. Accordingly, the kinetic energy is written in the standard form $T = \frac{1}{2}\boldsymbol{\Omega}\cdot\mathscr{J}\boldsymbol{\Omega}$. Then the relationship $\boldsymbol{\Omega} = 2\mathbf{G}(\mathbf{q})\dot{\mathbf{q}}$ from (14) is employed to arrive at $T = \frac{1}{2}\dot{\mathbf{q}}\cdot\widetilde{\mathbf{M}}_4(\mathbf{q})\dot{\mathbf{q}}$, where $\widetilde{\mathbf{M}}_4(\mathbf{q}) = 4\mathbf{G}(\mathbf{q})^{\mathrm{T}}\mathbf{J}\mathbf{G}(\mathbf{q})$. Since the 3×4 matrix $\mathbf{G}$ has rank three, the mass matrix $\widetilde{\mathbf{M}}_4$ is singular. The singular mass matrix $\widetilde{\mathbf{M}}_4$ can be linked to the present one through

$$\mathbf{M}_4(\mathbf{q}) = \widetilde{\mathbf{M}}_4(\mathbf{q}) + 2\operatorname{tr}(\mathscr{J})\mathbf{q}\otimes\mathbf{q}$$

Thus, the non-singularity of $\mathbf{M}_4$ is due to a rank-one augmentation of $\widetilde{\mathbf{M}}_4$.

4.1. Hamiltonian formulation

We next aim at a Hamiltonian formulation of the rigid body dynamics in terms of quaternions. To perform the transition to the Hamiltonian framework, we introduce the quaternion momentum

$$\mathbb{p} = \nabla_{\dot{\mathbb{q}}} T(\mathbb{q}, \dot{\mathbb{q}}) = \mathbf{M}_4(\mathbb{q})\dot{\mathbb{q}}$$

Inserting

$$\dot{\mathbb{q}} = \mathbf{M}_4(\mathbb{q})^{-1}\mathbb{p}$$

into expression (29) for the kinetic energy yields

$$T(\mathbb{q}, \mathbb{p}) = \tfrac{1}{2}\mathbb{p}^{\mathrm{T}}\mathbf{M}_4(\mathbb{q})^{-1}\mathbb{p}$$

For later use we provide alternative representations of $T(\mathbb{q}, \mathbb{p})$. Taking into account expression (33) for $\mathbf{M}_4(\mathbb{q})^{-1}$, we obtain

$$\begin{aligned} T(\mathbb{q}, \mathbb{p}) &= \tfrac{1}{8}\mathbb{p}^{\mathrm{T}}\mathbf{Q}_l(\mathbb{q})\mathscr{J}_4^{-1}\mathbf{Q}_l(\mathbb{q})^{\mathrm{T}}\mathbb{p} = \tfrac{1}{8}[\mathscr{J}_0^{-1}(\mathbb{q}\cdot\mathbb{p})^2 + \mathbb{p}^{\mathrm{T}}\mathbf{G}(\mathbb{q})^{\mathrm{T}}\mathscr{J}^{-1}\mathbf{G}(\mathbb{q})\mathbb{p}] \\ &= \tfrac{1}{8}[\mathscr{J}_0^{-1}(\mathbb{q}\cdot\mathbb{p})^2 + \mathbb{q}^{\mathrm{T}}\mathbf{G}(\mathbb{p})^{\mathrm{T}}\mathscr{J}^{-1}\mathbf{G}(\mathbb{p})\mathbb{q}] = \tfrac{1}{8}\mathbb{q}^{\mathrm{T}}\mathbf{Q}_l(\mathbb{p})\mathscr{J}_4^{-1}\mathbf{Q}_l(\mathbb{p})^{\mathrm{T}}\mathbb{q} \end{aligned} \tag{36}$$

where use has been made of $(10)_1$ and $(\mathrm{A2})_2$. We next introduce the augmented Hamiltonian

$$H_\lambda(\mathbb{q}, \mathbb{p}) = T(\mathbb{q}, \mathbb{p}) + V_\lambda(\mathbb{q}) \quad \text{with } V_\lambda(\mathbb{q}) = V(\mathbb{q}) + \lambda g(\mathbb{q})$$

Here, it has been tacitly assumed that the external loads can be derived from a potential function $V(\mathbb{q})$. Moreover, $g : \mathsf{R}^4 \to \mathsf{R}$ denotes a constraint function given by

$$g(\mathbb{q}) = \tfrac{1}{2}(\mathbb{q}\cdot\mathbb{q} - 1) \tag{37}$$

Now the Hamiltonian form of the equations governing the rotational motion of a rigid body can be written as

$$\begin{aligned} \dot{\mathbb{q}} &= \nabla_{\mathbb{p}} H_\lambda(\mathbb{q}, \mathbb{p}) \\ \dot{\mathbb{p}} &= -\nabla_{\mathbb{q}} H_\lambda(\mathbb{q}, \mathbb{p}) \\ 0 &= g(\mathbb{q}) \end{aligned} \tag{38}$$

Accordingly, the equations of motion assume the form of differential-algebraic equations (DAEs). Note that the algebraic constraint equation $(38)_3$ ensures that $\mathbb{q} \in \mathsf{S}^3 \subset \mathsf{R}^4$. With regard to (36), the differential part of the DAEs can also be written as

$$\begin{aligned} \dot{\mathbb{q}} &= \tfrac{1}{4}\mathbf{Q}_l(\mathbb{q})\mathscr{J}_4^{-1}\mathbf{Q}_l(\mathbb{q})^{\mathrm{T}}\mathbb{p} \\ \dot{\mathbb{p}} &= -\tfrac{1}{4}\mathbf{Q}_l(\mathbb{p})\mathscr{J}_4^{-1}\mathbf{Q}_l(\mathbb{p})^{\mathrm{T}}\mathbb{q} - \nabla V_\lambda(\mathbb{q}) \end{aligned}$$

or

$$\begin{aligned} \dot{\mathbb{q}} &= \tfrac{1}{4}[\mathscr{J}_0^{-1}(\mathbb{q}\cdot\mathbb{p})\mathbb{q} + \mathbf{G}(\mathbb{q})^{\mathrm{T}}\mathscr{J}^{-1}\mathbf{G}(\mathbb{q})\mathbb{p}] \\ \dot{\mathbb{p}} &= -\tfrac{1}{4}[\mathscr{J}_0^{-1}(\mathbb{q}\cdot\mathbb{p})\mathbb{p} + \mathbf{G}(\mathbb{p})^{\mathrm{T}}\mathscr{J}^{-1}\mathbf{G}(\mathbb{p})\mathbb{q}] - \nabla V(\mathbb{q}) - \lambda\mathbb{q} \end{aligned} \tag{39}$$

It is worth noting that the configuration-level constraint $(38)_3$ implies a hidden constraint on the momentum level, which can be obtained by differentiating (37) with respect to time:

$$\frac{\mathrm{d}}{\mathrm{d}t} g(\mathbb{q}) = Dg(\mathbb{q})\nabla_{\mathbb{p}} H_\lambda(\mathbb{q},\mathbb{p}) = \mathbb{q}^{\mathrm{T}} \tfrac{1}{4}\mathscr{I}_0^{-1}(\mathbb{q}\cdot\mathbb{p})\mathbb{q}$$

Here, use has been made of $(39)_1$ and $(\mathrm{A1})_1$. Accordingly, $(38)_3$ gives rise to the momentum-level constraint

$$\mathbb{q}\cdot\mathbb{p} = 0 \tag{40}$$

Correspondingly, the phase space coordinates $(\mathbb{q},\mathbb{p})$ are constrained to lie on the manifold

$$\mathsf{P} = \{(\mathbb{q},\mathbb{p}) \in \mathsf{R}^4 \times \mathsf{R}^4 \,|\, \mathbb{q}\cdot\mathbb{q} = 1,\ \mathbb{q}\cdot\mathbb{p} = 0\}$$

Remark 4.2
The Lagrange multiplier in the above Hamiltonian equations of motion may be expressed in terms of $\mathbb{q}\in\mathsf{S}^3$. To see this, differentiate (40) once more with respect to time to obtain

$$\mathbb{q}\cdot\dot{\mathbb{p}} + \mathbb{p}\cdot\dot{\mathbb{q}} = 0$$

Substituting from (39) into the last equation, a straightforward calculation yields the result

$$\lambda(\mathbb{q}) = -\mathbb{q}\cdot\nabla V(\mathbb{q})$$

4.2. Rotational invariance and conservation of angular momentum

We next verify that the augmented Hamiltonian of the free rigid body is invariant under rotations. In particular, the constraint $g(\mathbb{q})$ and the kinetic energy $T(\mathbb{q},\mathbb{p})$ are invariant under the group S^3 acting by rotations on $(\mathbb{q},\mathbb{p})$. Rotational invariance implies that

$$\begin{aligned} g(\mathbb{q}^\sharp) &= g(\mathbb{q}) \\ T(\mathbb{q}^\sharp,\mathbb{p}^\sharp) &= T(\mathbb{q},\mathbb{p}) \end{aligned} \tag{41}$$

where

$$\begin{aligned} \mathbb{q}^\sharp &= \mathbf{Q}_l(\mathbb{r})\mathbb{q} \\ \mathbb{p}^\sharp &= (\mathbf{Q}_l(\mathbb{r})^{\mathrm{T}})^{-1}\mathbb{p} = \mathbf{Q}_l(\mathbb{r})\mathbb{p} \end{aligned}$$

for $\mathbb{r}\in\mathsf{S}^3$. Concerning the constraint (37) we get

$$g(\mathbb{q}^\sharp) = \tfrac{1}{2}(\mathbb{q}^\sharp\cdot\mathbb{q}^\sharp - 1) = \tfrac{1}{2}(\mathbb{q}\cdot\mathbf{Q}_l(\mathbb{r})^{\mathrm{T}}\mathbf{Q}_l(\mathbb{r})\mathbb{q} - 1) = \tfrac{1}{2}(\mathbb{q}\cdot\mathbb{q} - 1) = g(\mathbb{q}) \tag{42}$$

where the orthogonality of $\mathbf{Q}_l(\mathbb{r})$, see $(\mathrm{A4})_1$, has been taken into account. With regard to the kinetic energy (36), we first show that $\mathbf{Q}_l(\mathbb{q})^{\mathrm{T}}\mathbb{p}$ is invariant under rotations. To this end we consider the corresponding quaternion multiplication $\overline{\mathbb{q}}\circ\mathbb{p}$. In particular,

$$\overline{\mathbb{q}}^\sharp\circ\mathbb{p}^\sharp = (\overline{\mathbb{r}\circ\mathbb{q}})\circ(\mathbb{r}\circ\mathbb{p}) = \overline{\mathbb{q}}\circ\overline{\mathbb{r}}\circ\mathbb{r}\circ\mathbb{p} = \mathbb{q}\circ\mathbb{p}$$

which implies that

$$\mathbf{Q}_l(\mathbb{q}^\sharp)^{\mathrm{T}}\mathbb{p}^\sharp = \mathbf{Q}_l(\mathbb{q})^{\mathrm{T}}\mathbb{p} \tag{43}$$

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Consequently, invariance property $(41)_2$ is satisfied as well. For the free rigid body, the above invariance properties imply rotational invariance of the augmented Hamiltonian

$$H_\lambda\left(\exp_{\mathsf{O}(4)}\left(\frac{\varepsilon}{2}\overset{+}{\boldsymbol{\xi}}\right)\mathbb{q}, \exp_{\mathsf{O}(4)}\left(\frac{\varepsilon}{2}\overset{+}{\boldsymbol{\xi}}\right)\mathbb{p}\right) = H_\lambda(\mathbb{q},\mathbb{p})$$

for $\varepsilon \in \mathsf{R}$ and $\boldsymbol{\xi} \in \mathsf{R}^3$. Here, the exponential map $\exp_{\mathsf{O}(4)}: \mathsf{R}^3 \rightarrow \mathsf{O}(4)$ is given by (A6). The last equation leads to

$$\begin{aligned}\left.\frac{\mathrm{d}}{\mathrm{d}\varepsilon}\right|_{\varepsilon=0} H_\lambda\left(\exp_{\mathsf{O}(4)}\left(\frac{\varepsilon}{2}\overset{+}{\boldsymbol{\xi}}\right)\mathbb{q}, \exp_{\mathsf{O}(4)}\left(\frac{\varepsilon}{2}\overset{+}{\boldsymbol{\xi}}\right)\mathbb{p}\right) &= 0 \\ \frac{1}{2}\nabla_{\mathbb{q}} H_\lambda(\mathbb{q},\mathbb{p})\cdot\overset{+}{\boldsymbol{\xi}}\mathbb{q} + \frac{1}{2}\nabla_{\mathbb{p}} H_\lambda(\mathbb{q},\mathbb{p})\cdot\overset{+}{\boldsymbol{\xi}}\mathbb{p} &= 0\end{aligned} \tag{44}$$

Rotational invariance of the augmented Hamiltonian can be linked to the conservation of a momentum map $\mathbf{J} \in \mathsf{R}^3$. To see this, consider $J_\xi(\mathbb{q},\mathbb{p}) = \mathbf{J}(\mathbb{q},\mathbb{p})\cdot\boldsymbol{\xi}$ and

$$\frac{\mathrm{d}}{\mathrm{d}t} J_\xi(\mathbb{q},\mathbb{p}) = -\nabla_{\mathbb{p}} J_\xi(\mathbb{q},\mathbb{p})\cdot\nabla_{\mathbb{q}} H_\lambda(\mathbb{q},\mathbb{p}) + \nabla_{\mathbb{q}} J_\xi(\mathbb{q},\mathbb{p})\cdot\nabla_{\mathbb{p}} H_\lambda(\mathbb{q},\mathbb{p})$$

Comparison of the last equation with $(44)_2$ leads to the conclusion that $J_\xi(\mathbb{q},\mathbb{p})$ is a first integral if the following conditions are satisfied:

$$\begin{aligned}\nabla_{\mathbb{p}} J_\xi(\mathbb{q},\mathbb{p}) &= \tfrac{1}{2}\overset{+}{\boldsymbol{\xi}}\mathbb{q} \\ \nabla_{\mathbb{q}} J_\xi(\mathbb{q},\mathbb{p}) &= -\tfrac{1}{2}\overset{+}{\boldsymbol{\xi}}\mathbb{p}\end{aligned}$$

To solve the above equations we choose

$$J_\xi(\mathbb{q},\mathbb{p}) = \tfrac{1}{2}\mathbb{p}\cdot\overset{+}{\boldsymbol{\xi}}\mathbb{q} = \tfrac{1}{2}\mathbb{p}\cdot\mathbf{E}(\mathbb{q})^{\mathrm{T}}\boldsymbol{\xi} \tag{45}$$

Note that on the right-hand side of the last equation property $(\mathrm{A}3)_1$ has been used. According to (45), the momentum map associated with rotational invariance of the system under consideration is given by

$$\mathbf{J}(\mathbb{q},\mathbb{p}) = \tfrac{1}{2}\mathbf{E}(\mathbb{q})\mathbb{p}$$

and thus is identical to the spatial angular momentum (35).

4.3. Introduction of invariants

Owing to the rotational invariance of the kinetic energy $T(\mathbb{q},\mathbb{p})$ and the constraint $g(\mathbb{q})$, it is possible to reparametrize both functions in terms of appropriate invariants. We shall employ these invariants in the numerical discretization of the equations of motion. With regard to (43) and (42), we introduce the invariants

$$\boldsymbol{\pi}(\mathbb{q},\mathbb{p}) = \mathbf{Q}_l(\mathbb{q})^{\mathrm{T}}\mathbb{p} = \begin{bmatrix}\mathbb{q}\cdot\mathbb{p} \\ \mathbf{G}(\mathbb{q})\mathbb{p}\end{bmatrix} = \begin{bmatrix}\pi_0(\mathbb{q},\mathbb{p}) \\ \boldsymbol{\Pi}(\mathbb{q},\mathbb{p})\end{bmatrix} \tag{46}$$

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and

$$\eta(\mathbf{q}) = \mathbf{q} \cdot \mathbf{q} \tag{47}$$

Accordingly, we get

$$T(\mathbf{q}, \mathbf{p}) = \tilde{T}(\boldsymbol{\pi}(\mathbf{q}, \mathbf{p})) = \tfrac{1}{8}\boldsymbol{\pi}(\mathbf{q}, \mathbf{p}) \cdot \mathscr{J}_4^{-1}\boldsymbol{\pi}(\mathbf{q}, \mathbf{p}) \tag{48}$$

and

$$g(\mathbf{q}) = \tilde{g}(\eta(\mathbf{q})) = \tfrac{1}{2}(\eta(\mathbf{q}) - 1)$$

In anticipation of the time discretization, it is illustrative to recast the differential part of the DAEs (38) in terms of the invariants (46) and (47). Accordingly,

$$\begin{aligned} \dot{\mathbf{q}} &= \nabla_{\mathbf{p}} T(\mathbf{q}, \mathbf{p}) \\ \dot{\mathbf{p}} &= -\nabla_{\mathbf{q}} T(\mathbf{q}, \mathbf{p}) - \nabla V(\mathbf{q}) - \lambda \nabla g(\mathbf{q}) \end{aligned}$$

can be written in the form

$$\begin{aligned} \dot{\mathbf{q}} &= \left(\frac{\partial \boldsymbol{\pi}}{\partial \mathbf{p}}\right)^{\mathrm{T}} \nabla \tilde{T}(\boldsymbol{\pi}) \\ \dot{\mathbf{p}} &= -\left(\frac{\partial \boldsymbol{\pi}}{\partial \mathbf{q}}\right)^{\mathrm{T}} \nabla \tilde{T}(\boldsymbol{\pi}) - \nabla V(\mathbf{q}) - \lambda \nabla \eta(\mathbf{q}) \tilde{g}'(\eta) \end{aligned}$$

or

$$\begin{aligned} \dot{\mathbf{q}} &= \tfrac{1}{4}[\mathbf{q} \quad \mathbf{G}(\mathbf{q})^{\mathrm{T}}]\mathscr{J}_4^{-1}\boldsymbol{\pi}(\mathbf{q}, \mathbf{p}) \\ \dot{\mathbf{p}} &= -\tfrac{1}{4}[\mathbf{p} \quad -\mathbf{G}(\mathbf{p})^{\mathrm{T}}]\mathscr{J}_4^{-1}\boldsymbol{\pi}(\mathbf{q}, \mathbf{p}) - \nabla V(\mathbf{q}) - \lambda \mathbf{q} \end{aligned} \tag{49}$$

Of course, the above equations are equivalent to those in (39).

4.4. Discretization

We next perform the time discretization of the DAEs (38). To this end, we apply the conserving one-step method due to Gonzalez [24], which fits into the framework of the mixed Galerkin method (specifically the mG(1) method) developed by Betsch and Steinmann [25]. Let the phase space coordinates $(\mathbf{q}_n, \mathbf{p}_n) \in \mathsf{P}$ at time t_n along with the step-size Δt be given. Then approximations of the quantities $(\mathbf{q}_{n+1}, \mathbf{p}_{n+1}) \in \mathsf{R}^4 \times \mathsf{R}^4$ and $\lambda \in \mathsf{R}$ at time t_{n+1} follow from the scheme:

$$\begin{aligned} \mathbf{q}_{n+1} - \mathbf{q}_n &= \Delta t \overline{\nabla}_{\mathbf{p}} H_\lambda(\mathbf{q}_n, \mathbf{p}_n, \mathbf{q}_{n+1}, \mathbf{p}_{n+1}) \\ \mathbf{p}_{n+1} - \mathbf{p}_n &= -\Delta t \overline{\nabla}_{\mathbf{q}} H_\lambda(\mathbf{q}_n, \mathbf{p}_n, \mathbf{q}_{n+1}, \mathbf{p}_{n+1}) \\ 0 &= g(\mathbf{q}_{n+1}) \end{aligned} \tag{50}$$

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Here, $\overline{\nabla}_{\mathbf{q}}$ and $\overline{\nabla}_{\mathbf{p}}$ denote discrete derivatives in the sense of Gonzalez [26]. In particular, the scheme (50) assumes the form

$$\begin{aligned}
\mathbf{q}_{n+1}-\mathbf{q}_n &= \frac{\Delta t}{8}[\mathbf{q}_{n+1/2}\mathbf{G}(\mathbf{q}_{n+1/2})^{\mathrm{T}}]\mathscr{I}_4^{-1}[\boldsymbol{\pi}_n+\boldsymbol{\pi}_{n+1}] \\
\mathbf{p}_{n+1}-\mathbf{p}_n &= -\frac{\Delta t}{8}[\mathbf{p}_{n+1/2}-\mathbf{G}(\mathbf{p}_{n+1/2})^{\mathrm{T}}]\mathscr{I}_4^{-1}[\boldsymbol{\pi}_n+\boldsymbol{\pi}_{n+1}]-\Delta t\overline{\nabla}V(\mathbf{q}_n,\mathbf{q}_{n+1})-\Delta t\lambda\mathbf{q}_{n+1/2} \\
0 &= \tfrac{1}{2}(\mathbf{q}_{n+1}\cdot\mathbf{q}_{n+1}-1)
\end{aligned} \tag{51}$$

where the abbreviations

$$\boldsymbol{\pi}_n=\boldsymbol{\pi}(\mathbf{q}_n,\mathbf{p}_n) \quad \text{and} \quad \boldsymbol{\pi}_{n+1}=\boldsymbol{\pi}(\mathbf{q}_{n+1},\mathbf{p}_{n+1})$$

together with $(\bullet)_{n+1/2}=\frac{1}{2}((\bullet)_n+(\bullet)_{n+1})$ have been introduced. Moreover, for the present purposes it suffices to choose $\overline{\nabla}V(\mathbf{q}_n,\mathbf{q}_{n+1})=\nabla V(\mathbf{q}_{n+1/2})$. Note that the first two equations in (51) can be viewed as discrete counterparts of those in (49).

By design, the scheme (51) conserves both angular momentum and energy (see Appendix C for a verification). Moreover, with regard to $(51)_3$, $\mathbf{q}_{n+1}\in\mathsf{S}^3$. In addition to that, in the present case, the momentum-level constraint (40) is satisfied too. To see this, pre-multiply $(51)_1$ by $\mathbf{q}_{n+1/2}^{\mathrm{T}}$ to get

$$\begin{aligned}
\mathbf{q}_{n+1/2}\cdot(\mathbf{q}_{n+1}-\mathbf{q}_n) &= \frac{\Delta t}{8}|\mathbf{q}_{n+1/2}|^2\mathscr{I}_0^{-1}[\pi_{0,n}+\pi_{0,n+1}] \\
\frac{1}{2}(\mathbf{q}_{n+1}\cdot\mathbf{q}_{n+1}-\mathbf{q}_n\cdot\mathbf{q}_n) &= \frac{\Delta t}{8}|\mathbf{q}_{n+1/2}|^2\mathscr{I}_0^{-1}[\mathbf{q}_n\cdot\mathbf{p}_n+\mathbf{q}_{n+1}\cdot\mathbf{p}_{n+1}]
\end{aligned}$$

where use has been made of (46) and $(\mathrm{A}1)_1$. Accordingly, provided that $(\mathbf{q}_n,\mathbf{p}_n)\in\mathsf{P}$ and $\mathbf{q}_{n+1}\in\mathsf{S}^3$, the last equation yields

$$\mathbf{q}_{n+1}\cdot\mathbf{p}_{n+1}=0$$

so that indeed $(\mathbf{q}_{n+1},\mathbf{p}_{n+1})\in\mathsf{P}$.

4.5. Implementation

The scheme (51) constitutes a system of nine non-linear algebraic equations for the determination of $\mathbf{q}_{n+1},\mathbf{p}_{n+1}\in\mathsf{R}^4$ and $\lambda\in\mathsf{R}$. Application of Newton's method leads to a generalized saddle point system, which has to be solved in each iteration. The solution of saddle point systems can be circumvented by eliminating the Lagrange multiplier λ from $(51)_2$. This task can be accomplished by applying the discrete null space method originally developed in [23, 27]. We first recast $(51)_{1,2}$ in the form

$$\begin{aligned}
\mathbf{q}_{n+1}-\mathbf{q}_n &= \frac{\Delta t}{8}\mathbf{Q}_l(\mathbf{q}_{n+1/2})\mathscr{I}_4^{-1}[\mathbf{Q}_l(\mathbf{q}_n)^{\mathrm{T}}\mathbf{p}_n+\mathbf{Q}_l(\mathbf{q}_{n+1})^{\mathrm{T}}\mathbf{p}_{n+1}] \\
\mathbf{p}_{n+1}-\mathbf{p}_n &= -\frac{\Delta t}{8}\mathbf{Q}_l(\mathbf{p}_{n+1/2})\mathscr{I}_4^{-1}[\mathbf{Q}_l(\mathbf{p}_n)^{\mathrm{T}}\mathbf{q}_n+\mathbf{Q}_l(\mathbf{p}_{n+1})^{\mathrm{T}}\mathbf{q}_{n+1}] \\
&\quad -\Delta t\nabla V(\mathbf{q}_{n+1/2})-\Delta t\lambda\mathbf{q}_{n+1/2}
\end{aligned} \tag{52}$$

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To achieve a first size-reduction of the algebraic system (52), we make use of the 3×4 matrix $\mathbf{G}(\mathbb{q}_{n+1/2})$, which plays the role of a discrete null space matrix. Pre-multiplying $(52)_2$ by $\mathbf{G}(\mathbb{q}_{n+1/2})$ annihilates the discrete constraint force due to property $(\mathrm{A}1)_1$:

$$\mathbf{G}(\mathbb{q}_{n+1/2})\{\mathbb{p}_{n+1}-\mathbb{p}_n\} = -\frac{\Delta t}{8}\mathbf{G}(\mathbb{q}_{n+1/2})\{\mathbf{Q}_l(\mathbb{p}_{n+1/2})\mathscr{I}_4^{-1}[\mathbf{Q}_l(\mathbb{p}_n)^{\mathrm{T}}\mathbb{q}_n+\mathbf{Q}_l(\mathbb{p}_{n+1})^{\mathrm{T}}\mathbb{q}_{n+1}]\}$$
$$-\Delta t\,\mathbf{G}(\mathbb{q}_{n+1/2})\nabla V(\mathbb{q}_{n+1/2}) \tag{53}$$

In a second step we perform a reparametrization of the unknowns

$$\mathbb{q}_{n+1}(\boldsymbol{\theta}) = \exp_{\mathsf{S}^3}((0, \tfrac{1}{2}\boldsymbol{\theta}))\circ\mathbb{q}_n \tag{54}$$

where $\exp_{\mathsf{S}^3}:\mathsf{R}^3\to\mathsf{S}^3$ has been introduced in Section 2.3. Accordingly, the four original unknowns $\mathbb{q}_{n+1}\in\mathsf{R}^4$ are replaced by $\boldsymbol{\theta}\in\mathsf{R}^3$, which plays the role of an incremental rotation vector. Note that the constraint $(51)_3$ is identically satisfied by employing the reparametrization (54). To summarize, application of the discrete null space method leads to the reduced system of seven non-linear algebraic equations consisting of $(52)_1$ and (53). In these equations $\mathbb{q}_{n+1}$ is expressed in terms of $\boldsymbol{\theta}\in\mathsf{R}^3$ via (54). The reduced system of equations can be solved iteratively by applying Newton's method. We refer to Appendix D for further details of the implementation.

Remark 4.3
Once $(\mathbb{q}_{n+1}, \mathbb{p}_{n+1})$ have been determined, the discrete Lagrange multiplier of the original scheme (51) may be calculated as follows. It can be easily shown by a straightforward calculation that

$$\mathbb{q}_{n+1/2}\cdot(\mathbb{p}_{n+1}-\mathbb{p}_n)+\mathbb{p}_{n+1/2}\cdot(\mathbb{q}_{n+1}-\mathbb{q}_n)=0$$

In this connection, the properties $(\mathbb{q}_n, \mathbb{p}_n)\in\mathsf{P}$ and $(\mathbb{q}_{n+1}, \mathbb{p}_{n+1})\in\mathsf{P}$ have been used. Inserting from $(51)_{1,2}$ into the last equation yields

$$\lambda(\mathbb{q}_n, \mathbb{q}_{n+1}) = -\frac{\mathbb{q}_{n+1/2}\cdot\overline{\nabla}V(\mathbb{q}_n, \mathbb{q}_{n+1})}{|\mathbb{q}_{n+1/2}|^2}$$

The last equation can be viewed as discrete analogue of the result outlined in Remark 4.2.

5. NUMERICAL EXAMPLES

In this section two representative numerical examples are presented. In this connection, the following integrators have been applied:

QUAT_EM Present quaternion-based energy–momentum scheme.
QUAT_VI Quaternion-based variational integrator summarized in Appendix E.
DIR_EM Director-based energy–momentum scheme, see References [7, 23] and Section 3.
ALGO_C1 Momentum conserving scheme due to Simo and Wong [14].

5.1. Free motion of a rigid body

The first example deals with the free rotational motion of a rigid body. The data for this example have been taken from Betsch and Steinmann [7]. Accordingly, the principal values of the convective

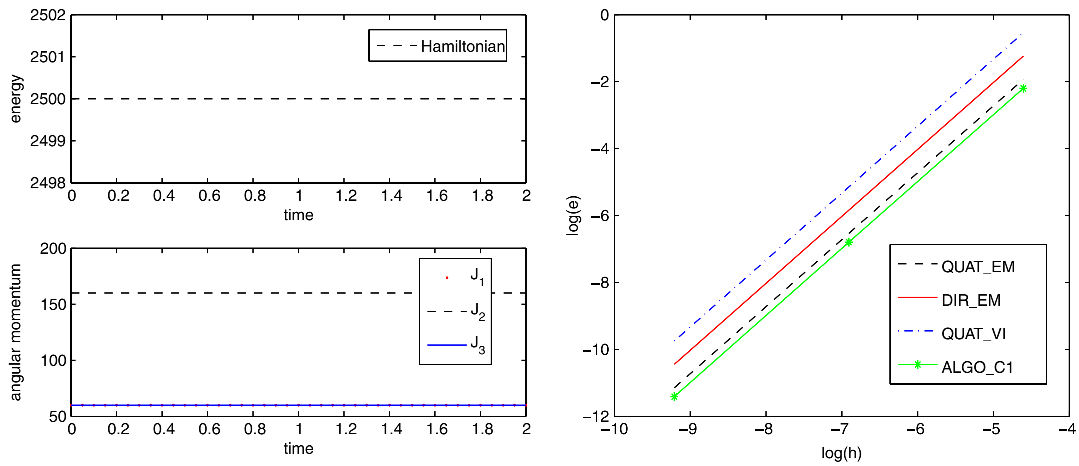

Figure 1. Free motion of a rigid body. Left: algorithmic conservation properties of **QUAT_EM** ($\Delta t = 0.05$). Right: comparison of the configuration error.

inertia tensor (20) are given by $\mathscr{J}_1 = 6$, $\mathscr{J}_2 = 8$ and $\mathscr{J}_3 = 3$. The initial values are specified by $\mathfrak{q}_0 = (1, \mathbf{0})$ and $\mathbf{\Omega}_0 = [10, 20, 20]$.

5.1.1. Algorithmic conservation properties. The newly developed time-stepping scheme **QUAT_EM** does indeed conserve energy and angular momentum. The algorithmic conservation properties can be observed from Figure 1. These results have been obtained by applying a fairly large step-size $\Delta t = 0.05$.

5.1.2. Accuracy. We next compare the accuracy of the present quaternion-based energy–momentum integrator **QUAT_EM** with that of the director-based integrator **DIR_EM**. In addition to that, comparison is made with the schemes **QUAT_VI** and **ALGO_C1**. To this end, a reference solution $\mathbf{R}_{\text{ref}}(T)$ at $T = 1$ is calculated with $\Delta t = 10^{-6}$. Then the configuration error is obtained by evaluating the formula $e = \| \mathbf{R}_{\text{ref}}(T) \cdot \mathbf{R}(T)^{\mathrm{T}} - \mathbf{I}_3 \|$, where $\| \ \|$ denotes the Frobenius norm. The results are depicted in Figure 1.

5.2. Steady precession of a gyro top

The second numerical example deals with a heavy symmetrical top and has been taken from Betsch and Leyendecker [23]. One point on the symmetry axis of the top is fixed to the origin of the inertial frame $\{\mathbf{e}_1, \mathbf{e}_2, \mathbf{e}_3\}$ (Figure 2). The shape of the top is assumed to be a cone with height $H = 0.1$ and radius $R = 0.05$. The total mass of the top is given by $M = \frac{1}{3}\rho\pi R^2 H$, where the mass density is assumed to be $\rho = 2700$. The principal moments of inertia relative to the center of mass are given by $\bar{\mathscr{J}}_1 = \bar{\mathscr{J}}_2 = (3M/80)(4R^2 + H^2)$ and $\bar{\mathscr{J}}_3 = (3M/10)R^2$. The principal values of the convective inertia tensor relative to the point of attachment follow from

$$\mathscr{J}_1 = \bar{\mathscr{J}}_1 + ML^2 \quad \text{and} \quad \mathscr{J}_3 = \bar{\mathscr{J}}_3$$

where $L = \frac{3}{4}H$ denotes the distance between the center of mass and the origin.

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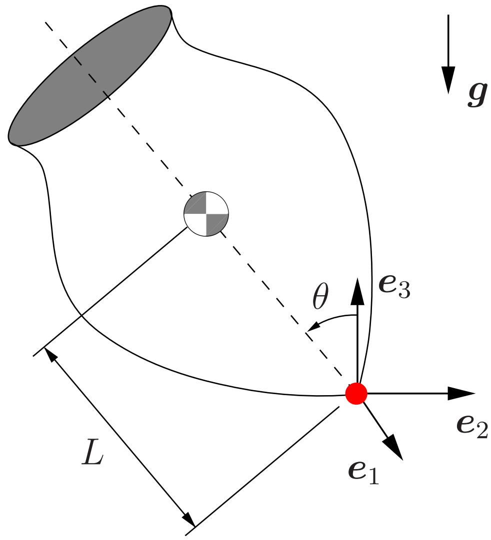

Figure 2. Symmetrical top.

Gravity is acting on the top such that the potential energy function is given by

$$V(\mathbf{q}) = MgL\mathbf{d}_3(\mathbf{q})\cdot\mathbf{e}_3$$

where $\mathbf{d}_3(\mathbf{q}) = \mathscr{R}(\mathbf{q})\mathbf{e}_3$ and $g = 9.81$ denotes the gravitational acceleration. A straightforward calculation along the lines of (26) yields

$$\nabla V(\mathbf{q}) = -2MgL\,\bar{\mathbf{e}}_3\,\mathbf{E}(\mathbf{q})^{\mathrm{T}}\mathbf{e}_3$$

5.2.1. Initial conditions. The initial configuration of the top is specified by

$$\mathbf{q}_0 = \left(\cos\left(\frac{\theta_0}{2}\right), \sin\left(\frac{\theta_0}{2}\right)\mathbf{e}_1\right) \quad \text{with } \theta_0 = \frac{\pi}{3}$$

In order to provide an analytical reference solution we consider the case of precession with no nutation. Let θ be the angle of nutation, ω_p the precession rate and ω_s the spin rate. Specifically, as initial values we choose

$$\theta = \theta_0 \quad \text{and} \quad \omega_p = 10$$

The condition for steady precession is given by (see, for example, Moon [28, Section 5.3])

$$\omega_s = \frac{MgL}{\mathscr{J}_3\omega_p} + \frac{\mathscr{J}_1 - \mathscr{J}_3}{\mathscr{J}_3}\omega_p\cos\theta$$

Accordingly, the initial angular velocity vector can be written as

$$\boldsymbol{\omega}_0 = \omega_p\mathbf{e}_3 + \omega_s\mathbf{d}_3$$

5.2.2. Algorithmic conservation properties. In the present example both the total energy and the 3-component of the angular momentum vector are first integrals of the motion. The newly developed quaternion-based energy–momentum scheme **QUAT_EM** does indeed conserve these quantities, independent of the step-size. This is shown in Figure 3 for a fairly large step-size of $\Delta t = 0.01$.

5.2.3. Accuracy. To evaluate the accuracy of the time-stepping schemes under consideration, we compare the numerical results with the analytical reference solution. To this end, we consider the

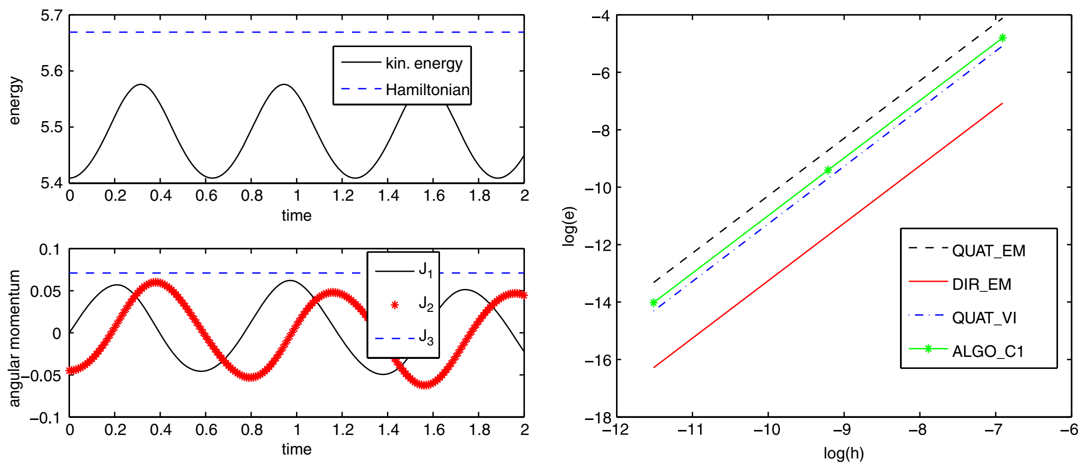

Figure 3. Steady precession of a gyro top: Left: conservation of the total energy and the 3-component of the angular momentum (**QUAT_EM**, $\Delta t = 0.01$). Right: relative error for the motion of the center of mass.

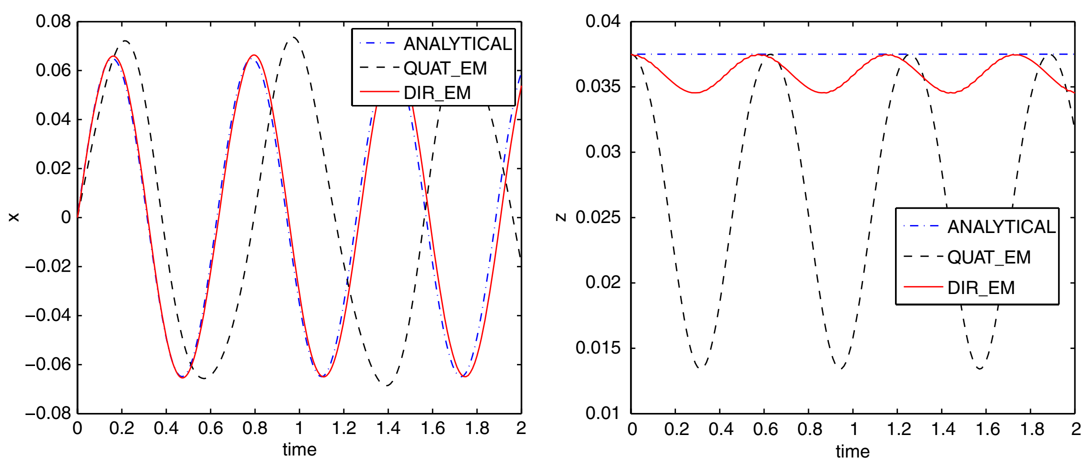

Figure 4. Steady precession of a gyro top: comparison between the analytical solution for the coordinates $x(t)$, $z(t)$ of the center of mass and the numerical results of **QUAT_EM** and **DIR_EM** ($\Delta t = 0.01$).

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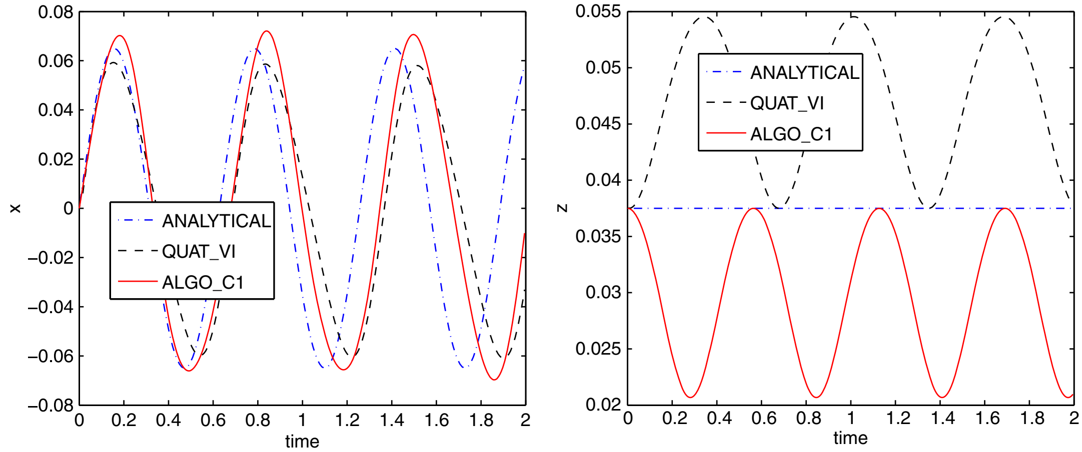

Figure 5. Steady precession of a gyro top: comparison between the analytical solution for the coordinates $x(t)$, $z(t)$ of the center of mass and the numerical results of **QUAT_VI** and **ALGO_C1** ($\Delta t = 0.007$).

position vector of the center of mass

$$\boldsymbol{\varphi}(t) = L\mathbf{d}_3(t) = x(t)\mathbf{e}_1 + y(t)\mathbf{e}_2 + z(t)\mathbf{e}_3$$

In the case of steady precession, the center of mass of the top moves on a circular trajectory in the plane $z = z(0) = L\cos(\theta_0)$. Accordingly, the analytical reference solution is given by

$$\boldsymbol{\varphi}_{\text{ref}}(t) = L\sin(\theta_0)\sin(\omega_p t)\mathbf{e}_1 - L\sin(\theta_0)\cos(\omega_p t)\mathbf{e}_2 + L\cos(\theta_0)\mathbf{e}_3$$

Figure 3 contains a log–log plot of the relative error $e = |\boldsymbol{\varphi}_{\text{ref}} - \boldsymbol{\varphi}|/|\boldsymbol{\varphi}_{\text{ref}}|$ at $t = 1$, calculated with the schemes under consideration. It can be observed that **DIR_EM** exhibits the best performance for a prescribed step-size. These results are further supported by Figures 4 and 5, in which the analytical solution for $x(t)$ and $z(t)$ is compared with the numerical results. In particular, in Figure 4 the results of **QUAT_EM** and **DIR_EM** obtained with $\Delta t = 0.01$ are shown. Similarly, Figure 5 shows the results of **QUAT_VI** and **ALGO_C1**. We remark that the step-size had to be reduced to $\Delta t = 0.007$, in order to reach convergence of the iterative solution procedure for **QUAT_VI**.

6. CONCLUSIONS

In this paper a new quaternion-based energy–momentum scheme for rigid body dynamics has been presented. The conserving scheme relies on (i) the direct discretization of the Hamiltonian form of the DAEs governing the rotational motion of the rigid body and (ii) the application of a discrete derivative in the sense of Gonzalez [26].

Owing to the availability of a non-singular quaternion mass matrix, the transition to the Hamiltonian framework has been accomplished in a straightforward way. In particular, the need to introduce undetermined inertia terms has been circumvented by performing a size-reduction of the director-based rigid body formulation. To apply the notion of the discrete derivative appropriate invariants of the quaternion-based rigid body formulation have been devised.

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Owing to the underlying DAE form of the equations of motion, quaternion-based rigid body formulations appear to be especially suitable for multibody systems. The interconnection of rigid bodies can be easily accounted for by appending additional algebraic joint constraints to the DAEs (see, for example, Nikravesh [1], Haug [2] and Rabier and Rheinboldt [5]). Similar observations hold for the director-based rigid body formulation (see Betsch and Leyendecker [23]).

In the past, quaternions have been preferred by virtue of their lower degree of redundancy. To quote Nikravesh [1, p. 156], 'While the direction cosines, subject to six constraints, could be adopted as rotational coordinates, this is neither practical nor convenient.' However, it should be mentioned that the DAEs in terms of quaternions are more elaborate than those in terms of directors. The latter indeed exhibit a striking simplicity (see Section 3).

The numerical examples presented herein confirm that the quaternion-based approach as well as the director-based approach can compete with alternative methods relying on the discretization of the classical Euler's equations. We further remark that all schemes employed in the numerical examples are SO(3)-equivariant by design. This desirable feature ensures that the numerical results do not depend on the choice of coordinate frames. For example, numerical schemes based on the Euler angles are not SO(3)-equivariant in general.

APPENDIX A: SUMMARY OF ALGEBRAIC RELATIONSHIPS

This appendix contains useful algebraic relationships between the matrices introduced in Section 2.5. It can be easily verified by straightforward calculations that the following identities hold for any $\mathbb{q}\in\mathsf{R}^4$:

$$\begin{aligned}\mathbf{E}(\mathbb{q})\mathbb{q} &= \mathbf{G}(\mathbb{q})\mathbb{q}=\mathbf{0}\\ \mathbf{E}(\mathbb{q})\mathbf{E}(\mathbb{q})^{\mathrm{T}} &= \mathbf{G}(\mathbb{q})\mathbf{G}(\mathbb{q})^{\mathrm{T}}=|\mathbb{q}|^2\mathbf{I}_3\\ \mathbf{E}(\mathbb{q})^{\mathrm{T}}\mathbf{E}(\mathbb{q}) &= \mathbf{G}(\mathbb{q})^{\mathrm{T}}\mathbf{G}(\mathbb{q})=|\mathbb{q}|^2\mathbf{I}_4-\mathbb{q}\otimes\mathbb{q}\end{aligned}\tag{A1}$$

Moreover, for $\mathbb{q},\mathbb{p}\in\mathsf{R}^4$,

$$\begin{aligned}\mathbf{E}(\mathbb{q})\mathbb{p} &= -\mathbf{E}(\mathbb{p})\mathbb{q}\\ \mathbf{G}(\mathbb{q})\mathbb{p} &= -\mathbf{G}(\mathbb{p})\mathbb{q}\\ \mathbf{E}(\mathbb{q})\mathbf{G}(\mathbb{p})^{\mathrm{T}} &= \mathbf{E}(\mathbb{p})\mathbf{G}(\mathbb{q})^{\mathrm{T}}\end{aligned}\tag{A2}$$

and

$$\begin{aligned}\overset{+}{\mathbf{a}}\,\mathbb{q} &= \mathbf{E}(\mathbb{q})^{\mathrm{T}}\mathbf{a}\\ \overset{-}{\mathbf{a}}\,\mathbb{q} &= \mathbf{G}(\mathbb{q})^{\mathrm{T}}\mathbf{a}\end{aligned}\tag{A3}$$

where $\mathbf{a}\in\mathsf{R}^3$. The inverse of $\mathbf{Q}_l$ and $\mathbf{Q}_r$ is given by

$$\begin{aligned}\mathbf{Q}_l(\mathbb{q})^{-1} &= \frac{1}{|\mathbb{q}|^2}\mathbf{Q}_l(\mathbb{q})^{\mathrm{T}}=\frac{1}{|\mathbb{q}|^2}\mathbf{Q}_l(\overline{\mathbb{q}})\\ \mathbf{Q}_r(\mathbb{q})^{-1} &= \frac{1}{|\mathbb{q}|^2}\mathbf{Q}_r(\mathbb{q})^{\mathrm{T}}=\frac{1}{|\mathbb{q}|^2}\mathbf{Q}_r(\overline{\mathbb{q}})\end{aligned}\tag{A4}$$

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Accordingly, for $\mathbf{q} \in \mathsf{S}^3 \subset \mathsf{R}^4$, both $\mathbf{Q}_l$ and $\mathbf{Q}_r$ are orthogonal. For $\mathbf{a}, \mathbf{b} \in \mathsf{R}^3$ we have

$$\bar{\bar{\mathbf{a}}}\bar{\mathbf{b}} = -(\mathbf{a}\cdot\mathbf{b})\mathbf{I}_4 + \begin{bmatrix} 0 & (\mathbf{a}\times\mathbf{b})^{\mathrm{T}} \\ -\mathbf{a}\times\mathbf{b} & \widehat{\mathbf{a}\times\mathbf{b}} \end{bmatrix} \tag{A5}$$

$$\bar{\mathbf{a}}\bar{\mathbf{b}} = -(\mathbf{a}\cdot\mathbf{b})\mathbf{I}_4 - (\mathbf{a}\times\mathbf{b})^{-}$$

We further remark that the exponential map dealt with in Section 2.3 can be written in matrix form as well. For example,

$$\exp_{\mathsf{O}(4)}\left(\frac{1}{2}\overset{+}{\mathbf{w}}\right) = \sum_{k=0}^{\infty} \frac{\left(\frac{1}{2}\overset{+}{\mathbf{w}}\right)^k}{k!} = \cos\left(\frac{1}{2}|\mathbf{w}|\right)\mathbf{I}_4 + \frac{\sin\left(\frac{1}{2}|\mathbf{w}|\right)}{|\mathbf{w}|}\overset{+}{\mathbf{w}} \tag{A6}$$

Note that, in analogy to the exponential map on S^3, the tangent space to the orthogonal group $\mathsf{O}(4)$ at the identity consists of skew-symmetric matrices $\overset{+}{\mathbf{w}}$, which can be identified with $\mathbf{w} \in \mathsf{R}^3$ through $(11)_1$.

APPENDIX B: PROOF OF FORMULA (34)

In view of (24), the body frame $\{\mathbf{d}_I\}$ attached to the rigid body at its center of mass can be parametrized in terms of quaternions via the relationship $\mathbf{d}_I = \mathscr{R}(\mathbf{q})\mathbf{e}_I$. The corresponding quaternion representation is given by (cf. Equation (7))

$$(0, \mathbf{d}_I) = \mathbf{q} \circ (0, \mathbf{e}_I) \circ \bar{\mathbf{q}}$$

Accordingly,

$$\mathbf{a} \circ (0, \mathbf{d}_I) = \mathbf{a} \circ \mathbf{q} \circ (0, \mathbf{e}_I) \circ \bar{\mathbf{q}}$$

for any $\mathbf{a} \in \mathsf{H}$. Using the matrix form (9) of quaternion multiplication, the last equation can be written as

$$\mathbf{Q}_r((0, \mathbf{d}_I))\mathbf{a} = \mathbf{Q}_r(\bar{\mathbf{q}})\mathbf{Q}_r((0, \mathbf{e}_I))\mathbf{Q}_r(\mathbf{q})\mathbf{a}$$

or

$$\bar{\mathbf{d}}_I = \mathbf{Q}_r(\mathbf{q})^{\mathrm{T}}\,\bar{\mathbf{e}}_I\,\mathbf{Q}_r(\mathbf{q}) = \begin{bmatrix} 0 & -\mathbf{d}_I^{\mathrm{T}} \\ \mathbf{d}_I & -\widehat{\mathbf{d}}_I \end{bmatrix}$$

where use has been made of $(10)_2$, $(\mathrm{A4})_2$ and $(11)_2$. Multiplying the last equation by $[0, \mathbf{a}^{\mathrm{T}}]$ from the left and by $[0, \mathbf{b}^{\mathrm{T}}]^{\mathrm{T}}$ from the right yields

$$[0 \;\; \mathbf{a}^{\mathrm{T}}]\,\bar{\mathbf{d}}_I \begin{bmatrix} 0 \\ \mathbf{b} \end{bmatrix} = [0 \;\; \mathbf{a}^{\mathrm{T}}]\mathbf{Q}_r(\mathbf{q})^{\mathrm{T}}\,\bar{\mathbf{e}}_I\,\mathbf{Q}_r(\mathbf{q}) \begin{bmatrix} 0 \\ \mathbf{b} \end{bmatrix}$$

$$-\mathbf{a}^{\mathrm{T}}\widehat{\mathbf{d}}_I\mathbf{b} = \mathbf{a}^{\mathrm{T}}\mathbf{E}(\mathbf{q})\,\bar{\mathbf{e}}_I\,\mathbf{E}(\mathbf{q})^{\mathrm{T}}\mathbf{b}$$

for any $\mathbf{a},\ \mathbf{b}\in\mathsf{R}^3$. Note that in the above use has been made of $(10)_2$. From the last equation it follows that:

$$\widehat{\mathbf{d}}_I=-\mathbf{E}(\mathbb{q})\,\bar{\mathbf{e}}_I\,\mathbf{E}(\mathbb{q})^{\mathrm{T}}$$

APPENDIX C: VERIFICATION OF THE ALGORITHMIC CONSERVATION PROPERTIES

In this appendix we verify that the scheme (51) conserves both angular momentum and energy. For simplicity of exposition we restrict our considerations to the free rigid body, i.e. $V(\mathbb{q})=0$.

C.1. Conservation of angular momentum

To verify algorithmic conservation of angular momentum consider

$$\begin{aligned}
J_{\xi,n+1}-J_{\xi,n}&=J_\xi(\mathbb{q}_{n+1},\mathbb{p}_{n+1})-J_\xi(\mathbb{q}_n,\mathbb{p}_n)=\frac{1}{2}\mathbb{p}_{n+1}\cdot\overset{+}{\boldsymbol{\xi}}\,\mathbb{q}_{n+1}-\frac{1}{2}\mathbb{p}_n\cdot\overset{+}{\boldsymbol{\xi}}\,\mathbb{q}_n\\
&=\frac{1}{2}(\mathbb{p}_{n+1}-\mathbb{p}_n)\cdot\overset{+}{\boldsymbol{\xi}}\,\mathbb{q}_{n+1/2}-\frac{1}{2}(\mathbb{q}_{n+1}-\mathbb{q}_n)\cdot\overset{+}{\boldsymbol{\xi}}\,\mathbb{p}_{n+1/2}\\
&=-\frac{\Delta t}{2}\overline{\nabla}_{\mathbb{q}}H_\lambda\cdot\overset{+}{\boldsymbol{\xi}}\,\mathbb{q}_{n+1/2}-\frac{\Delta t}{2}\overline{\nabla}_{\mathbb{p}}H_\lambda\cdot\overset{+}{\boldsymbol{\xi}}\,\mathbb{p}_{n+1/2}
\end{aligned}\tag{C1}$$

for $\boldsymbol{\xi}\in\mathsf{R}^3$. In the above use has been made of (45) and $(50)_{1,2}$. The discrete partial derivatives of the augmented Hamiltonian may be written in the form

$$\begin{aligned}
\overline{\nabla}_{\mathbb{q}}H_\lambda&=\left(\frac{\partial\boldsymbol{\pi}}{\partial\mathbb{q}}\right)^{\mathrm{T}}_{(\mathbb{q}_{n+1/2},\mathbb{p}_{n+1/2})}\overline{\nabla}\tilde{T}(\boldsymbol{\pi}_n,\boldsymbol{\pi}_{n+1})+\lambda\mathbb{q}_{n+1/2}\\
\overline{\nabla}_{\mathbb{p}}H_\lambda&=\left(\frac{\partial\boldsymbol{\pi}}{\partial\mathbb{p}}\right)^{\mathrm{T}}_{(\mathbb{q}_{n+1/2},\mathbb{p}_{n+1/2})}\overline{\nabla}\tilde{T}(\boldsymbol{\pi}_n,\boldsymbol{\pi}_{n+1})
\end{aligned}\tag{C2}$$

where, with regard to (51), $\overline{\nabla}\tilde{T}(\boldsymbol{\pi}_n,\boldsymbol{\pi}_{n+1})=\frac{1}{8}\mathscr{J}_4^{-1}[\boldsymbol{\pi}_n+\boldsymbol{\pi}_{n+1}]=\nabla\tilde{T}(\boldsymbol{\pi}_{n+1/2})$. Inserting from (C2) into (C1) and taking into account the skew-symmetry of $\overset{+}{\boldsymbol{\xi}}$, we obtain

$$\begin{aligned}
J_{\xi,n+1}-J_{\xi,n}=-\frac{\Delta t}{2}\overline{\nabla}\tilde{T}(\boldsymbol{\pi}_n,\boldsymbol{\pi}_{n+1})\cdot\Bigg\{&\left.\frac{\partial\boldsymbol{\pi}}{\partial\mathbb{q}}\right|_{(\mathbb{q}_{n+1/2},\mathbb{p}_{n+1/2})}\overset{+}{\boldsymbol{\xi}}\,\mathbb{q}_{n+1/2}\\
&+\left.\frac{\partial\boldsymbol{\pi}}{\partial\mathbb{p}}\right|_{(\mathbb{q}_{n+1/2},\mathbb{p}_{n+1/2})}\overset{+}{\boldsymbol{\xi}}\,\mathbb{p}_{n+1/2}\Bigg\}
\end{aligned}\tag{C3}$$

On the other hand, the invariance property of $\boldsymbol{\pi}$ leads to

$$\left.\frac{\mathrm{d}}{\mathrm{d}\varepsilon}\right|_{\varepsilon=0}\boldsymbol{\pi}\left(\exp_{\mathsf{O}(4)}\left(\frac{\varepsilon}{2}\overset{+}{\boldsymbol{\xi}}\right)\mathbb{q},\exp_{\mathsf{O}(4)}\left(\frac{\varepsilon}{2}\overset{+}{\boldsymbol{\xi}}\right)\mathbb{p}\right)=0$$

$$\frac{1}{2}\frac{\partial\boldsymbol{\pi}}{\partial\mathbb{q}}\overset{+}{\boldsymbol{\xi}}\,\mathbb{q}+\frac{1}{2}\frac{\partial\boldsymbol{\pi}}{\partial\mathbb{p}}\overset{+}{\boldsymbol{\xi}}\,\mathbb{p}=0$$

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This implies that the curly bracket in (C3) vanishes, so that

$$J_{\xi,n+1}-J_{\xi,n}=0$$

which holds for arbitrary $\overline{\nabla}\tilde{T}(\boldsymbol{\pi}_n,\boldsymbol{\pi}_{n+1})$.

C.2. Conservation of energy

We next verify algorithmic conservation of energy. To this end, pre-multiply $(50)_1$ by $(\mathbb{p}_{n+1}^{\mathrm{T}}-\mathbb{p}_n^{\mathrm{T}})$, $(50)_2$ by $-(\mathbb{q}_{n+1}^{\mathrm{T}}-\mathbb{q}_n^{\mathrm{T}})$ and subsequently add both equations to obtain

$$0=\Delta t\,(\mathbb{p}_{n+1}-\mathbb{p}_n)\cdot\overline{\nabla}_{\mathbb{p}}H_\lambda+\Delta t\,(\mathbb{q}_{n+1}-\mathbb{q}_n)\cdot\overline{\nabla}_{\mathbb{q}}H_\lambda$$

Taking into account (C2), the last equation yields

$$\begin{aligned}
0&=\Delta t\overline{\nabla}\tilde{T}(\boldsymbol{\pi}_n,\boldsymbol{\pi}_{n+1})\cdot\left\{\left.\frac{\partial\boldsymbol{\pi}}{\partial\mathbb{q}}\right|_{(\mathbb{q}_{n+1/2},\mathbb{p}_{n+1/2})}(\mathbb{q}_{n+1}-\mathbb{q}_n)+\left.\frac{\partial\boldsymbol{\pi}}{\partial\mathbb{p}}\right|_{(\mathbb{q}_{n+1/2},\mathbb{p}_{n+1/2})}(\mathbb{p}_{n+1}-\mathbb{p}_n)\right\}\\
&\quad+\Delta t\,\lambda\mathbb{q}_{n+1/2}\cdot(\mathbb{q}_{n+1}-\mathbb{q}_n)\\
0&=\frac{\Delta t}{2}\nabla\tilde{T}(\boldsymbol{\pi}_{n+1/2})\cdot\{\boldsymbol{\pi}_{n+1}-\boldsymbol{\pi}_n\}+\frac{\Delta t}{2}\lambda(\mathbb{q}_{n+1}\cdot\mathbb{q}_{n+1}-\mathbb{q}_n\cdot\mathbb{q}_n)
\end{aligned}$$

Taking into account expression (48) for the kinetic energy and the fact that $\mathbb{q}_{n+1}\in\mathsf{S}^3$ is enforced by $(51)_3$, the last equation leads to the result

$$\tilde{T}(\boldsymbol{\pi}_{n+1})-\tilde{T}(\boldsymbol{\pi}_n)=T(\mathbb{q}_{n+1},\mathbb{p}_{n+1})-T(\mathbb{q}_n,\mathbb{p}_n)=0$$

which confirms algorithmic conservation of energy in the case of the free rigid body.

APPENDIX D: DETAILS OF THE IMPLEMENTATION

This appendix contains an outline of the iterative solution procedure. To solve the system of non-linear algebraic equations, Newton's method may be applied. To this end, consider the residual vector

$$\mathbf{R}(\boldsymbol{\theta},\mathbb{p}_{n+1})=\begin{bmatrix}\mathbf{R}_{\mathbb{q}}(\mathbb{q}_{n+1},\mathbb{p}_{n+1})\\ \mathbf{G}(\mathbb{q}_{n+1/2})\mathbf{R}_{\mathbb{p}}(\mathbb{q}_{n+1},\mathbb{p}_{n+1})\end{bmatrix}$$

where, with regard to $(52)_1$ and (53),

$$\begin{aligned}
\mathbf{R}_{\mathbb{q}}&=\mathbb{q}_{n+1}-\mathbb{q}_n-\frac{\Delta t}{8}\mathbf{Q}_l(\mathbb{q}_{n+1/2})\mathscr{I}_4^{-1}[\mathbf{Q}_l(\mathbb{q}_n)^{\mathrm{T}}\mathbb{p}_n+\mathbf{Q}_l(\mathbb{q}_{n+1})^{\mathrm{T}}\mathbb{p}_{n+1}]\\
\mathbf{R}_{\mathbb{p}}&=\mathbb{p}_{n+1}-\mathbb{p}_n+\frac{\Delta t}{8}\mathbf{Q}_l(\mathbb{p}_{n+1/2})\mathscr{I}_4^{-1}[\mathbf{Q}_l(\mathbb{p}_n)^{\mathrm{T}}\mathbb{q}_n+\mathbf{Q}_l(\mathbb{p}_{n+1})^{\mathrm{T}}\mathbb{q}_{n+1}]+\Delta t\nabla V(\mathbb{q}_{n+1/2})
\end{aligned}$$

Note that in the above equations $\mathbb{q} \in \mathsf{S}^3$ is expressed in terms of $\boldsymbol{\theta} \in \mathsf{R}^3$ via formula (54). In each Newton iteration, the following linear system has to be solved:

$$\begin{bmatrix} \mathbf{K}_{\mathbb{q}\theta} & \mathbf{K}_{\mathbb{q}\mathbb{p}} \\ \mathbf{K}_{p\theta} & \mathbf{K}_{p\mathbb{p}} \end{bmatrix} \begin{bmatrix} \Delta\boldsymbol{\theta} \\ \Delta\mathbb{p} \end{bmatrix} = -\mathbf{R} \tag{D1}$$

where

$$\mathbf{K}_{\mathbb{q}\theta} = \tfrac{1}{2}\mathbf{K}_{\mathbb{q}\mathbb{q}}\mathbf{E}(\mathbb{q}_{n+1})^{\mathrm{T}}\mathbf{H}(\boldsymbol{\theta})$$

$$\mathbf{K}_{\mathbb{q}\mathbb{q}} = \mathbb{I}_4 - \frac{\Delta t}{8}(\mathbf{Q}_r(\mathbb{o}) + \mathbf{Q}_l(\mathbb{q}_{n+1/2})\mathscr{I}_4^{-1}\overline{\mathbf{Q}}(\mathbb{p}_{n+1})^{\mathrm{T}})$$

$$\mathbf{K}_{\mathbb{q}\mathbb{p}} = -\frac{\Delta t}{8}\mathbf{Q}_l(\mathbb{q}_{n+1/2})\mathscr{I}_4^{-1}\mathbf{Q}_l(\mathbb{q}_{n+1})^{\mathrm{T}}$$

$$\mathbf{K}_{p\theta} = \tfrac{1}{2}\mathbf{K}_{p\mathbb{q}}\mathbf{E}(\mathbb{q}_{n+1})^{\mathrm{T}}\mathbf{H}(\boldsymbol{\theta})$$

$$\mathbf{K}_{p\mathbb{q}} = \mathbf{G}(\mathbb{q}_{n+1/2})\left\{\frac{\Delta t}{8}\mathbf{Q}_l(\mathbb{p}_{n+1/2})\mathscr{I}_4^{-1}\mathbf{Q}_l(\mathbb{p}_{n+1})^{\mathrm{T}} + \frac{\Delta t}{2}\nabla^2 V(\mathbb{q}_{n+1/2})\right\} - \frac{1}{2}\mathbf{G}(\mathbf{R}_{\mathbb{p}})$$

$$\mathbf{K}_{p\mathbb{p}} = \mathbf{G}(\mathbb{q}_{n+1/2})\left\{\mathbb{I}_4 + \frac{\Delta t}{8}(\mathbf{Q}_r(\mathbb{k}) + \mathbf{Q}_l(\mathbb{p}_{n+1/2})\mathscr{I}_4^{-1}\overline{\mathbf{Q}}(\mathbb{q}_{n+1})^{\mathrm{T}})\right\}$$

and

$$\mathbb{o} = \tfrac{1}{2}\mathscr{I}_4^{-1}[\mathbf{Q}_l(\mathbb{q}_n)^{\mathrm{T}}\mathbb{p}_n + \mathbf{Q}_l(\mathbb{q}_{n+1})^{\mathrm{T}}\mathbb{p}_{n+1}] \qquad \overline{\mathbf{Q}}(\mathbb{q}) = [\mathbb{q} \quad -\mathbf{G}(\mathbb{q})^{\mathrm{T}}]$$
$$\mathbb{k} = \tfrac{1}{2}\mathscr{I}_4^{-1}[\mathbf{Q}_l(\mathbb{p}_n)^{\mathrm{T}}\mathbb{q}_n + \mathbf{Q}_l(\mathbb{p}_{n+1})^{\mathrm{T}}\mathbb{q}_{n+1}]$$

Once the iterative increments $(\Delta\boldsymbol{\theta}, \Delta\mathbb{p})$ have been determined by solving the linear system of equations (D1), the update of the unknowns is given by

$$\begin{aligned} \boldsymbol{\theta}^{(l+1)} &= \boldsymbol{\theta}^{(l)} + \Delta\boldsymbol{\theta} \\ \mathbb{p}_{n+1}^{(l+1)} &= \mathbb{p}_{n+1}^{(l)} + \Delta\mathbb{p} \end{aligned} \quad \text{and} \quad \mathbb{q}_{n+1}^{(l+1)} = \exp_{\mathsf{S}^3}\left(\left(0, \frac{1}{2}\boldsymbol{\theta}^{(l+1)}\right)\right) \circ \mathbb{q}_n$$

where l denotes the iteration counter.

We eventually remark that in the above the following relationship between $\Delta\mathbb{q}_{n+1} \in T_{\mathbb{q}_{n+1}}\mathsf{S}^3$ and $\Delta\boldsymbol{\theta} \in \mathsf{R}^3$ has been used:

$$\Delta\mathbb{q}_{n+1} = \tfrac{1}{2}\mathbf{E}(\mathbb{q}_{n+1})^{\mathrm{T}}\mathbf{H}(\boldsymbol{\theta})\Delta\boldsymbol{\theta} \tag{D2}$$

The last equation can be derived by considering one-parameter curves $\mathbb{q}_\varepsilon \in \mathsf{S}^3$ of the form

$$\mathbb{q}_\varepsilon = \exp_{\mathsf{S}^3}\left(\left(0, \frac{1}{2}\{\boldsymbol{\theta} + \varepsilon\Delta\boldsymbol{\theta}\}\right)\right) \circ \mathbb{q}_n = \exp_{\mathsf{S}^3}\left(\left(0, \frac{1}{2}\{\boldsymbol{\theta} + \varepsilon\Delta\boldsymbol{\theta}\}\right)\right) \circ \exp_{\mathsf{S}^3}\left(\left(0, -\frac{1}{2}\boldsymbol{\theta}\right)\right) \circ \mathbb{q}$$

By definition, tangent vectors $\Delta\mathbb{q} \in T_{\mathbb{q}}\mathsf{S}^3$ are given by

$$\Delta\mathbb{q} = \left.\frac{\mathrm{d}}{\mathrm{d}\varepsilon}\right|_{\varepsilon=0} \mathbb{q}_\varepsilon = \left.\frac{\mathrm{d}}{\mathrm{d}\varepsilon}\right|_{\varepsilon=0} \exp_{\mathsf{S}^3}\left(\left(0, \frac{1}{2}\{\boldsymbol{\theta} + \varepsilon\Delta\boldsymbol{\theta}\}\right)\right) \circ \exp_{\mathsf{S}^3}\left(\left(0, -\frac{1}{2}\boldsymbol{\theta}\right)\right) \circ \mathbb{q} \tag{D3}$$

With regard to (6), a straightforward calculation yields

$$\begin{aligned}
\left.\frac{\mathrm{d}}{\mathrm{d}\varepsilon}\right|_{\varepsilon=0} & \exp_{\mathbb{S}^3}\left(\left(0,\frac{1}{2}\{\boldsymbol{\theta}+\varepsilon\Delta\boldsymbol{\theta}\}\right)\right)\\
&= \left.\frac{\mathrm{d}}{\mathrm{d}\varepsilon}\right|_{\varepsilon=0}\left[\cos\left(\frac{1}{2}|\boldsymbol{\theta}+\varepsilon\Delta\boldsymbol{\theta}|\right)(1,\mathbf{0})+\frac{\sin(\frac{1}{2}|\boldsymbol{\theta}+\varepsilon\Delta\boldsymbol{\theta}|)}{|\boldsymbol{\theta}+\varepsilon\Delta\boldsymbol{\theta}|}(0,\boldsymbol{\theta}+\varepsilon\Delta\boldsymbol{\theta})\right]\\
&= -\sin\left(\frac{1}{2}|\boldsymbol{\theta}|\right)\frac{\boldsymbol{\theta}\cdot\Delta\boldsymbol{\theta}}{2|\boldsymbol{\theta}|}(1,\mathbf{0})+\left[\cos\left(\frac{1}{2}|\boldsymbol{\theta}|\right)\frac{\boldsymbol{\theta}\cdot\Delta\boldsymbol{\theta}}{2|\boldsymbol{\theta}|^2}-\sin\left(\frac{1}{2}|\boldsymbol{\theta}|\right)\frac{\boldsymbol{\theta}\cdot\Delta\boldsymbol{\theta}}{|\boldsymbol{\theta}|^3}\right](0,\boldsymbol{\theta})\\
&\quad +\frac{\sin(\frac{1}{2}|\boldsymbol{\theta}|)}{|\boldsymbol{\theta}|}(0,\Delta\boldsymbol{\theta})
\end{aligned}$$

Now, making use of

$$\exp_{\mathbb{S}^3}\left(\left(0,-\frac{1}{2}\boldsymbol{\theta}\right)\right)=\cos\left(\frac{1}{2}|\boldsymbol{\theta}|\right)(1,\mathbf{0})-\frac{\sin(\frac{1}{2}|\boldsymbol{\theta}|)}{|\boldsymbol{\theta}|}(0,\boldsymbol{\theta})$$

it can be easily verified that

$$\left.\frac{\mathrm{d}}{\mathrm{d}\varepsilon}\right|_{\varepsilon=0}\exp_{\mathbb{S}^3}\left(\left(0,\frac{1}{2}\{\boldsymbol{\theta}+\varepsilon\Delta\boldsymbol{\theta}\}\right)\right)\circ\exp_{\mathbb{S}^3}\left(\left(0,-\frac{1}{2}\boldsymbol{\theta}\right)\right)=\frac{1}{2}(0,\mathbf{H}(\boldsymbol{\theta})\Delta\boldsymbol{\theta}) \tag{D4}$$

where

$$\mathbf{H}(\boldsymbol{\theta})=\frac{\sin(|\boldsymbol{\theta}|)}{|\boldsymbol{\theta}|}\mathbf{I}+\frac{1-\cos(|\boldsymbol{\theta}|)}{|\boldsymbol{\theta}|}\frac{\widehat{\boldsymbol{\theta}}}{|\boldsymbol{\theta}|}+\left(1-\frac{\sin(|\boldsymbol{\theta}|)}{|\boldsymbol{\theta}|}\right)\frac{\boldsymbol{\theta}\otimes\boldsymbol{\theta}}{|\boldsymbol{\theta}|^2}$$

Inserting (D4) into $(\mathrm{D3})_2$ we obtain

$$\Delta\mathbb{q}=\tfrac{1}{2}(0,\mathbf{H}(\boldsymbol{\theta})\Delta\boldsymbol{\theta})\circ\mathbb{q}$$

or, employing (9),

$$\Delta\mathbb{q}=\frac{1}{2}\mathbf{Q}_r(\mathbb{q})\begin{bmatrix}0\\ \mathbf{H}(\boldsymbol{\theta})\Delta\boldsymbol{\theta}\end{bmatrix}=\frac{1}{2}\mathbf{E}(\mathbb{q})^{\mathrm{T}}\mathbf{H}(\boldsymbol{\theta})\Delta\boldsymbol{\theta}$$

where use has been made of $(10)_2$. The last equation confirms the validity of (D2).

APPENDIX E: QUATERNION-BASED VARIATIONAL INTEGRATOR

This appendix outlines the application of the variational integrator proposed by Leyendecker *et al.* [29] (see also Wendlandt and Marsden [3]) to the present quaternion formulation of rigid body dynamics. The variational integrator emanates from the discrete Euler–Lagrange equations

$$D_2L_d(\mathbb{q}_{n-1},\mathbb{q}_n)+D_1L_d(\mathbb{q}_n,\mathbb{q}_{n+1})-\Delta t\,\mathbb{q}_n\lambda_n=\mathbf{0} \tag{E1}$$

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which have to be supplemented with $g(\mathbf{q}_{n+1})=0$. The discrete Lagrangian is defined by

$$L_d(\mathbf{q}_n,\mathbf{q}_{n+1})=T_d(\mathbf{q}_n,\mathbf{q}_{n+1})-\Delta t\,V\left(\frac{\mathbf{q}_n+\mathbf{q}_{n+1}}{2}\right)$$

where the discrete kinetic energy assumes the form

$$T_d(\mathbf{q}_n,\mathbf{q}_{n+1})=\Delta t\,T\left(\frac{\mathbf{q}_n+\mathbf{q}_{n+1}}{2},\frac{\mathbf{q}_{n+1}-\mathbf{q}_n}{\Delta t}\right)$$

The kinetic energy function $T(\mathbf{q},\dot{\mathbf{q}})$ is given by (29), with configuration-dependent mass matrix (32). Accordingly,

$$\begin{aligned}T_d(\mathbf{q}_n,\mathbf{q}_{n+1})&=\frac{1}{2\Delta t}(\mathbf{q}_{n+1}-\mathbf{q}_n)\cdot\mathbf{M}_4\left(\frac{\mathbf{q}_n+\mathbf{q}_{n+1}}{2}\right)(\mathbf{q}_{n+1}-\mathbf{q}_n)\\&=\frac{2}{\Delta t}(\mathbf{q}_{n+1}-\mathbf{q}_n)\cdot\mathbf{Q}_l\left(\frac{\mathbf{q}_n+\mathbf{q}_{n+1}}{2}\right)\mathscr{J}_4\mathbf{Q}_l\left(\frac{\mathbf{q}_n+\mathbf{q}_{n+1}}{2}\right)^{\mathrm{T}}(\mathbf{q}_{n+1}-\mathbf{q}_n)\end{aligned}$$

Now calculate

$$\begin{aligned}\mathbf{Q}_l\left(\frac{\mathbf{q}_n+\mathbf{q}_{n+1}}{2}\right)^{\mathrm{T}}(\mathbf{q}_{n+1}-\mathbf{q}_n)&=\frac{1}{2}(\mathbf{Q}_l(\mathbf{q}_n)^{\mathrm{T}}+\mathbf{Q}_l(\mathbf{q}_{n+1})^{\mathrm{T}})(\mathbf{q}_{n+1}-\mathbf{q}_n)\\&=\frac{1}{2}\begin{bmatrix}\mathbf{q}_{n+1}\cdot\mathbf{q}_{n+1}-\mathbf{q}_n\cdot\mathbf{q}_n\\\mathbf{G}(\mathbf{q}_n)\mathbf{q}_{n+1}-\mathbf{G}(\mathbf{q}_{n+1})\mathbf{q}_n\end{bmatrix}\\&=\begin{bmatrix}0\\\mathbf{G}(\mathbf{q}_n)\mathbf{q}_{n+1}\end{bmatrix}=\begin{bmatrix}0\\-\mathbf{G}(\mathbf{q}_{n+1})\mathbf{q}_n\end{bmatrix}\end{aligned}$$

where use has been made of $(10)_1$, $(\mathrm{A2})_2$ and the fact that the variational integrator enforces the quaternion unit-length constraint at the time nodes, i.e. $\mathbf{q}_n,\mathbf{q}_{n+1}\in\mathsf{S}^3$. Accordingly, the expression for the discrete kinetic energy boils down to

$$T_d(\mathbf{q}_n,\mathbf{q}_{n+1})=\frac{1}{2\Delta t}\mathbf{q}_{n+1}\cdot\widetilde{\mathbf{M}}_4(\mathbf{q}_n)\mathbf{q}_{n+1}=\frac{1}{2\Delta t}\mathbf{q}_n\cdot\widetilde{\mathbf{M}}_4(\mathbf{q}_{n+1})\mathbf{q}_n$$

where $\widetilde{\mathbf{M}}_4(\mathbf{q})=4\mathbf{G}(\mathbf{q})^{\mathrm{T}}\mathbf{J}\mathbf{G}(\mathbf{q})$ has already been introduced in Remark 4.1. The partial derivatives of the discrete Lagrangian can now be calculated to be

$$\begin{aligned}D_1L_d(\mathbf{q}_n,\mathbf{q}_{n+1})&=\frac{1}{\Delta t}\widetilde{\mathbf{M}}_4(\mathbf{q}_{n+1})\mathbf{q}_n-\frac{\Delta t}{2}\nabla V\left(\frac{\mathbf{q}_n+\mathbf{q}_{n+1}}{2}\right)\\D_2L_d(\mathbf{q}_n,\mathbf{q}_{n+1})&=\frac{1}{\Delta t}\widetilde{\mathbf{M}}_4(\mathbf{q}_n)\mathbf{q}_{n+1}-\frac{\Delta t}{2}\nabla V\left(\frac{\mathbf{q}_n+\mathbf{q}_{n+1}}{2}\right)\end{aligned}$$

so that the discrete Euler–Lagrange equations (E1) assume the specific form

$$\frac{1}{\Delta t}(\widetilde{\mathbf{M}}_4(\mathbf{q}_{n-1})+\widetilde{\mathbf{M}}_4(\mathbf{q}_{n+1}))\mathbf{q}_n-\frac{\Delta t}{2}\nabla V\left(\frac{\mathbf{q}_{n-1}+\mathbf{q}_n}{2}\right)-\frac{\Delta t}{2}\nabla V\left(\frac{\mathbf{q}_n+\mathbf{q}_{n+1}}{2}\right)-\Delta t\,\mathbf{q}_n\lambda_n=\mathbf{0}$$

Given $\mathbf{q}_{n-1}, \mathbf{q}_n \in S^3$, the above equations, together with $g(\mathbf{q}_{n+1}) = 0$, provide five algebraic equations for the determination of $\mathbf{q}_{n+1} \in S^3 \subset R^4$ and $\lambda_n \in R$. To initialize the present algorithm, the initial values $(\mathbf{q}_0, \mathbf{p}_0) \in P$ can be used to determine $\mathbf{q}_1 \in S^3$ (along with $\lambda_0 \in R$), by solving the following algebraic system of non-linear equations:

$$\begin{aligned} \mathbf{p}_0 &= -D_1 L_d(\mathbf{q}_0, \mathbf{q}_1) + \frac{\Delta t}{2} \mathbf{q}_0 \lambda_0 \\ 0 &= g(\mathbf{q}_1) \end{aligned}$$

We finally remark that the discrete angular momentum map

$$\mathbf{J}^-(\mathbf{q}_n, \mathbf{q}_{n+1}) = \tfrac{1}{2}\mathbf{E}(\mathbf{q}_n)\mathbf{p}^-_{n,n+1} \quad \text{with } \mathbf{p}^-_{n,n+1} = -D_1 L_d(\mathbf{q}_n, \mathbf{q}_{n+1}) + \frac{\Delta t}{2} \mathbf{q}_n \lambda_n$$

is conserved in the sense that $\mathbf{J}^-(\mathbf{q}_{n-1}, \mathbf{q}_n) = \mathbf{J}^-(\mathbf{q}_n, \mathbf{q}_{n+1})$, provided that the underlying system is invariant under rotations (cf. Section 4.2).

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