Singularity-free rotational Brownian dynamics

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1 Background

- The configuration of a patchy particle is determined by the center of mass position $\mathbf{R}^{\mathrm{s}}$ in the laboratory frame and the rotation matrix $\mathbf{A}$ relative to the lab frame. This matrix is parameterized by the rotational coordinates $\boldsymbol{\alpha}$; possible choices include the Euler angles $\boldsymbol{\Psi}$, the rotation vector $\boldsymbol{a}$ (see Appendix 8.1), or the quaternions $\mathbf{q}$ (see Appendix 8.3).
- The structure of a patchy particle is determined by the positions of the P patches, relative to the center of mass, in the body-fixed frame: $\underline{\mathbf{r}}_p^{\mathrm{b}}$, with the bar highlighting a constant. The positions of the patches in the space or lab frame are calculated as $\mathbf{r}_p^{\mathrm{s}} = \mathbf{R}^{\mathrm{s}} + \mathbf{A}\underline{\mathbf{r}}_p^{\mathrm{b}}$.
- The use of Euler angles is hampered by strong singularities.
- Using a rotation vector to define the rotation matrix softens the strong singularities to weak singularities. On the down side, the equations of motion become rather involved.
- The quaternions are singularity free, 'but because there are four quaternions and only three degrees of rotational motion for a rigid body, the quaterions do not constitute a set of generalized coordinates that describes the angular orientation of rigid bodies' [Naess et al, Physica A 294 323 (2001)]. 'The Brownian dynamics of nanoparticles cannot therefore be readily described by quaternions' [Naess and Elgsaeter, Macromol. Theory Simul. 13 419 (2004)].
- Given the lab-based Cartesian forces $\mathbf{f}_p^{\mathrm{s}}$ on the patches, the total lab-based Cartesian force on the particle is given by $\mathbf{F}^{\mathrm{s}} = \sum_p \mathbf{f}_p^{\mathrm{s}}$ and the total lab-based Cartesian torque relative to the particle's center of mass by $\mathbf{T}^{\mathrm{s}} = \sum_p (\mathbf{r}_p^{\mathrm{s}} - \mathbf{R}^{\mathrm{s}}) \times \mathbf{f}_p^{\mathrm{s}} = \sum_p (\mathbf{A}\underline{\mathbf{r}}_p^{\mathrm{b}}) \times \mathbf{f}_p^{\mathrm{s}}$.
- The translational and rotational mobility tensors, $\boldsymbol{\mu}^{\mathrm{t}}(\boldsymbol{\alpha})$ and $\boldsymbol{\mu}^{\mathrm{r},\alpha}(\boldsymbol{\alpha})$, respectively, vary with the orientation of the particle. Given their values in the body-fixed frame, $\underline{\boldsymbol{\mu}}^{\mathrm{t}}$ and $\underline{\boldsymbol{\mu}}^{\mathrm{r}}$, one readily shows (see below) that in the laboratory frame $\boldsymbol{\mu}^{\mathrm{t}}(\alpha) = \mathbf{A}\underline{\boldsymbol{\mu}}^{\mathrm{t}}\mathbf{A}^{\mathrm{T}}$ and $\boldsymbol{\mu}^{\mathrm{r},\alpha} = \mathbf{A}\underline{\boldsymbol{\mu}}^{\mathrm{r}}\mathbf{A}^{\mathrm{T}}$. The superscript $\boldsymbol{\alpha}$ to the rotational mobility matrix stresses that this matrix depends on the chosen set of rotational coordinates.
- We will use $\boldsymbol{\Theta}(t)$ to denote two time-dependent column vectors whose elements each have zero mean, unit variance and are delta-correlated in time.

2 Classical mechanics

In classical mechanics, the angular momentum is related to the inertia tensor $\mathbf{I}$ and angular velocity $\boldsymbol{\omega}$ by

$$\mathbf{L} = \mathbf{I}\boldsymbol{\omega}. \tag{1}$$

Its time derivtive reads in an inertial frame as

$$\dot{\mathbf{L}} = \mathbf{T}^{\mathrm{s}}. \tag{2}$$

This equation of motion is readily solved[1] using the following low order integration algorithm, where for clarity we have added superscripts s and b to distinguish between vectors in the space- or laboratory-fixed frame and vectors in the non-inertial body-fixed frame:[2]

$$\mathbf{L}^{\mathrm{s}}(t+\Delta t) = \mathbf{L}^{\mathrm{s}}(t) + \mathbf{T}^{\mathrm{s}}(t)\Delta t, \tag{3}$$

$$\boldsymbol{\omega}^{\mathrm{b}}(t+\Delta t) = \left(\mathbf{I}^{\mathrm{b}}(t+\Delta t)\right)^{-1}\mathbf{L}^{\mathrm{b}}(t+\Delta t) \approx \left(\underline{\mathbf{I}}^{\mathrm{b}}\right)^{-1}\mathbf{A}^{-1}(t)\mathbf{L}^{\mathrm{s}}(t+\Delta t), \tag{4}$$

$$\mathbf{q}(t+\Delta t) = \mathbf{q}(t) + \tilde{\mathbf{B}}(t)\boldsymbol{\omega}^{\mathrm{b}}(t+\Delta t)\Delta t, \tag{5}$$

$$\mathbf{q}(t+\Delta t) = \mathbf{q}(t+\Delta t)/|\mathbf{q}(t+\Delta t)| \tag{6}$$

$$\mathbf{A}(t+\Delta t) = \mathbf{A}(\mathbf{q}(t+\Delta t)). \tag{7}$$

Here $\tilde{\mathbf{B}}$ is the 4×3 matrix obtained by eliminating the first column of the $\mathbf{B}$ matrix; both are detailed in Appendix 8.4. Note that this approach does not require the inertia tensor to be diagonal. Rather then simply rescaling $\mathbf{q}$ to its proper length, as in Eq. (6), it would be more appropriate to constrain.

There exists a similar scheme that uses lab-fixed quantities only, of the form

$$\mathbf{L}^{\mathrm{s}}(t+\Delta t) = \mathbf{L}^{\mathrm{s}}(t) + \mathbf{T}^{\mathrm{s}}(t)\Delta t, \tag{8}$$

$$\boldsymbol{\omega}^{\mathrm{s}}(t+\Delta t) = \left(\mathbf{I}^{\mathrm{s}}(t+\Delta t)\right)^{-1}\mathbf{L}^{\mathrm{s}}(t+\Delta t) \approx \mathbf{A}(t)\left(\underline{\mathbf{I}}^{\mathrm{b}}\right)^{-1}\mathbf{A}^{-1}(t)\mathbf{L}^{\mathrm{s}}(t+\Delta t), \tag{9}$$

$$\mathbf{q}(t+\Delta t) = \mathbf{q}(t) + \tilde{\mathbf{C}}(t)\boldsymbol{\omega}^{\mathrm{s}}(t+\Delta t)\Delta t, \tag{10}$$

$$\mathbf{q}(t+\Delta t) = \mathbf{q}(t+\Delta t)/|\mathbf{q}(t+\Delta t)| \tag{11}$$

$$\mathbf{A}(t+\Delta t) = \mathbf{A}(\mathbf{q}(t+\Delta t)). \tag{12}$$

A problem surfacing in Eqs. (4) and (9) is that both employ the rotation matrix at t rather then at $t+\Delta t$. One solution would be to iterate. Forward extrapolation can be used to start with an improved initial value of $\mathbf{A}(\mathbf{q}(t)+\dot{\mathbf{q}}(t)\Delta t)$.

3 Brownian dynamics

3.1 Equation of motion

The generic equation of motion for Brownian dynamics of any set of generalized coordinates $\mathbf{Q}$ has the form

$$\mathbf{Q}(t+\Delta t) - \mathbf{Q}(t) = -\boldsymbol{\mu}^{Q}\frac{\partial\mathcal{A}}{\partial\mathbf{Q}}\Delta t + k_B T\frac{\partial}{\partial\mathbf{Q}}\cdot\boldsymbol{\mu}^{Q}\Delta t + \left(\boldsymbol{\mu}^{Q}\right)^{1/2}\boldsymbol{\Theta}(t)\sqrt{2k_BT\Delta t}, \tag{13}$$

where the terms on the right hand side represent

- the average velocity, resulting from the force balance between free-energy 'forces' and friction forces, as discussed in more detail below;
- a term to compensate for the spurious-drift that arises in BD algorithms with a coordinate-dependent friction;
- a Markovian stochastic contribution, related to the friction and the temperature by the fluctuation-dissipation theorem.

[1] The conventional way, e.g. in Goldstein section 5.5, is to translate time derivatives of vectors from one frame to the next: $\mathbf{T}^{\mathrm{s}} = \dot{\mathbf{L}}^{\mathrm{s}} = [\dot{\mathbf{L}}^{\mathrm{b}} + \boldsymbol{\omega}\times\mathbf{L}]^{\mathrm{s}}$. In the body-fixed frame that diagonalizes the inertia tensor, $L^{\mathrm{b}}_{\alpha} = \underline{I}^{\mathrm{b}}_{\alpha\alpha}\omega^{\mathrm{b}}_{\alpha}$, this yields the Euler equations $\dot{\boldsymbol{\omega}}^{\mathrm{b}} = \left(\underline{\mathbf{I}}^{\mathrm{b}}\right)^{-1}\left(\mathbf{T}^{\mathrm{b}} - \boldsymbol{\omega}^{\mathrm{b}}\times\underline{\mathbf{I}}^{\mathrm{b}}\boldsymbol{\omega}^{\mathrm{b}}\right)$.

[2] Is this in the body fixed frame or in the frame that momentarily shares the body's orientation, or ...?

From Eulerian angular velocities to body-fixed angular velocities, Goldstein Eq. (4.87):

$$\begin{pmatrix} \omega_1^{\mathrm{b}} \\ \omega_2^{\mathrm{b}} \\ \omega_3^{\mathrm{b}} \end{pmatrix} = \begin{pmatrix} \sin\theta\sin\psi & \cos\psi & 0 \\ \sin\theta\cos\psi & -\sin\psi & 0 \\ \cos\theta & 0 & 1 \end{pmatrix} \begin{pmatrix} \dot{\phi} \\ \dot{\theta} \\ \dot{\psi} \end{pmatrix} \tag{227}$$

Jacobian

$$\left| \frac{\partial \boldsymbol{\omega}^{\mathrm{b}}}{\partial \mathbf{Q}} \right| = \sin\theta \tag{228}$$

8.3 Quaternions

Euler-Rodriques formula:

$$\begin{aligned} \mathbf{A} &= \begin{pmatrix} q_0^2 + q_1^2 - q_2^2 - q_3^2 & 2q_1q_2 - 2q_0q_3 & 2q_1q_3 + 2q_0q_2 \\ 2q_1q_2 + 2q_0q_3 & q_0^2 - q_1^2 + q_2^2 - q_3^2 & 2q_2q_3 - 2q_0q_1 \\ 2q_1q_3 - 2q_0q_2 & 2q_2q_3 + 2q_0q_1 & q_0^2 - q_1^2 - q_2^2 + q_3^2 \end{pmatrix} && (229) \\ &= \begin{pmatrix} 1 - 2q_2^2 - 2q_3^2 & 2q_1q_2 - 2q_0q_3 & 2q_1q_3 + 2q_0q_2 \\ 2q_1q_2 + 2q_0q_3 & 1 - 2q_1^2 - 2q_3^2 & 2q_2q_3 - 2q_0q_1 \\ 2q_1q_3 - 2q_0q_2 & 2q_2q_3 + 2q_0q_1 & 1 - 2q_1^2 - 2q_2^2 \end{pmatrix} && (230) \end{aligned}$$

The first form is called ‘homogeneous’, the second form ‘inhomogeneous’.

In index notation:

$$A_{\alpha\beta} = \delta_{\alpha\beta}\left(q_0^2 - q_1^2 - q_2^2 - q_3^2\right) + 2q_\alpha q_\beta - 2q_0\epsilon_{\alpha\beta\gamma}q_\gamma. \tag{231}$$

Relation to other sets of rotation coordinates:

- Rotation by an angle a around a unit vector $\hat{\boldsymbol{a}}$.

$$\begin{aligned} q_0 &= \cos(a/2) \\ q_1 &= \hat{a}_x \sin(a/2) \\ q_2 &= \hat{a}_y \sin(a/2) \\ q_3 &= \hat{a}_z \sin(a/2) \end{aligned} \tag{232}$$

- Euler angles

$$\begin{aligned} q_0 &= \cos\tfrac{1}{2}\theta\cos\tfrac{1}{2}(\phi+\psi) \\ q_1 &= \sin\tfrac{1}{2}\theta\cos\tfrac{1}{2}(\phi-\psi) \\ q_2 &= \sin\tfrac{1}{2}\theta\sin\tfrac{1}{2}(\phi-\psi) \\ q_3 &= \cos\tfrac{1}{2}\theta\sin\tfrac{1}{2}(\phi+\psi) \end{aligned} \tag{233}$$

(Copied from Allen and Tildesley as is.)

8.4 Quaternion time derivatives

With q_0 referred to as the scalar parameter and $\tilde{\mathbf{q}} = (q_1, q_2, q_3)$ as the vector parameter,

$$\mathbf{r}' = \mathbf{A}\mathbf{r} = \mathbf{r} + 2q_0\left(\tilde{\mathbf{q}} \times \mathbf{r}\right) + 2\left(\tilde{\mathbf{q}} \times \left(\tilde{\mathbf{q}} \times \mathbf{r}\right)\right). \tag{234}$$

The rotation matrix $\mathbf{A}$ turns the body-fixed vector $\mathbf{r}^{\mathrm{b}}$ into the space-fixed vector $\mathbf{r}^{\mathrm{s}} = \mathbf{A}\mathbf{r}^{\mathrm{b}}$. Combining the two expressions for the velocity of this point in the lab frame,

$$\dot{\mathbf{r}}^{\mathrm{s}} = \dot{\mathbf{A}}\mathbf{r}^{\mathrm{b}}, \tag{235}$$

$$\dot{\mathbf{r}}^{\mathrm{s}} = [\boldsymbol{\omega} \times \mathbf{r}]^{\mathrm{s}} = \mathbf{A}[\boldsymbol{\omega} \times \mathbf{r}]^{\mathrm{b}}, \tag{236}$$

it follows that

$$\boldsymbol{\omega}^{\mathrm{b}} \times \mathbf{r}^{\mathrm{b}} = \mathbf{A}^{-1}\dot{\mathbf{A}}\mathbf{r}^{\mathrm{b}}. \tag{237}$$

Evaluation of the matrix product yields

$$\left(\mathbf{A}^{-1}\right)_{1\alpha}\left(\frac{d\mathbf{A}}{dt}\right)_{\alpha 1} = 2q^2\left(\mathbf{q}\cdot\dot{\mathbf{q}}\right) \tag{238}$$

$$\left(\mathbf{A}^{-1}\right)_{2\alpha}\left(\frac{d\mathbf{A}}{dt}\right)_{\alpha 2} = \left(\mathbf{A}^{-1}\right)_{3\alpha}\left(\frac{d\mathbf{A}}{dt}\right)_{\alpha 3} = 2q^2\left(\mathbf{q}\cdot\dot{\mathbf{q}}\right) \tag{239}$$

$$\left(\mathbf{A}^{-1}\right)_{2\alpha}\left(\frac{d\mathbf{A}}{dt}\right)_{\alpha 1} = 2q^2\left(-\dot{q}_0 q_3 + \dot{q}_1 q_2 - \dot{q}_2 q_1 + \dot{q}_3 q_0\right) \tag{240}$$

$$\left(\mathbf{A}^{-1}\right)_{3\alpha}\left(\frac{d\mathbf{A}}{dt}\right)_{\alpha 1} = 2q^2\left(+\dot{q}_0 q_2 + \dot{q}_1 q_3 - \dot{q}_2 q_0 - \dot{q}_3 q_1\right) \tag{241}$$

$$\left(\mathbf{A}^{-1}\right)_{3\alpha}\left(\frac{d\mathbf{A}}{dt}\right)_{\alpha 2} = 2q^2\left(-\dot{q}_0 q_1 + \dot{q}_1 q_0 + \dot{q}_2 q_3 - \dot{q}_3 q_2\right) \tag{242}$$

$$\left(\mathbf{A}^{-1}\right)_{\beta\alpha}\left(\frac{d\mathbf{A}}{dt}\right)_{\alpha\gamma} = -\left(\mathbf{A}^{-1}\right)_{\gamma\alpha}\left(\frac{d\mathbf{A}}{dt}\right)_{\alpha\beta}. \tag{243}$$

Element-by-element comparison with

$$\boldsymbol{\omega}^{\mathrm{b}} \times \mathbf{r}^{\mathrm{b}} = \begin{pmatrix} 0 & -\omega_z^{\mathrm{b}} & \omega_y^{\mathrm{b}} \\ \omega_z^{\mathrm{b}} & 0 & -\omega_x^{\mathrm{b}} \\ -\omega_y^{\mathrm{b}} & \omega_x^{\mathrm{b}} & 0 \end{pmatrix} \mathbf{r}^{\mathrm{b}} \tag{244}$$

then gives[12]

$$\begin{pmatrix} \omega_x^{\mathrm{b}} \\ \omega_y^{\mathrm{b}} \\ \omega_z^{\mathrm{b}} \end{pmatrix} = 2q^2 \begin{pmatrix} -q_1 & q_0 & q_3 & -q_2 \\ -q_2 & -q_3 & q_0 & q_1 \\ -q_3 & q_2 & -q_1 & q_0 \end{pmatrix} \begin{pmatrix} \dot{q}_0 \\ \dot{q}_1 \\ \dot{q}_2 \\ \dot{q}_3 \end{pmatrix} \quad \text{or} \quad \boldsymbol{\omega}^{\mathrm{b}} = \tilde{\mathbf{B}}^{-1}\dot{\mathbf{q}}, \tag{245}$$

with the unit length constraint translating into $\mathbf{q}\cdot\dot{\mathbf{q}} = 0$. The latter two equations can be combined into

$$\begin{pmatrix} 0 \\ \boldsymbol{\omega}^{\mathrm{b}} \end{pmatrix} = \begin{pmatrix} \mathbf{q}^{\mathrm{T}} \\ \tilde{\mathbf{B}}^{-1} \end{pmatrix} \dot{\mathbf{q}} = \mathbf{B}^{-1}\dot{\mathbf{q}} \tag{246}$$

where

$$\mathbf{B}^{-1} = 2q^2 \begin{pmatrix} q_0 & q_1 & q_2 & q_3 \\ -q_1 & q_0 & q_3 & -q_2 \\ -q_2 & -q_3 & q_0 & q_1 \\ -q_3 & q_2 & -q_1 & q_0 \end{pmatrix}. \tag{247}$$

[12] Caution: any vector $\dot{\mathbf{q}}$ yields a vector $\boldsymbol{\omega}$, but proper rotations require $\mathbf{q}\cdot\dot{\mathbf{q}} = 0$.

Inversion gives[13]

$$\dot{\mathbf{q}} = \mathbf{B}\begin{pmatrix} 0 \\ \boldsymbol{\omega}^{\mathrm{b}} \end{pmatrix} = \begin{pmatrix} \mathbf{q} & \tilde{\mathbf{B}} \end{pmatrix}\begin{pmatrix} 0 \\ \boldsymbol{\omega}^{\mathrm{b}} \end{pmatrix} \quad \text{or} \quad \dot{\mathbf{q}} = \tilde{\mathbf{B}}\boldsymbol{\omega}^{\mathrm{b}} \tag{248}$$

with

$$\mathbf{B} = \frac{1}{2q^4}\begin{pmatrix} q_0 & -q_1 & -q_2 & -q_3 \\ q_1 & q_0 & -q_3 & q_2 \\ q_2 & q_3 & q_0 & -q_1 \\ q_3 & -q_2 & q_1 & q_0 \end{pmatrix} \quad \text{and} \quad \tilde{\mathbf{B}} = \frac{1}{2q^4}\begin{pmatrix} -q_1 & -q_2 & -q_3 \\ q_0 & -q_3 & q_2 \\ q_3 & q_0 & -q_1 \\ -q_2 & q_1 & q_0 \end{pmatrix}. \tag{249}$$

Comparing these matrices with their inverse yields

$$\mathbf{B}^{-1} = 4q^6\mathbf{B}^{\mathrm{T}}, \tag{250}$$

$$\tilde{\mathbf{B}}^{-1} = 4q^6\tilde{\mathbf{B}}^{\mathrm{T}}. \tag{251}$$

For rotation matrices $q^2 = 1$, in which case

$$\mathbf{B}^{-1} = 4\mathbf{B}^{\mathrm{T}}, \tag{252}$$

$$\tilde{\mathbf{B}}^{-1} = 4\tilde{\mathbf{B}}^{\mathrm{T}}. \tag{253}$$

and even

$$\tilde{\mathbf{B}}^{-1}\tilde{\mathbf{B}} = \mathbf{1}, \tag{254}$$

though the 3×4 matrix $\tilde{\mathbf{B}}^{-1}$ and the 4×3 matrix $\tilde{\mathbf{B}}$ are clearly not eachother's inverse.

By analogy with Eq. (237), it is also possible to link the time derivatives of the quaternions directly to the lab-based angular velocities:

$$\boldsymbol{\omega}^{\mathrm{s}} \times \mathbf{r}^{\mathrm{s}} = \dot{\mathbf{A}}\mathbf{r}^{\mathrm{b}} = \dot{\mathbf{A}}\mathbf{A}^{-1}\mathbf{r}^{\mathrm{s}}, \tag{255}$$

etcetera.

For the quaternion equations of motion in the lab frame,

$$\dot{\mathbf{r}}^{\mathrm{s}} = \dot{\mathbf{A}}\mathbf{r}^{\mathrm{b}} = \dot{\mathbf{A}}\mathbf{A}^{-1}\mathbf{r}^{\mathrm{s}}, \tag{256}$$

$$\dot{\mathbf{r}}^{\mathrm{s}} = [\boldsymbol{\omega} \times \mathbf{r}]^{\mathrm{s}}. \tag{257}$$

Evaluation of the matrix product yields

$$\left(\frac{d\dot{\mathbf{A}}}{dt}\right)_{1\alpha} \left(\mathbf{A}^{-1}\right)_{\alpha 1} = 2q^2\left(\mathbf{q} \cdot \dot{\mathbf{q}}\right) \tag{258}$$

$$\left(\frac{d\dot{\mathbf{A}}}{dt}\right)_{2\alpha} \left(\mathbf{A}^{-1}\right)_{\alpha 1} = 2q^2(-\dot{q}_0 q_3 - \dot{q}_1 q_2 + \dot{q}_2 q_1 + \dot{q}_3 q_0) \tag{259}$$

$$\left(\frac{d\dot{\mathbf{A}}}{dt}\right)_{3\alpha} \left(\mathbf{A}^{-1}\right)_{\alpha 1} = 2q^2(+\dot{q}_0 q_2 - \dot{q}_1 q_3 - \dot{q}_2 q_0 + \dot{q}_3 q_1) \tag{260}$$

$$\left(\frac{d\dot{\mathbf{A}}}{dt}\right)_{3\alpha} \left(\mathbf{A}^{-1}\right)_{\alpha 2} = 2q^2(-\dot{q}_0 q_1 + \dot{q}_1 q_0 - \dot{q}_2 q_3 + \dot{q}_3 q_2) \tag{261}$$

[13] This is exactly identical to Eq. (3.37) in Allen and Tildesley. Note that they use the transposed definition of **A**, because their **A** rotates from space fixed to body fixed.

Element-by-element comparison with

$$\boldsymbol{\omega}^{\mathrm{s}} \times \mathbf{r}^{\mathrm{s}} = \begin{pmatrix} 0 & -\omega_z^{\mathrm{s}} & \omega_y^{\mathrm{s}} \\ \omega_z^{\mathrm{s}} & 0 & -\omega_x^{\mathrm{s}} \\ -\omega_y^{\mathrm{s}} & \omega_x^{\mathrm{s}} & 0 \end{pmatrix} \mathbf{r}^{\mathrm{s}} \tag{262}$$

then gives[12]

$$\begin{pmatrix} \omega_x^{\mathrm{s}} \\ \omega_y^{\mathrm{s}} \\ \omega_z^{\mathrm{s}} \end{pmatrix} = 2q^2 \begin{pmatrix} -q_1 & q_0 & -q_3 & q_2 \\ -q_2 & q_3 & q_0 & -q_1 \\ -q_3 & -q_2 & q_1 & q_0 \end{pmatrix} \begin{pmatrix} \dot{q}_0 \\ \dot{q}_1 \\ \dot{q}_2 \\ \dot{q}_3 \end{pmatrix} \quad \text{or} \quad \boldsymbol{\omega}^{\mathrm{s}} = \tilde{\mathbf{C}}^{-1}\dot{\mathbf{q}}, \tag{263}$$

provided $\mathbf{q} \cdot \dot{\mathbf{q}} = 0$. Combining the last two equations,

$$\begin{pmatrix} 0 \\ \boldsymbol{\omega}^{\mathrm{s}} \end{pmatrix} = \begin{pmatrix} \mathbf{q}^{\mathrm{T}} \\ \tilde{\mathbf{C}}^{-1} \end{pmatrix} \dot{\mathbf{q}} = \mathbf{C}^{-1}\dot{\mathbf{q}} \tag{264}$$

where

$$\mathbf{C}^{-1} = 2q^2 \begin{pmatrix} q_0 & q_1 & q_2 & q_3 \\ -q_1 & q_0 & -q_3 & q_2 \\ -q_2 & q_3 & q_0 & -q_1 \\ -q_3 & -q_2 & q_1 & q_0 \end{pmatrix} \tag{265}$$

Inversion gives

$$\dot{\mathbf{q}} = \mathbf{C} \begin{pmatrix} 0 \\ \boldsymbol{\omega}^{\mathrm{s}} \end{pmatrix} \quad \text{or} \quad \dot{\mathbf{q}} = \tilde{\mathbf{C}}\boldsymbol{\omega}^{\mathrm{s}}, \tag{266}$$

with

$$\mathbf{C} = \frac{1}{2q^4} \begin{pmatrix} q_0 & -q_1 & -q_2 & -q_3 \\ q_1 & q_0 & q_3 & -q_2 \\ q_2 & -q_3 & q_0 & q_1 \\ q_3 & q_2 & -q_1 & q_0 \end{pmatrix} \quad \text{and} \quad \tilde{\mathbf{C}} = \frac{1}{2q^4} \begin{pmatrix} -q_1 & -q_2 & -q_3 \\ q_0 & q_3 & -q_2 \\ -q_3 & q_0 & q_1 \\ q_2 & -q_1 & q_0 \end{pmatrix} \tag{267}$$

An alternative derivation, by comparing the equations of motion in the lab frame with those in the body frame, gives

$$\tilde{\mathbf{C}} = \tilde{\mathbf{B}}\mathbf{A}^{-1} = \frac{1}{2q^4} \begin{pmatrix} -q_1 & -q_2 & -q_3 \\ q_0 & q_3 & -q_2 \\ -q_3 & q_0 & q_1 \\ q_2 & -q_1 & q_0 \end{pmatrix}, \tag{268}$$

in perfect agreement.

8.5 Inertia tensor

The 4×4 product of the tilded matrices gives

$$\tilde{\mathbf{B}}\tilde{\mathbf{B}}^{-1} = \frac{1}{q^2} \begin{pmatrix} q_1^2 + q_2^2 + q_3^2 & -q_0 q_1 & -q_0 q_2 & -q_0 q_3 \\ -q_1 q_0 & q_0^2 + q_2^2 + q_3^2 & -q_1 q_2 & -q_1 q_3 \\ -q_2 q_0 & -q_2 q_1 & q_0^2 + q_1^2 + q_3^2 & -q_2 q_3 \\ -q_3 q_0 & -q_3 q_1 & -q_3 q_2 & q_0^2 + q_1^2 + q_2^2 \end{pmatrix} \tag{269}$$

$$= \mathbf{1} - \frac{1}{q^2}\mathbf{q}\mathbf{q}^{\mathrm{T}}, \tag{270}$$