9

Algorithmic schemes for finite rotations

This chapter presents the topics related to the algorithmic treatment of finite rotations. Mostly static (time-independent) problems are considered, although angular velocity and acceleration also are defined in Sect. 9.4.

We assume that the Newton method is used to solve the non-linear equilibrium equations. To generate the tangent matrix and the residual vector, the total rotation and the increment of rotation are needed.

1. For the total rotation, we use either the rotations matrices or quaternions. Both are used in the most general Scheme 2, when the total rotation is composed of the part which is a result of the update and the part which is parameterized.
2. For increments of rotations, we use the rotation vector to avoid additional orthogonality constraints.

The respective formulas are provided for the parametrization by the canonical rotation vector and by the semi-tangential vector. For both, it is essential use the formulae which are free of numerical indeterminacy; this applies not only to the rotation tensor but also to its first and second differentials.

Besides, the formulae to convert the parameters used for the increment to those used for the total rotation are required; we show that the aforementioned rotation vectors and quaternions can be conveniently matched together. Note that the rotation vector and its increment can belong to different tangent planes to SO(3), which is a matter of choice and can affect the effectiveness and stability of computations.

Several update schemes of rotational parameters can be considered but not all of them perform equally well. This cannot be fully predicted theoretically and a numerical verification is always needed. The answer to the question which type of update is optimal, multiplicative or additive, is quite convoluted, see [30].

Note that the situation in dynamics is more complicated, due to the presence of the angular velocity and acceleration. The time-stepping (e.g. Newmark) scheme must be extended to incorporate the rotational dofs, which can be done in various ways. This is illustrated by the examples for the rigid-body dynamics in Sect. 9.4 but the dynamics of shells remains beyond the scope of this work.

9.1 Increments of rotation vectors in two tangent planes

In this section, we consider the tangent spaces at two different rotations, $\mathbf{R}_A$ and $\mathbf{R}_B$, and establish the relation between the infinitesimal rotation vectors belonging to these spaces, using either a left or right composition rule. The tangent operators $\mathbf{T}$ and their inverses are given for the semi-tangential and canonical rotation vectors. Finally, the differentials $\chi\mathbf{T}$, which are needed in the second variation of the rotation tensor, are obtained.

Tangent plane. The set of all infinitesimal rotations $\tilde{\boldsymbol{\theta}}$ superposed onto the finite rotation $\mathbf{R}$ is referred to as the plane tangent to $\mathrm{SO}(3)$ at $\mathbf{R}$, and denoted by $T_R\mathrm{SO}(3) \doteq \{\tilde{\boldsymbol{\theta}}\,\mathbf{R} \mid \text{for } \tilde{\boldsymbol{\theta}} \in \mathrm{so}(3)\}$. The plane tangent at $\mathbf{R} = \mathbf{I}$ is called the initial tangent plane and denoted by $T_I\mathrm{SO}(3) \doteq \{\tilde{\boldsymbol{\theta}} \mid \text{for } \tilde{\boldsymbol{\theta}} \in \mathrm{so}(3)\}$.

The definitions are analogous for the right composition rule; the tangent plane at $\mathbf{R}$ is defined as $T_R\mathrm{SO}(3) \doteq \{\mathbf{R}\,\tilde{\boldsymbol{\Theta}} \mid \text{for } \tilde{\boldsymbol{\Theta}} \in \mathrm{so}(3)\}$, and the initial tangent plane as $T_I\mathrm{SO}(3) \doteq \{\tilde{\boldsymbol{\Theta}} \mid \text{for } \tilde{\boldsymbol{\Theta}} \in \mathrm{so}(3)\}$.

9.1.1 Operator $\mathbf{T}$

Generally, in this section we use the notation similar to that of [44], with the exception of the tangent operator $\mathbf{T}$, which we associate with the left composition. In [44], the operator for the right composition rule is designated by $\mathbf{T}$, see eq. (38) therein, while we denote it by $\mathbf{T}^T$. Our $\mathbf{T}$ is identical to $\boldsymbol{\Gamma}$ of [9], eq. (8.31), and $\mathbf{T}$ of [40], eq. (68). The operator $\mathbf{T}$ used in [219] and [221], eq. (88), is equivalent to our $\mathbf{T}^{-T}$. Note that, in these papers, the tangent operators are given only for the canonical rotation vector, while we also provide the operators for the semi-tangential parametrization.

A. Left composition rule

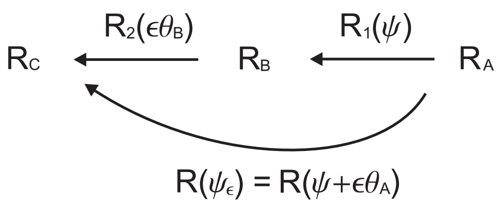

Fig. 9.1 Scheme of increments of rotations for the left composition rule.

We adopt the left composition rule and express $\mathbf{R}_B = \mathbf{R}_1(\boldsymbol{\psi})\,\mathbf{R}_A$, where $\boldsymbol{\psi}$ is the rotation vector, see Fig. 9.1. The perturbed rotation $\mathbf{R}_C$ can be related either to $\mathbf{R}_A$ or to $\mathbf{R}_B$,

$$\mathbf{R}_C = \mathbf{R}(\boldsymbol{\psi}_\epsilon)\,\mathbf{R}_A, \qquad \mathbf{R}_C = \mathbf{R}_2(\epsilon\boldsymbol{\theta}_B)\,\mathbf{R}_B, \tag{9.1}$$

where $\boldsymbol{\psi}_\epsilon \doteq \boldsymbol{\psi} + \epsilon\boldsymbol{\theta}_A$ and ϵ is a scalar parameter. Note that, using the notation established in mechanics, we can also designate $\boldsymbol{\theta}_A$ as $\Delta\boldsymbol{\psi}$. Besides, $\boldsymbol{\theta}_A$ and $\boldsymbol{\theta}_B$ are infinitesimal rotation vectors, and

$$\tilde{\boldsymbol{\psi}}_\epsilon\,\mathbf{R}_A = \left(\tilde{\boldsymbol{\psi}} + \epsilon\tilde{\boldsymbol{\theta}}_A\right)\mathbf{R}_A \in T_{R_A}\mathrm{SO}(3), \qquad \epsilon\tilde{\boldsymbol{\theta}}_B\,\mathbf{R}_B \in T_{R_B}\mathrm{SO}(3), \tag{9.2}$$

i.e. the perturbations $\epsilon\tilde{\boldsymbol{\theta}}_A$ and $\epsilon\tilde{\boldsymbol{\theta}}_B$ belong to different tangent planes, see Fig. 9.2.
Because both relations (9.1) must yield the same $\mathbf{R}_C$, we obtain

$$\mathbf{R}_2(\epsilon\boldsymbol{\theta}_B)\,\mathbf{R}_B = \mathbf{R}(\boldsymbol{\psi}_\epsilon)\,\mathbf{R}_A, \tag{9.3}$$

which, using $\mathbf{R}_B = \mathbf{R}_1(\boldsymbol{\psi})\,\mathbf{R}_A$, reduces to

$$\mathbf{R}_2(\epsilon\boldsymbol{\theta}_B) = \mathbf{R}(\boldsymbol{\psi}_\epsilon)\,\mathbf{R}_1^T(\boldsymbol{\psi}). \tag{9.4}$$

This is a non-linear equation of $\boldsymbol{\theta}_A$ and $\boldsymbol{\theta}_B$, and to find the relation between $\boldsymbol{\theta}_A$ and $\boldsymbol{\theta}_B$, we have to

1. select a specific parametrization of $\mathbf{R}$,
2. convert the tensorial equation to the vectorial form, and
3. locally linearize it using the scheme defined below to obtain the tangent operator.

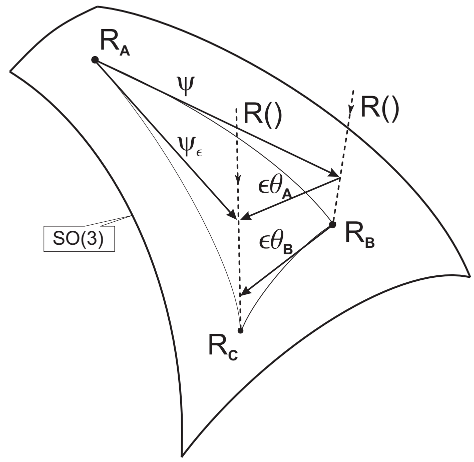

Fig. 9.2 Geometrical interpretation of SO(3) and increments of rotation. $\boldsymbol{\theta}_A$ and $\boldsymbol{\theta}_B$ are not parallel!

Scheme of calculation of operator T. Assume that the l.h.s. of an equation, such as, e.g., eq. (9.8), depends on $\boldsymbol{\theta}_B$ while the r.h.s. depends on $\boldsymbol{\theta}_A$. Hence, the equation can be rewritten as $\mathbf{l}(\boldsymbol{\theta}_B) = \mathbf{r}(\boldsymbol{\theta}_A)$, where $\mathbf{l}$ and $\mathbf{r}$ are, in general, non-linear functions. The differentials of both sides of the considered equation must be equal,

$$D\mathbf{l} \cdot \boldsymbol{\theta}_B = D\mathbf{r} \cdot \boldsymbol{\theta}_A. \tag{9.5}$$

Hence, we calculate two directional derivatives and obtain two tangent operators,

$$\mathbf{T}_l : \quad D\mathbf{l} \cdot \boldsymbol{\theta}_B = \mathbf{T}_l\, \boldsymbol{\theta}_B, \qquad \mathbf{T}_r : \quad D\mathbf{r} \cdot \boldsymbol{\theta}_B = \mathbf{T}_r\, \boldsymbol{\theta}_A, \tag{9.6}$$

where $\mathbf{T}_l$ is the left tangent operator, while $\mathbf{T}_r$ is the right tangent operator. By using them, from eq. (9.5), we obtain

$$\boldsymbol{\theta}_B = \mathbf{T}\, \boldsymbol{\theta}_A, \quad \text{where} \qquad \mathbf{T} \doteq \mathbf{T}_l^{-1} \mathbf{T}_r. \tag{9.7}$$

The directional derivative is calculated in a standard manner, i.e. we differentiate the perturbed expression with respect to the perturbation parameter ϵ and evaluate it for $\epsilon = 0$.

Remark. The hand derivation of tangent operators is, in general, quite tedious work and prone to errors. The same operators can be obtained in a relatively easier way using a symbolic manipulation program, such as *Mathematica* or *Maple*. Using such programs, we can differentiate a vectorial expression w.r.t. a scalar variable and evaluate it for $\epsilon = 0$, so they are well suited to calculate the directional derivative. Then, it remains to recast the obtained expressions into a concise tensorial form and extract the tangent operator.

Semi-tangential parametrization. Assume that $\boldsymbol{\theta}_A$, $\boldsymbol{\theta}_B$, $\boldsymbol{\psi}$ and $\boldsymbol{\psi}_\epsilon$ are semi-tangential rotation vectors. For the semi-tangential parametrization, we can apply the composition formula (8.189), use the identity $\mathbf{R}_1^T(\boldsymbol{\psi}) = \mathbf{R}_1(-\boldsymbol{\psi})$ in eq. (9.4), and write its vectorial counterpart as follows:

$$\epsilon\boldsymbol{\theta}_B = \frac{1}{1+\boldsymbol{\psi}_\epsilon\cdot\boldsymbol{\psi}}\left[\boldsymbol{\psi}_\epsilon - \boldsymbol{\psi} - \boldsymbol{\psi}_\epsilon\times\boldsymbol{\psi}\right]. \tag{9.8}$$

This is an equation non-linear in $\boldsymbol{\theta}_A$ which we can linearize by using the scheme explained in eq. (9.7). Then

$$\boldsymbol{\theta}_B = \mathbf{T}(\boldsymbol{\psi})\ \boldsymbol{\theta}_A, \qquad \mathbf{T} \doteq \frac{\partial\boldsymbol{\theta}_B}{\partial\boldsymbol{\theta}_A}, \tag{9.9}$$

where the tangent operator is

$$\mathbf{T}(\boldsymbol{\psi}) = \frac{1}{1+\boldsymbol{\psi}\cdot\boldsymbol{\psi}}(\mathbf{I}+\tilde{\boldsymbol{\psi}}). \tag{9.10}$$

The operator $\mathbf{T}$ has the following properties:

1. It is non-singular for arbitrary $\boldsymbol{\psi}$, as $\det\mathbf{T} = 1/(1+\|\boldsymbol{\psi}\|^2)^2$.
2. If $\boldsymbol{\psi} = \mathbf{0}$, then $\mathbf{T}(\boldsymbol{\psi}) = \mathbf{I}$. Then we obtain $\boldsymbol{\theta}_B = \boldsymbol{\theta}_A$, as expected.
3. If $\boldsymbol{\psi}$ and $\boldsymbol{\theta}_A$ are coaxial, i.e. $\boldsymbol{\theta}_A = \alpha\,\boldsymbol{\psi}$, where α is an arbitrary scalar, then

$$\boldsymbol{\theta}_B = \mathbf{T}(\boldsymbol{\psi})\,\boldsymbol{\theta}_A = \alpha\,\mathbf{T}(\boldsymbol{\psi})\,\boldsymbol{\psi} = \frac{1}{1+\boldsymbol{\psi}\cdot\boldsymbol{\psi}}\boldsymbol{\theta}_A, \tag{9.11}$$

   i.e. $\mathbf{T}(\boldsymbol{\psi})$ only shortens $\boldsymbol{\theta}_A$. In the proof, we used $\tilde{\boldsymbol{\psi}}\boldsymbol{\psi} = \mathbf{0}$.
4. For $\|\boldsymbol{\psi}\| \to \infty$, $\mathbf{T}(\boldsymbol{\psi}) \to \mathbf{0}$. Hence, we cannot use very long rotation vectors, the norms of which are big numbers.
5. $\mathbf{T}(\boldsymbol{\psi})$ is not a periodic function of $\|\boldsymbol{\psi}\|$. To show this, we use $\tilde{\boldsymbol{\psi}} = \|\boldsymbol{\psi}\|\,\tilde{\mathbf{e}}$ in eq. (9.10), where $\tilde{\mathbf{e}} = \mathbf{S}$, to obtain

$$\mathbf{T}(\boldsymbol{\psi}) = \frac{1}{1+\|\boldsymbol{\psi}\|^2}\mathbf{I} + \frac{\|\boldsymbol{\psi}\|}{1+\|\boldsymbol{\psi}\|^2}\,\tilde{\mathbf{e}}, \tag{9.12}$$

where $\tilde{\mathbf{e}}$ does not depend on $\|\boldsymbol{\psi}\|$. For example, for $\mathbf{e} = [0, 0, 1]^T$, we obtain the following representation:

$$(\mathbf{T})_{ij} = \begin{bmatrix} \frac{1}{1+t^2} & -\frac{t}{1+t^2} & 0 \\ \frac{t}{1+t^2} & \frac{1}{1+t^2} & 0 \\ 0 & 0 & \frac{1}{1+t^2} \end{bmatrix}, \tag{9.13}$$

where its components are not periodical functions of $t \doteq \|\boldsymbol{\psi}\|$. (Note that the coefficients in this matrix are equal to c_1 and c_2 of eq. (8.101) divided by $2t$.) In consequence, we cannot use the shortened rotation vector.

6. The inverse operator is as follows:

$$\mathbf{T}^{-1}(\boldsymbol{\psi}) = \mathbf{I} - \tilde{\boldsymbol{\psi}} + \boldsymbol{\psi} \otimes \boldsymbol{\psi}. \tag{9.14}$$

Note that the derivation of $\mathbf{T}$ is relatively simple for semi-tangential vectors due to the vectorial form of eq. (9.8).

Finally, our $\mathbf{T}$ of eq. (9.10) is different from the $\mathbf{T}$ operator of [76], eq. (4.32), in which the additional multiplier 2 appears. Both operators are correct and their various forms result from different definitions.

Canonical parametrization. Assume that $\boldsymbol{\theta}_A$, $\boldsymbol{\theta}_B$, $\boldsymbol{\psi}$, and $\boldsymbol{\psi}_\epsilon$ are canonical rotation vectors. For the canonical parametrization, we do not have a vectorial composition formula, such as for the semi-tangential parametrization. Therefore, in order to use eq. (8.189), we shall first introduce auxiliary semi-tangential vectors as functions of the canonical vectors

$$\overline{\boldsymbol{\psi}} \doteq \tan(\|\boldsymbol{\psi}\|/2)\, \frac{\boldsymbol{\psi}}{\|\boldsymbol{\psi}\|}, \qquad \overline{\boldsymbol{\psi}_\epsilon} \doteq \tan(\|\boldsymbol{\psi}_\epsilon\|/2)\, \frac{\boldsymbol{\psi}_\epsilon}{\|\boldsymbol{\psi}_\epsilon\|},$$

$$\overline{\epsilon\boldsymbol{\theta}_B} \doteq \tan(\|\epsilon\boldsymbol{\theta}_B\|/2)\, \frac{\epsilon\boldsymbol{\theta}_B}{\|\epsilon\boldsymbol{\theta}_B\|}, \tag{9.15}$$

marked by a horizontal overbar. Using these auxiliary vectors and exploiting $\mathbf{R}_1^T(\overline{\boldsymbol{\psi}}) = \mathbf{R}_1(-\overline{\boldsymbol{\psi}})$ in eq. (9.4), we can write its vectorial counterpart as

$$\overline{\epsilon\boldsymbol{\theta}_B} = \frac{1}{1 + \overline{\boldsymbol{\psi}_\epsilon} \cdot \overline{\boldsymbol{\psi}}} \left[\overline{\boldsymbol{\psi}_\epsilon} - \overline{\boldsymbol{\psi}} - \overline{\boldsymbol{\psi}_\epsilon} \times \overline{\boldsymbol{\psi}} \right]. \tag{9.16}$$

Analogously, as in eq. (9.9), the operator $\mathbf{T}$ is defined as

$$\boldsymbol{\theta}_B = \mathbf{T}(\boldsymbol{\psi})\, \boldsymbol{\theta}_A, \qquad \mathbf{T} \doteq \frac{\partial \boldsymbol{\theta}_B}{\partial \boldsymbol{\theta}_A}. \tag{9.17}$$

To obtain the operator $\mathbf{T}$, we use the earlier-described scheme of eq. (9.7), which yields

$$\mathbf{T}(\boldsymbol{\psi}) = c_1 \mathbf{I} + (1 - c_1)\, \mathbf{e} \otimes \mathbf{e} + c_2 \tilde{\boldsymbol{\psi}}, \tag{9.18}$$

where $\mathbf{e} = \boldsymbol{\psi}/\|\boldsymbol{\psi}\|$ and the scalar coefficients c_1 and c_2 are the same as in the rotation tensor of eqs. (8.81) and (8.83). Another, equivalent form of this operator is obtained by using $\tilde{\boldsymbol{\psi}}^2 = \|\boldsymbol{\psi}\|^2 \mathbf{S}^2 = \|\boldsymbol{\psi}\|^2 (\mathbf{e} \otimes \mathbf{e} - \mathbf{I})$, and is as follows:

$$\mathbf{T}(\boldsymbol{\psi}) = \mathbf{I} + c_2 \tilde{\boldsymbol{\psi}} + c_3 \tilde{\boldsymbol{\psi}}^2, \tag{9.19}$$

where $c_3 \doteq (1 - c_1)/\|\boldsymbol{\psi}\|^2$. The operator $\mathbf{T}$ has the following properties:

1. If $\boldsymbol{\psi} \rightarrow \mathbf{0}$, then $\mathbf{T}(\boldsymbol{\psi}) \rightarrow \mathbf{I}$, i.e. the operator tends to the identity operator.
2. At $\|\boldsymbol{\psi}\| = 0$, the coefficients of $\mathbf{T}$ are numerically indeterminate. This problem also appeared for the rotation tensor, see eq. (8.85), and was already solved for c_1 and c_2. For c_3, the problem can be solved in the same way, by defining it for $\|\boldsymbol{\psi}\| = 0$ as the limit value, i.e.

   $$\lim_{\|\boldsymbol{\psi}\| \rightarrow 0} c_3 = \frac{1}{6}. \tag{9.20}$$

   We have to consider the first derivative of c_3, which is used in the tangent operator. Again, we can use either the perturbation, $\|\boldsymbol{\psi}\| = \sqrt{\boldsymbol{\psi} \cdot \boldsymbol{\psi} + \tau}$, where $\tau = 10^{-8}$, or the truncated Taylor series expansion at $x = 0$, e.g.

   $$c_3 = \frac{1 - (\sin x / x)}{x^2} \approx \frac{1}{6} - \frac{1}{120} x^2 + \frac{1}{5040} x^4,$$

   where $x \doteq \|\boldsymbol{\psi}\|$. The above three-term expansion preserves a good accuracy of c_3 and its first derivative for the range exceeding $|x| = 1$. In consequence, we have $\mathbf{T}(\boldsymbol{\psi} = \mathbf{0}) = \mathbf{I}$.
3. $\mathbf{T}(\boldsymbol{\psi})$ is singular at $\|\boldsymbol{\psi}\| = 2k\pi$, $(k = 1, 2, ...)$, at which the determinant $\det \mathbf{T} = 2(1 - \cos \|\boldsymbol{\psi}\|)/\|\boldsymbol{\psi}\|^2$ is equal to zero. At $\|\boldsymbol{\psi}\| = 0$, $\det \mathbf{T}$ is indeterminate although $\lim_{\|\boldsymbol{\psi}\| \rightarrow 0} \det \mathbf{T} = 1$.
4. If $\boldsymbol{\psi}$ and $\boldsymbol{\theta}_A$ are coaxial, i.e. $\boldsymbol{\theta}_A = \alpha\, \boldsymbol{\psi}$, where α is an arbitrary scalar, then

   $$\boldsymbol{\theta}_B = \mathbf{T}(\boldsymbol{\psi})\, \boldsymbol{\theta}_A = \alpha\, \mathbf{T}(\boldsymbol{\psi})\, \boldsymbol{\psi} = \boldsymbol{\theta}_A, \tag{9.21}$$

   i.e. $\mathbf{T}(\boldsymbol{\psi})$ acts as the identity operator. In the proof, we used $\tilde{\boldsymbol{\psi}} \boldsymbol{\psi} = \mathbf{0}$ and $\mathbf{e}(\mathbf{e} \cdot \boldsymbol{\psi}) = \boldsymbol{\psi}$.

5. $\mathbf{T}(\boldsymbol{\psi})$ is not a periodic function of $\|\boldsymbol{\psi}\|$. To show this, we use $\tilde{\boldsymbol{\psi}} = \|\boldsymbol{\psi}\|\,\tilde{\mathbf{e}}$ in eq. (9.18), where $\tilde{\mathbf{e}} = \mathbf{S}$, to obtain

$$\mathbf{T}(\boldsymbol{\psi}) = c_1\,\mathbf{I} + (1-c_1)\;\mathbf{e}\otimes\mathbf{e} + c_2\|\boldsymbol{\psi}\|\,\tilde{\mathbf{e}}, \tag{9.22}$$

where $\mathbf{e}$ and $\tilde{\mathbf{e}}$ do not depend on $\|\boldsymbol{\psi}\|$. For example, for $\mathbf{e} = [0,0,1]^T$, we obtain the following representation:

$$(\mathbf{T})_{ij} = \begin{bmatrix} \frac{\sin\omega}{\omega} & -\frac{\sin^2(\omega/2)}{(\omega/2)} & 0 \\ \frac{\sin^2(\omega/2)}{(\omega/2)} & \frac{\sin\omega}{\omega} & 0 \\ 0 & 0 & 1 \end{bmatrix}, \tag{9.23}$$

and we see that its components are not periodical functions of $\omega \doteq \|\boldsymbol{\psi}\|$. In consequence, we cannot use the shortened canonical rotation vector $\boldsymbol{\psi}^*$ of eq. (8.82) because $\mathbf{T}(\boldsymbol{\psi}) \neq \mathbf{T}(\boldsymbol{\psi}^*)$.

6. $\mathbf{T}(\boldsymbol{\psi})$ is singular for $\|\boldsymbol{\psi}\| \to \infty$. Note that for $\omega \doteq \|\boldsymbol{\psi}\| \to \infty$, eq. (9.22) yields

$$\mathbf{T}(\boldsymbol{\psi}) \to \mathbf{e}\otimes\mathbf{e}, \tag{9.24}$$

where $\det(\mathbf{e}\otimes\mathbf{e}) = 0$, so the representation of $\mathbf{T}(\boldsymbol{\psi})$ is singular. Hence, it is not advisable to use very long rotation vectors as their norms are big numbers.

7. $\mathbf{T}(\boldsymbol{\psi})$ can be represented as the following series:

$$\mathbf{T}(\boldsymbol{\psi}) = \mathbf{I} + \frac{1}{2!}\tilde{\boldsymbol{\psi}} + \frac{1}{3!}\tilde{\boldsymbol{\psi}}^2 + \ldots + \frac{1}{(n+1)!}\tilde{\boldsymbol{\psi}}^n \ldots, \tag{9.25}$$

which can be truncated for small $\boldsymbol{\psi}$.

8. The inverse operator is

$$\mathbf{T}^{-1}(\boldsymbol{\psi}) = c_3\mathbf{I} + c_4\,\boldsymbol{\psi}\otimes\boldsymbol{\psi} - \tfrac{1}{2}\tilde{\boldsymbol{\psi}}, \tag{9.26}$$

where

$$c_3 \doteq \frac{\|\boldsymbol{\psi}\|/2}{\tan(\|\boldsymbol{\psi}\|/2)}, \qquad c_4 \doteq \frac{1-c_3}{\|\boldsymbol{\psi}\|^2}.$$

In terms of components of $\boldsymbol{\psi} \doteq [\psi_1, \psi_2, \psi_3]^T$, the operator $\mathbf{T}$ is as follows:

$$(\mathbf{T})_{ij} = \begin{bmatrix} c_1 + A\psi_1^2 & -c_2\psi_3 + A\psi_1\psi_2 & c_2\psi_2 + A\psi_1\psi_3 \\ c_2\psi_3 + A\psi_2\psi_1 & c_1 + A\psi_2^2 & -c_2\psi_1 + A\psi_2\psi_3 \\ -c_2\psi_2 + A\psi_3\psi_1 & c_2\psi_1 + A\psi_3\psi_2 & c_1 + A\psi_3^2 \end{bmatrix}, \tag{9.27}$$

where $A \doteq (1-c_1)/\|\boldsymbol{\psi}\|^2 = (1-c_1)/(\psi_1^2 + \psi_2^2 + \psi_3^2)$.

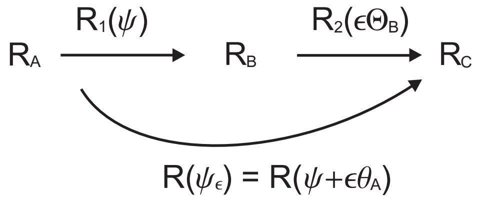

Fig. 9.3 Scheme of increments of rotations for the right composition rule.

B. Right composition rule

We adopt the right composition rule and express $\mathbf{R}_B = \mathbf{R}_A \, \mathbf{R}_1(\boldsymbol{\psi})$, where $\boldsymbol{\psi}$ is the rotation vector, see Fig. 9.3. The perturbed rotation $\mathbf{R}_C$ can be related either to $\mathbf{R}_A$ or to $\mathbf{R}_B$,

$$\mathbf{R}_C = \mathbf{R}_A \, \mathbf{R}(\boldsymbol{\psi}_\epsilon), \qquad \mathbf{R}_C = \mathbf{R}_B \, \mathbf{R}_2(\epsilon \boldsymbol{\Theta}_B), \tag{9.28}$$

where $\boldsymbol{\psi}_\epsilon \doteq \boldsymbol{\psi} + \epsilon \boldsymbol{\theta}_A$ and ϵ is a scalar parameter. Besides, $\boldsymbol{\theta}_A$ and $\boldsymbol{\Theta}_B$ are infinitesimal rotation vectors, and

$$\mathbf{R}_A \, \tilde{\boldsymbol{\psi}}_\epsilon = \mathbf{R}_A \left(\tilde{\boldsymbol{\psi}} + \epsilon \tilde{\boldsymbol{\theta}}_A \right) \in T_{R_A} \mathrm{SO}(3), \quad \mathbf{R}_B \, \epsilon \tilde{\boldsymbol{\Theta}}_B \in T_{R_B} \mathrm{SO}(3), \tag{9.29}$$

i.e. the perturbations $\epsilon \tilde{\boldsymbol{\theta}}_A$ and $\epsilon \tilde{\boldsymbol{\Theta}}_B$ belong to different tangent planes. Because both relations (9.28) must yield the same $\mathbf{R}_C$, we obtain

$$\mathbf{R}_B \, \mathbf{R}_2(\epsilon \boldsymbol{\Theta}_B) = \mathbf{R}_A \, \mathbf{R}(\boldsymbol{\psi}_\epsilon), \tag{9.30}$$

which, using $\mathbf{R}_B = \mathbf{R}_A \, \mathbf{R}_1(\boldsymbol{\psi})$, is reduced to

$$\mathbf{R}_2(\epsilon \boldsymbol{\Theta}_B) = \mathbf{R}_1^T(\boldsymbol{\psi}) \, \mathbf{R}(\boldsymbol{\psi}_\epsilon). \tag{9.31}$$

To find the relation between $\boldsymbol{\theta}_A$ and $\boldsymbol{\Theta}_B$ from this non-linear equation, we have to use the same steps as for the left composition rule, outlined below eq. (9.4).

Semi-tangential parametrization. Assume that $\boldsymbol{\theta}_A$, $\boldsymbol{\Theta}_B$, $\boldsymbol{\psi}$, and $\boldsymbol{\psi}_\epsilon$ are semi-tangential rotation vectors. For the semi-tangential parametrization, we use $\mathbf{R}_1^T(\boldsymbol{\psi}) = \mathbf{R}_1(-\boldsymbol{\psi})$, apply the composition formula (8.189), and directly write a vectorial counterpart of eq. (9.31) as follows:

$$\epsilon \boldsymbol{\Theta}_B = \frac{1}{1 + \boldsymbol{\psi}_\epsilon \cdot \boldsymbol{\psi}} \left[\boldsymbol{\psi}_\epsilon - \boldsymbol{\psi} - \boldsymbol{\psi} \times \boldsymbol{\psi}_\epsilon \right]. \tag{9.32}$$

Comparing with eq. (9.8), we note that $\boldsymbol{\psi}_\epsilon$ and $\boldsymbol{\psi}$ in the cross-product are interchanged. To obtain the relation between $\boldsymbol{\theta}_A$ and $\boldsymbol{\Theta}_B$, we use the earlier-described scheme of eq. (9.7), which yields

$$\boldsymbol{\Theta}_B = \mathbf{T}^T(\boldsymbol{\psi})\ \boldsymbol{\theta}_A, \tag{9.33}$$

where $\mathbf{T}$ was defined in eq. (9.10). Finally, we note that transposition of $\mathbf{T}$ changes the sign of the skew-symmetric $\tilde{\boldsymbol{\psi}}$ so this term needs special attention.

Canonical parametrization. Assume that $\boldsymbol{\theta}_A$, $\boldsymbol{\Theta}_B$, $\boldsymbol{\psi}$, and $\boldsymbol{\psi}_\epsilon$ are canonical rotation vectors. For the canonical parametrization, we do not have a vectorial composition formula as for the semi-tangential one. Therefore, in order to use eq. (8.189), we shall first introduce auxiliary semi-tangential vectors as functions of the canonical vectors

$$\overline{\boldsymbol{\psi}} \doteq \tan(\|\boldsymbol{\psi}\|/2)\,\frac{\boldsymbol{\psi}}{\|\boldsymbol{\psi}\|}, \qquad \overline{\boldsymbol{\psi}_\epsilon} \doteq \tan(\|\boldsymbol{\psi}_\epsilon\|/2)\,\frac{\boldsymbol{\psi}_\epsilon}{\|\boldsymbol{\psi}_\epsilon\|},$$

$$\overline{\epsilon\boldsymbol{\Theta}_B} \doteq \tan(\|\epsilon\boldsymbol{\Theta}_B\|/2)\,\frac{\epsilon\boldsymbol{\Theta}_B}{\|\epsilon\boldsymbol{\Theta}_B\|}, \tag{9.34}$$

marked by a horizontal overbar. On use of the auxiliary vectors, and $\mathbf{R}_1^T(\overline{\boldsymbol{\psi}}) = \mathbf{R}_1(-\overline{\boldsymbol{\psi}})$, we can write a vectorial counterpart of eq. (9.31), as follows:

$$\overline{\epsilon\boldsymbol{\Theta}_B} = \frac{1}{1 + \overline{\boldsymbol{\psi}_\epsilon}\cdot\overline{\boldsymbol{\psi}}}\left[\overline{\boldsymbol{\psi}_\epsilon} - \overline{\boldsymbol{\psi}} - \overline{\boldsymbol{\psi}} \times \overline{\boldsymbol{\psi}_\epsilon}\right]. \tag{9.35}$$

Comparing with eq. (9.16), we note that $\overline{\boldsymbol{\psi}_\epsilon}$ and $\overline{\boldsymbol{\psi}}$ in the cross-product are interchanged. To obtain the relation between $\boldsymbol{\theta}_A$ and $\boldsymbol{\Theta}_B$, we use the earlier-described scheme of eq. (9.7), which yields

$$\boldsymbol{\Theta}_B = \mathbf{T}^T(\boldsymbol{\psi})\ \boldsymbol{\theta}_A, \tag{9.36}$$

where $\mathbf{T}$ was defined in eq. (9.18).

Remark. Note that the multiplicative right update of rotations and the relation of eq. (9.36) are used, e.g., in the energy and momentum conserving algorithm for rigid-body dynamics, see Sect. 9.4.3.

Numerical verification of $\mathbf{T}$. To verify correctness of the form of $\mathbf{T}$, in particular of the sign in front of the skew-symmetric term, we can numerically calculate the value of $\boldsymbol{\Theta}_B$ in two different ways. Let us assume, e.g., that $\boldsymbol{\psi} = [0,0,1]^T$, $\boldsymbol{\theta}_A = [1,0,0]^T$ and $\epsilon = 10^{-8}$. Then

1. Using $\mathbf{T}$, we obtain $\epsilon\boldsymbol{\Theta}_B = \mathbf{T}^T \epsilon\boldsymbol{\theta}_A \approx [8.41,\ -4.59,\ 0]^T \times 10^{-9}$.
2. For $\boldsymbol{\psi}_\epsilon = \boldsymbol{\psi} + \epsilon\boldsymbol{\theta}_A = [10^{-8},0,1]^T$, we calculate $\overline{\epsilon\boldsymbol{\Theta}_B}$ using the vectorial eq. (9.35) and, next, by the approximation

$$\overline{\epsilon\boldsymbol{\Theta}_B} \doteq \tan(\|\epsilon\boldsymbol{\Theta}_B\|/2)\,\frac{\epsilon\boldsymbol{\Theta}_B}{\|\epsilon\boldsymbol{\Theta}_B\|} \approx \frac{\|\epsilon\boldsymbol{\Theta}_B\|}{2}\,\frac{\epsilon\boldsymbol{\Theta}_B}{\|\epsilon\boldsymbol{\Theta}_B\|} = \frac{\epsilon\boldsymbol{\Theta}_B}{2}, \tag{9.37}$$

we obtain $(\epsilon\boldsymbol{\Theta}_B) \approx 2\,(\overline{\epsilon\boldsymbol{\Theta}_B}) \approx [8.41,\ -4.59,\ 0]^T \times 10^{-9}$.

Hence, both methods yield the same value. If we change the sign at the skew-symmetric term in $\mathbf{T}$, then we obtain: $\epsilon\boldsymbol{\Theta}_B = \mathbf{T}^T\,\epsilon\boldsymbol{\theta}_A \approx [8.41,\ +4.59,\ 0]^T \times 10^{-9}$, with a plus at the second component.

9.1.2 Differential $\chi\mathbf{T}$

In calculations of the second variation of the rotation tensor in Sect. 9.2.4, we will need the directional derivative of the tangent operator $\mathbf{T}$, which is defined as

$$\chi\mathbf{T} \doteq D\mathbf{T}(\boldsymbol{\psi}) \cdot \boldsymbol{\theta}^+, \tag{9.38}$$

where the direction $\boldsymbol{\theta}^+$ is defined in eq. (9.73).

A. For the semi-tangential parametrization, and the operator $\mathbf{T}$ of eq. (9.10), we obtain

$$\chi\mathbf{T}(\boldsymbol{\psi},\boldsymbol{\theta}^+) = -2a_1^2\,(\boldsymbol{\theta}^+ \cdot \boldsymbol{\psi})\,(\mathbf{I} + \tilde{\boldsymbol{\psi}}) + a_1\,\tilde{\boldsymbol{\theta}}^+, \tag{9.39}$$

where $a_1 \doteq 1/(1 + \boldsymbol{\psi}\cdot\boldsymbol{\psi})$. For $\boldsymbol{\psi} \to \mathbf{0}$, $\chi\mathbf{T} \to \tilde{\boldsymbol{\theta}}^+ \in \mathrm{so}(3)$.

B. For the canonical rotation vector, and the operator $\mathbf{T}$ of eq. (9.18), we obtain

$$\begin{aligned}\chi\mathbf{T}(\boldsymbol{\psi},\boldsymbol{\theta}^+) = {} & a_1\,(\mathbf{e}\cdot\boldsymbol{\theta}^+)\,\mathbf{I} + a_2\,(\boldsymbol{\theta}^+ \otimes \mathbf{e} + \mathbf{e} \otimes \boldsymbol{\theta}^+) \\ & + a_3\,(\mathbf{e}\cdot\boldsymbol{\theta}^+)(\mathbf{e}\otimes\mathbf{e}) + a_4\,(\mathbf{e}\cdot\boldsymbol{\theta}^+)\tilde{\boldsymbol{\psi}} + a_5\,\tilde{\boldsymbol{\theta}}^+, \end{aligned} \tag{9.40}$$

where $\mathbf{e} = \boldsymbol{\psi}/\|\boldsymbol{\psi}\|$, $\omega = \|\boldsymbol{\psi}\| = \sqrt{\boldsymbol{\psi}\cdot\boldsymbol{\psi}}$, and the scalar coefficients are

$$
\begin{aligned}
&a_1 = b_2 - b_1, \qquad a_2 = b_3 - b_1, \\
&a_3 = 3b_1 - b_2 - 2b_3, \qquad a_4 = -b_3 b_4 + b_1, \qquad a_5 = \tfrac{1}{2} b_4, \\
&b_1 = \frac{\sin\omega}{\omega^2}, \quad b_2 = \frac{\cos\omega}{\omega}, \quad b_3 = \frac{1}{\omega}, \quad b_4 = \left[\frac{\sin(\omega/2)}{(\omega/2)}\right]^2. \qquad (9.41)
\end{aligned}
$$

We see that the coefficients $b_i \ (i = 1, \ldots, 4)$ are numerically indeterminate at $\omega = 0$. For $\boldsymbol{\psi} \to \mathbf{0}$, $\chi\mathbf{T} \to \frac{1}{2}\tilde{\boldsymbol{\theta}}^+ \in \mathrm{so}(3)$.

Remark. The derivation of formula (9.40) is cumbersome, see [44], but its correctness can be verified easier. For instance, we can assume $(\boldsymbol{\psi})_i = \{0, 0, 1\}$ and $(\boldsymbol{\theta}^+)_i = \{0, 0, \tau\}$, where τ is a small value chosen in the way established for the finite difference operators, see [65]. Then we can calculate $D\mathbf{T} \cdot \boldsymbol{\theta}^+$ in two ways: first, using eq. (9.40) and next, by an approximate difference formula $D\mathbf{T} \cdot \boldsymbol{\theta}^+ \approx \mathbf{T}(\boldsymbol{\psi} + \boldsymbol{\theta}^+) - \mathbf{T}(\boldsymbol{\psi})$.

A summary of the tangent operators is provided in Table 9.1 where the variations of the rotation tensor in which they are used are indicated.

Table 9.1 Tangent operators and variations of rotation tensor.

Tangent operator	Semi-tangential parametrization	Canonical parametrization	Used in variations of rotation
$\mathbf{T}(\boldsymbol{\psi})$	eq. (9.10)	eq. (9.18)	first, second
$\chi\mathbf{T}(\boldsymbol{\psi}, \boldsymbol{\theta}^+)$	eq. (9.39)	eq. (9.40)	second

9.2 Variation of rotation tensor

In this section we derive the formulae for the variation of the rotation tensor assuming the additive and multiplicative (left and right) compositions of the semi-tangential and canonical rotation vectors. Then we can relate the obtained variation to each other using the tangent operators derived in the preceding section.

The notation used below is the same as in the preceding section, see Figs. 9.1 and 9.3.

9.2.1 Variation of rotation tensor for additive composition

For the additive composition of the rotation parameters, $\boldsymbol{\psi}_\epsilon = \boldsymbol{\psi} + \epsilon\boldsymbol{\theta}_A \in T_I\mathrm{SO}(3)$, we define the variation as the following directional derivative:

$$\delta_{\tilde{\theta}_A} \mathbf{R}(\boldsymbol{\psi}) \doteq D\mathbf{R}(\boldsymbol{\psi}) \cdot \tilde{\boldsymbol{\theta}}_A = \frac{\mathrm{d}}{\mathrm{d}\epsilon}[\mathbf{R}(\boldsymbol{\psi}_\epsilon)]_{\epsilon=0}, \tag{9.42}$$

where ϵ is a scalar perturbation parameter. Note that we can also denote $\boldsymbol{\theta}_A \doteq \delta\boldsymbol{\psi}$, following the established convention in mechanics. Because the function $\mathbf{R}(\boldsymbol{\psi})$ is different for each parametrization, the variation must be derived separately for the semi-tangential and canonical parametrization.

The above directional derivative can be calculated using a symbolic manipulation program, such as *Mathematica* or *Maple*, but then we obtain long and complicated formulas. On the other hand, concise forms can be derived using the multiplicative composition of rotation tensors, as we show below.

9.2.2 Variation of rotation tensor for multiplicative composition

We derive the formulae for the variation of the rotation tensor w.r.t. the rotation vectors (semi-tangential and canonical), at two characteristic points: (A) at $\mathbf{R}_B = \mathbf{I}$ (or for $\mathbf{R}_1 = \mathbf{I}$) and (B) at arbitrary $\mathbf{R}_B$.

A. Variation of rotation tensor $\mathbf{R}_B = \mathbf{I}$

Define the variation of $\mathbf{R}_B$ w.r.t. the skew-symmetric $\tilde{\boldsymbol{\theta}}_B \in \mathrm{so}(3)$, as the directional derivative of $\mathbf{R}_2$ in the direction $\tilde{\boldsymbol{\theta}}_B$,

$$\delta_{\tilde{\psi}} \mathbf{R}_B \doteq D\mathbf{R}_B \cdot \tilde{\boldsymbol{\theta}}_B = \frac{\mathrm{d}}{\mathrm{d}\epsilon}[\mathbf{R}_2(\epsilon\tilde{\boldsymbol{\theta}}_B)]_{\epsilon=0}, \tag{9.43}$$

where ϵ is a scalar perturbation parameter.

Semi-tangential rotation vector. For the skew-symmetric $\tilde{\boldsymbol{\theta}}_B \in \mathrm{so}(3)$ associated with the semi-tangential rotation vector of eq. (8.97), we obtain

$$\delta_{\tilde{\theta}_B} \mathbf{R}_B = 2\,\tilde{\boldsymbol{\theta}}_B, \tag{9.44}$$

where the form of $\mathbf{R}_B$ for the semi-tangential vector was used. The proof is as follows. For $\epsilon\tilde{\boldsymbol{\theta}}_B$, eq. (8.99) becomes

$$\mathbf{R}(\epsilon\tilde{\boldsymbol{\theta}}_B) = \mathbf{I} + \frac{2}{1 + \|\epsilon\boldsymbol{\theta}_B\|^2}\left(\epsilon\tilde{\boldsymbol{\theta}}_B + \epsilon^2\tilde{\boldsymbol{\theta}}_B^2\right), \qquad \|\epsilon\boldsymbol{\theta}_B\|^2 = \tfrac{1}{2}\epsilon^2\tilde{\boldsymbol{\theta}}_B \cdot \tilde{\boldsymbol{\theta}}_B \geq 0. \tag{9.45}$$

Denoting the nominator by $N \doteq 2\left(\epsilon\tilde{\boldsymbol{\theta}}_B + \epsilon^2\tilde{\boldsymbol{\theta}}_B^2\right)$ and the denominator by $D \doteq 1 + \frac{1}{2}\epsilon^2\tilde{\boldsymbol{\theta}}_B \cdot \tilde{\boldsymbol{\theta}}_B$, we calculate the derivative

$$\frac{\mathrm{d}}{\mathrm{d}\epsilon}\left[\mathbf{R}_B(\epsilon\tilde{\boldsymbol{\theta}}_B)\right] = \frac{1}{D^2}\left(\frac{\mathrm{dN}}{\mathrm{d}\epsilon}D - \frac{\mathrm{dD}}{\mathrm{d}\epsilon}N\right), \tag{9.46}$$

where $\frac{\mathrm{dN}}{\mathrm{d}\epsilon} = 2\left(\tilde{\boldsymbol{\theta}}_B + 2\epsilon\tilde{\boldsymbol{\theta}}_B^2\right)$, and $\frac{\mathrm{dD}}{\mathrm{d}\epsilon} = \epsilon\tilde{\boldsymbol{\theta}}_B \cdot \tilde{\boldsymbol{\theta}}_B$. For $\epsilon = 0$, we obtain

$$[N]_{\epsilon=0} = 0, \qquad [D]_{\epsilon=0} = 1, \qquad \left[\frac{\mathrm{dN}}{\mathrm{d}\epsilon}\right]_{\epsilon=0} = 2\tilde{\boldsymbol{\theta}}_B, \qquad \left[\frac{\mathrm{dD}}{\mathrm{d}\epsilon}\right]_{\epsilon=0} = 0,$$

and eq. (9.46) yields the r.h.s. of eq. (9.44). □

Canonical rotation vector. For the skew-symmetric $\tilde{\boldsymbol{\theta}}_B \in \mathrm{so}(3)$ associated with the canonical rotation vector of eq. (8.79), we obtain

$$\delta_{\tilde{\theta}_B}\mathbf{R}_B = \tilde{\boldsymbol{\theta}}_B. \tag{9.47}$$

The proof is immediate, as for $\mathbf{R}_B$ we may use the exponential representation, i.e. $\mathbf{R}_{B\epsilon} = \exp(\epsilon\tilde{\boldsymbol{\theta}}_B) = \mathbf{I} + \epsilon\tilde{\boldsymbol{\theta}}_B + ... + \frac{1}{n!}(\epsilon\tilde{\boldsymbol{\theta}}_B)^n + ...$. Then

$$\frac{\mathrm{d}}{\mathrm{d}\epsilon}[\exp(\epsilon\tilde{\boldsymbol{\theta}}_B)] = \left[\mathbf{I} + \epsilon\tilde{\boldsymbol{\theta}}_B + ... + \frac{1}{(n-1)!}(\epsilon\tilde{\boldsymbol{\theta}}_B)^{n-1} + ...\right]\tilde{\boldsymbol{\theta}}_B, \tag{9.48}$$

and, by setting $\epsilon = 0$, we obtain the r.h.s. of eq. (9.47). □

B. Variation of arbitrary rotation tensor $\mathbf{R}_B$

To calculate the variation of an arbitrary rotation $\mathbf{R}_B$, we use the composition rules for the rotation tensors of eqs. (8.176) and (8.177) with $\mathbf{R}_1 = \mathbf{R}(\boldsymbol{\psi})$, and the variations of the rotation tensor $\mathbf{R}_B = \mathbf{I}$ of eqs. (9.44) and (9.47).

Left (or spatial) variation. For the left composition rule, the perturbed rotation is defined as $\mathbf{R}_{B\epsilon} \doteq \mathbf{R}_2(\epsilon\tilde{\boldsymbol{\theta}}_B)\,\mathbf{R}_B$, where $\tilde{\boldsymbol{\theta}}_B \in \mathrm{so}(3)$. The variation of $\mathbf{R}_B$ w.r.t. $\tilde{\boldsymbol{\theta}}_B$ is defined as the derivative of $\mathbf{R}_B$ in the direction $\tilde{\boldsymbol{\theta}}_B$,

$$\delta_{\tilde{\theta}_B}\mathbf{R}_B \doteq D\mathbf{R}_B \cdot \tilde{\boldsymbol{\theta}}_B = \frac{\mathrm{d}}{\mathrm{d}\epsilon}[\mathbf{R}_2(\epsilon\tilde{\boldsymbol{\theta}}_B)\,\mathbf{R}_B]_{\epsilon=0} = \frac{\mathrm{d}}{\mathrm{d}\epsilon}[\mathbf{R}_2(\epsilon\tilde{\boldsymbol{\theta}}_B)]_{\epsilon=0}\,\mathbf{R}_B. \tag{9.49}$$

Right (Lagrangian, or material) variation. For the right composition rule, the perturbed rotation is defined as $\mathbf{R}_{B\epsilon} \doteq \mathbf{R}_B \mathbf{R}_2(\epsilon \tilde{\boldsymbol{\Theta}}_B)$, where $\tilde{\boldsymbol{\Theta}}_B \in \mathrm{so}(3)$. The variation of $\mathbf{R}_B$ w.r.t. $\tilde{\boldsymbol{\Theta}}_B$ is defined as the derivative of $\mathbf{R}_B$ in the direction $\tilde{\boldsymbol{\Theta}}_B$,

$$\delta_{\tilde{\Theta}_B} \mathbf{R}_B \doteq D\mathbf{R} \cdot \tilde{\boldsymbol{\Theta}}_B = \frac{\mathrm{d}}{\mathrm{d}\epsilon} [\mathbf{R}_B \mathbf{R}_2(\epsilon \tilde{\boldsymbol{\Theta}}_B)]_{\epsilon=0} = \mathbf{R}_B \frac{\mathrm{d}}{\mathrm{d}\epsilon} [\mathbf{R}_2(\epsilon \tilde{\boldsymbol{\Theta}}_B)]_{\epsilon=0}. \tag{9.50}$$

In the above two definitions, we should use the directional derivative of $\mathbf{R}_2$ given for the semi-tangential vector by eq. (9.44) and for the canonical vector by eq. (9.47).

9.2.3 Relations between variations for various composition rules

In this section, we establish the relations between variations for the additive composition and the multiplicative composition of the canonical rotational parameters. For the semi-tangential vector, the procedure is analogous and the results are in eq. (9.60).

The composition equations for the rotation tensors, eqs. (8.176) and (8.177), can be rewritten together as

$$\mathbf{R}_t = \mathbf{R}_2^* \, \mathbf{R}_1 = \mathbf{R}_1 \, \mathbf{R}_2. \tag{9.51}$$

Let us define $\mathbf{R}_t \doteq \mathbf{R}(\boldsymbol{\psi} + \epsilon \boldsymbol{\theta}_A)$, $\mathbf{R}_1 \doteq \mathbf{R}(\boldsymbol{\psi})$, $\mathbf{R}_2^* \doteq \mathbf{R}_2(\epsilon \tilde{\boldsymbol{\theta}}_B)$, and $\mathbf{R}_2 \doteq \mathbf{R}_2(\epsilon \tilde{\boldsymbol{\Theta}}_B)$, where $\boldsymbol{\theta}_A$, $\boldsymbol{\theta}_B$, and $\boldsymbol{\Theta}_B$ are the infinitesimal rotation vectors, shown in Figs. 9.1 and 9.3. Then eq. (9.51) becomes

$$\mathbf{R} \underbrace{(\boldsymbol{\psi} + \epsilon \boldsymbol{\theta}_A)}_{\text{additive}} = \underbrace{\mathbf{R}_2(\epsilon \tilde{\boldsymbol{\theta}}_B) \, \mathbf{R}(\boldsymbol{\psi})}_{\text{multiplicative, left}} = \underbrace{\mathbf{R}(\boldsymbol{\psi}) \, \mathbf{R}_2(\epsilon \tilde{\boldsymbol{\Theta}}_B)}_{\text{multiplicative, right}} , \tag{9.52}$$

where the additive and multiplicative compositions of rotational parameters were used.

Below, we calculate three variations (directional derivatives) of eq. (9.52): (1) in the direction $\tilde{\boldsymbol{\theta}}_A \in T_I\mathrm{SO}(3)$, (2) in the direction $\tilde{\boldsymbol{\theta}}_B \mathbf{R} \in T_R\mathrm{SO}(3)$, and (3) in the direction $\mathbf{R} \tilde{\boldsymbol{\Theta}}_B \in T_R\mathrm{SO}(3)$. The relations are derived for the canonical rotation vector.

Variation in direction $\tilde{\boldsymbol{\theta}}_A \in T_I\mathrm{SO}(3)$. We can calculate the derivative of eq. (9.52) in the direction $\tilde{\boldsymbol{\theta}}_A$ in a standard manner and the derivatives of particular parts are as follows:

a) For the additive composition, $\mathbf{R}(\boldsymbol{\psi}+\epsilon\boldsymbol{\theta}_A)$, we obtain the derivative of eq. (9.42).

b) For the left multiplicative composition, $\mathbf{R}_2(\epsilon\tilde{\boldsymbol{\theta}}_B)\,\mathbf{R}(\boldsymbol{\psi})$,

$$\delta_{\tilde{\theta}_A}\left[\mathbf{R}_2(\epsilon\tilde{\boldsymbol{\theta}}_B)\,\mathbf{R}(\boldsymbol{\psi})\right] = \frac{\mathrm{d}}{\mathrm{d}\epsilon}\left[\mathbf{R}_2(\epsilon\tilde{\boldsymbol{\theta}}_B)\,\mathbf{R}(\boldsymbol{\psi})\right]_{\epsilon=0}, \tag{9.53}$$

in which we must express $\tilde{\boldsymbol{\theta}}_B$ as a function of the perturbation $\tilde{\boldsymbol{\theta}}_A$. Note that $\boldsymbol{\theta}_B = \mathbf{T}(\boldsymbol{\psi})\,\boldsymbol{\theta}_A$, where the tangent operator $\mathbf{T}$ is defined in eqs. (9.10) and (9.18) and we can write $\epsilon\tilde{\boldsymbol{\theta}}_B = [\mathbf{T}(\boldsymbol{\psi})\,\epsilon\boldsymbol{\theta}_A]\times\mathbf{I}$ to obtain

$$\delta_{\tilde{\theta}_A}\left[\mathbf{R}_2(\epsilon\tilde{\boldsymbol{\theta}}_B)\,\mathbf{R}(\boldsymbol{\psi})\right] = \underbrace{\{[\mathbf{T}(\boldsymbol{\psi})\,\boldsymbol{\theta}_A]\times\mathbf{I}\}}_{\text{skew-symm.}}\,\mathbf{R}(\boldsymbol{\psi}). \tag{9.54}$$

c) For the right multiplicative composition, $\mathbf{R}(\boldsymbol{\psi})\,\mathbf{R}_2(\epsilon\tilde{\boldsymbol{\Theta}}_B)$, we obtain

$$\delta_{\tilde{\theta}_A}\left[\mathbf{R}(\boldsymbol{\psi})\,\mathbf{R}_2(\epsilon\tilde{\boldsymbol{\Theta}}_B)\right] = \frac{\mathrm{d}}{\mathrm{d}\epsilon}\left[\mathbf{R}(\boldsymbol{\psi})\,\mathbf{R}_2(\epsilon\tilde{\boldsymbol{\Theta}}_B)\right]_{\epsilon=0}, \tag{9.55}$$

in which we must express $\epsilon\tilde{\boldsymbol{\Theta}}_B$ as a function of the perturbation $\epsilon\tilde{\boldsymbol{\theta}}_A$. Note that $\boldsymbol{\Theta}_B = \mathbf{T}^T(\boldsymbol{\psi})\,\boldsymbol{\theta}_A$, by eqs. (9.33) and (9.36), and we can write $\epsilon\tilde{\boldsymbol{\Theta}}_B = [\mathbf{T}^T(\boldsymbol{\psi})\,\epsilon\boldsymbol{\theta}_A]\times\mathbf{I}$ to obtain

$$\delta_{\tilde{\theta}_A}\left[\mathbf{R}(\boldsymbol{\psi})\mathbf{R}_2(\epsilon\tilde{\boldsymbol{\Theta}}_B)\right] = \mathbf{R}(\boldsymbol{\psi})\,\underbrace{\{[\mathbf{T}^T(\boldsymbol{\psi})\,\boldsymbol{\theta}_A]\times\mathbf{I}\}}_{\text{skew-symm.}}. \tag{9.56}$$

Writing the above results together, we have the relation linking the variations for various compositions of rotations

$$\underbrace{\delta_{\tilde{\theta}_A}\mathbf{R}(\boldsymbol{\psi})}_{\text{additive}} = \underbrace{\{[\mathbf{T}(\boldsymbol{\psi})\,\boldsymbol{\theta}_A]\times\mathbf{I}\}\,\mathbf{R}(\boldsymbol{\psi})}_{\text{left, multiplicative}} = \underbrace{\mathbf{R}(\boldsymbol{\psi})\,\{[\mathbf{T}^T(\boldsymbol{\psi})\,\boldsymbol{\theta}_A]\times\mathbf{I}\}}_{\text{right, multiplicative}}. \tag{9.57}$$

Note that this relation allows us to express the variation for the additive composition of eq. (9.42) in the concise forms of variations for multiplicative compositions to avoid long and complicated formulas.

Remark 1. Note that writing the above relation in the short form as

$$\underbrace{\delta_{\tilde{\theta}_A}\mathbf{R}}_{\text{additive}} = \underbrace{\delta_{\tilde{\theta}_B}\mathbf{R}}_{\text{left}} = \underbrace{\delta_{\tilde{\Theta}_B}\mathbf{R}}_{\text{right}}, \tag{9.58}$$

we must remember that it holds only if $\boldsymbol{\theta}_B = \mathbf{T}(\boldsymbol{\psi})\,\boldsymbol{\theta}_A$ and $\boldsymbol{\Theta}_B = \mathbf{T}^T(\boldsymbol{\psi})\,\boldsymbol{\theta}_A$.

Remark 2. The forms of the variations for the multiplicative rules specified above are not suitable for numerical implementations. However, if these variations are multiplied by a vector, e.g. the shell director $\mathbf{t}_3$, then $\boldsymbol{\theta}_A$ can be separated. For instance, for the variation of a shell director, we can perform the following transformations:

$$\begin{aligned} \delta \mathbf{a}_3 &= \delta_{\tilde{\theta}_A} \mathbf{R}\, \mathbf{t}_3 = \mathbf{R}(\boldsymbol{\psi}) \{[\mathbf{T}^T(\boldsymbol{\psi})\, \boldsymbol{\theta}_A] \times \mathbf{I}\}\, \mathbf{t}_3 = \mathbf{R}(\boldsymbol{\psi}) \{[\mathbf{T}^T(\boldsymbol{\psi})\, \boldsymbol{\theta}_A] \times \mathbf{t}_3\} \\ &= -\mathbf{R}(\boldsymbol{\psi}) \{\mathbf{t}_3 \times [\mathbf{T}^T(\boldsymbol{\psi})\, \boldsymbol{\theta}_A]\} = -\underbrace{\mathbf{R}(\boldsymbol{\psi})\, (\mathbf{t}_3 \times \mathbf{I})\, \mathbf{T}^T(\boldsymbol{\psi})}_{3\times 3 \text{ matrix}}\ \underbrace{\boldsymbol{\theta}_A}_{\text{vector}}, \end{aligned} \tag{9.59}$$

where, in the final form, we have a product of the matrix and $\boldsymbol{\theta}_A$.

Variations for the semi-tangential rotation vector. For the semi-tangential rotation vector, the procedure is analogous and eq. (9.57) linking the variations for various compositions of rotations, becomes

$$\underbrace{\delta_{\tilde{\theta}_A} \mathbf{R}(\boldsymbol{\psi})}_{\text{additive}} = \underbrace{\{[2\, \mathbf{T}(\boldsymbol{\psi})\, \boldsymbol{\theta}_A] \times \mathbf{I}\}\, \mathbf{R}(\boldsymbol{\psi})}_{\text{left, multiplicative}} = \underbrace{\mathbf{R}(\boldsymbol{\psi}) \{[2\, \mathbf{T}^T(\boldsymbol{\psi})\, \boldsymbol{\theta}_A] \times \mathbf{I}\}}_{\text{right, multiplicative}}. \tag{9.60}$$

Note the multiplier 2; it appeared earlier in eq. (9.44), as compared to eq. (9.47).

Variation in direction $\tilde{\boldsymbol{\theta}}_B \mathbf{R} \in T_R\mathrm{SO}(3)$. We calculate a derivative of eq. (9.52) in the direction $\tilde{\boldsymbol{\theta}}_B \mathbf{R} \in T_R\mathrm{SO}(3)$ in a standard manner and obtain the following derivatives of each side:

a) For the additive composition, $\mathbf{R}(\boldsymbol{\psi} + \epsilon \boldsymbol{\theta}_A)$, we must express $\tilde{\boldsymbol{\theta}}_A$ as a function of the perturbation $\tilde{\boldsymbol{\theta}}_B$. Note that $\boldsymbol{\theta}_A = \mathbf{T}^{-1}(\boldsymbol{\psi})\, \boldsymbol{\theta}_B$ and we can write

$$\delta_{\tilde{\theta}_B} \mathbf{R}(\boldsymbol{\psi}) = \frac{\mathrm{d}}{\mathrm{d}\epsilon} [\mathbf{R}(\boldsymbol{\psi} + \mathbf{T}^{-1} \epsilon \boldsymbol{\theta}_B)]_{\epsilon=0}, \tag{9.61}$$

b) For the left multiplicative composition, $\mathbf{R}_2(\epsilon \tilde{\boldsymbol{\theta}}_B)\, \mathbf{R}(\boldsymbol{\psi})$, we obtain eq. (9.49), i.e.

$$\delta_{\tilde{\theta}_B} \mathbf{R} = \frac{\mathrm{d}}{\mathrm{d}\epsilon} [\mathbf{R}_2(\epsilon \tilde{\boldsymbol{\theta}}_B)]_{\epsilon=0}\, \mathbf{R}, \tag{9.62}$$

where the directional derivative of $\mathbf{R}_2$ is given either by eq. (9.44) or by eq. (9.47), but with $\tilde{\boldsymbol{\psi}}$ replaced by $\tilde{\boldsymbol{\theta}}_B$.

Hence, the variation for the additive composition and the left multiplicative composition are mutually related as follows:

$$\underbrace{\delta_{\tilde{\theta}_B}\mathbf{R}(\boldsymbol{\psi})}_{\text{additive}} = a\,\underbrace{\tilde{\boldsymbol{\theta}}_B\,\mathbf{R}(\boldsymbol{\psi})}_{\text{left}}, \tag{9.63}$$

where $a = 2$ for the semi-tangential vector and $a = 1$ for the canonical vector. Note that we could have also calculated a variation for the right multiplicative composition $\mathbf{R}(\boldsymbol{\psi})\,\mathbf{R}_2(\epsilon\tilde{\boldsymbol{\Theta}}_B)$, using $\boldsymbol{\Theta}_B = \mathbf{T}^T\mathbf{T}^{-1}\boldsymbol{\theta}_B$, but it is not used in subsequent calculations.

Variation in direction $\mathbf{R}\tilde{\boldsymbol{\Theta}}_B \in T_R\mathrm{SO}(3)$. We calculate a derivative of eq. (9.52) in the direction $\mathbf{R}\tilde{\boldsymbol{\Theta}}_B \in T_R\mathrm{SO}(3)$ in a standard manner, and obtain the following derivatives of each side.

a) For the additive composition, $\mathbf{R}(\boldsymbol{\psi}+\epsilon\boldsymbol{\theta}_A)$, we must express $\tilde{\boldsymbol{\theta}}_A$ as a function of the perturbation $\tilde{\boldsymbol{\Theta}}_B$. Note that $\boldsymbol{\theta}_A = \mathbf{T}^{-T}(\boldsymbol{\psi})\,\boldsymbol{\Theta}_B$ and we can write

$$\delta_{\tilde{\Theta}_B}\mathbf{R}(\boldsymbol{\psi}) \;=\; \frac{\mathrm{d}}{\mathrm{d}\epsilon}[\mathbf{R}(\boldsymbol{\psi} + \mathbf{T}^{-T}\epsilon\boldsymbol{\Theta}_B)]_{\epsilon=0}. \tag{9.64}$$

b) For the right multiplicative composition, $\mathbf{R}(\boldsymbol{\psi})\,\mathbf{R}_2(\epsilon\tilde{\boldsymbol{\Theta}}_B)$, we obtain eq. (9.50), i.e.

$$\delta_{\tilde{\Theta}_B}\mathbf{R} = \mathbf{R}\,\frac{\mathrm{d}}{\mathrm{d}\epsilon}[\mathbf{R}_2(\epsilon\tilde{\boldsymbol{\Theta}}_B)]_{\epsilon=0}, \tag{9.65}$$

where the directional derivative of $\mathbf{R}_2$ is given either by eq. (9.44) or by eq. (9.47) but with $\tilde{\boldsymbol{\psi}}$ replaced by $\tilde{\boldsymbol{\Theta}}_B$.

Hence, the variation for the additive composition and the right multiplicative composition are mutually related as follows:

$$\underbrace{\delta_{\tilde{\Theta}_B}\mathbf{R}(\boldsymbol{\psi})}_{\text{additive}} = a\,\underbrace{\mathbf{R}(\boldsymbol{\psi})\,\tilde{\boldsymbol{\Theta}}_B}_{\text{right}}, \tag{9.66}$$

where $a = 2$ for the semi-tangential vector and $a = 1$ for the canonical vector. Note that we could also calculate a variation for the left multiplicative composition $\mathbf{R}_2(\epsilon\tilde{\boldsymbol{\theta}}_B)\,\mathbf{R}(\boldsymbol{\psi})$, using $\boldsymbol{\theta}_B = \mathbf{T}\mathbf{T}^{-T}\boldsymbol{\Theta}_B$, but it is not used in calculations.

Remark. By using $\boldsymbol{\theta}_B = \mathbf{T}(\boldsymbol{\psi})\,\boldsymbol{\theta}_A$ and $\boldsymbol{\Theta}_B = \mathbf{T}^T(\boldsymbol{\psi})\,\boldsymbol{\theta}_A$, eq. (9.57) yields,

$$\tilde{\boldsymbol{\theta}}_B \;=\; \mathbf{R}\,\tilde{\boldsymbol{\Theta}}_B\,\mathbf{R}^T, \qquad \boldsymbol{\theta}_B \;=\; \mathbf{R}\,\boldsymbol{\Theta}_B, \tag{9.67}$$

where $\boldsymbol{\Theta}_B$ and $\boldsymbol{\theta}_B$ are the axial vectors of $\tilde{\boldsymbol{\Theta}}_B$ and $\tilde{\boldsymbol{\theta}}_B$, respectively. We see that $\tilde{\boldsymbol{\theta}}_B$ is the forward-rotated $\tilde{\boldsymbol{\Theta}}_B$, hence their properties are linked, as discussed in Sect. 8.3.1. In particular, if we assume two Cartesian bases, the reference basis $\{\mathbf{i}_i\}$ and the rotated basis $\{\mathbf{t}_i\}$, where $\mathbf{t}_i \doteq \mathbf{R}\,\mathbf{i}_i$, and the representations,

$$\tilde{\boldsymbol{\Theta}} = \tilde{\Theta}_{ij}\,\mathbf{i}_i \otimes \mathbf{i}_j, \qquad \tilde{\boldsymbol{\theta}} = \tilde{\theta}_{ij}\,\mathbf{t}_i \otimes \mathbf{t}_j, \tag{9.68}$$

then eq. (9.67) implies

$$\tilde{\mathbf{\Theta}} = \mathbf{R}^T(\tilde{\theta}_{ij}\,\mathbf{t}_i \otimes \mathbf{t}_j)\,\mathbf{R} = \tilde{\theta}_{ij}\,(\mathbf{R}^T\mathbf{t}_i \otimes \mathbf{R}^T\mathbf{t}_j) = \tilde{\theta}_{ij}\,\mathbf{i}_i \otimes \mathbf{i}_j. \tag{9.69}$$

Hence, $\tilde{\Theta}_{ij} = \tilde{\theta}_{ij}$, i.e. the components of $\tilde{\mathbf{\Theta}}$ in the basis $\{\mathbf{i}_i\}$ and the components of $\tilde{\boldsymbol{\theta}}$ in the basis $\{\mathbf{t}_i\}$ are identical. In other words, $\tilde{\boldsymbol{\Theta}}$ can be considered as $\tilde{\boldsymbol{\theta}}$ parallel transported from the rotated basis to the reference basis.

Example. Consider the case when the rotation and the variations are performed around the axis $\mathbf{t}_3$ of the basis $\{\mathbf{t}_i\}$. Assume the following representations of two canonical rotation vectors $\boldsymbol{\psi} = [0, 0, \psi_3]^T$ and $\boldsymbol{\theta}_A = [0, 0, \theta_3]^T$, which yield

$$\mathbf{R}(\psi_3) = \begin{bmatrix} \cos\psi_3 & -\sin\psi_3 & 0 \\ +\sin\psi_3 & \cos\psi_3 & 0 \\ 0 & 0 & 1 \end{bmatrix}, \qquad \tilde{\boldsymbol{\theta}}_A = \theta_3 \begin{bmatrix} 0 & -1 & 0 \\ +1 & 0 & 0 \\ 0 & 0 & 0 \end{bmatrix}.$$

For the additive variation, on use of eq. (9.42), we can calculate,

$$\delta_{\tilde{\theta}_A}\mathbf{R}(\boldsymbol{\psi}) \doteq D\mathbf{R}(\psi_3)\cdot\tilde{\boldsymbol{\theta}}_A = \frac{\mathrm{d}}{\mathrm{d}\epsilon}[\mathbf{R}(\psi_3 + \epsilon\theta_3)]_{\epsilon=0} = \frac{\mathrm{d}\mathbf{R}}{\mathrm{d}\psi_3}\,\theta_3, \tag{9.70}$$

where

$$\frac{\mathrm{d}\mathbf{R}}{\mathrm{d}\psi_3} = \begin{bmatrix} -\sin\psi_3 & -\cos\psi_3 & 0 \\ \cos\psi_3 & -\sin\psi_3 & 0 \\ 0 & 0 & 0 \end{bmatrix}.$$

For the left variation of $\mathbf{R}$, we only perform a multiplication, which yields

$$\delta_{\tilde{\theta}_B}\mathbf{R} = \tilde{\boldsymbol{\theta}}_A\,\mathbf{R} = \theta_3 \begin{bmatrix} -\sin\psi_3 & -\cos\psi_3 & 0 \\ \cos\psi_3 & -\sin\psi_3 & 0 \\ 0 & 0 & 0 \end{bmatrix}. \tag{9.71}$$

Similarly for the right variation of $\mathbf{R}$,

$$\delta_{\tilde{\Theta}_B}\mathbf{R} = \mathbf{R}\,\tilde{\boldsymbol{\theta}}_A = \theta_3 \begin{bmatrix} -\sin\psi_3 & -\cos\psi_3 & 0 \\ \cos\psi_3 & -\sin\psi_3 & 0 \\ 0 & 0 & 0 \end{bmatrix}. \tag{9.72}$$

Note that $\delta_{\tilde{\Theta}_B}\mathbf{R} = \delta_{\tilde{\theta}_B}\mathbf{R},$ indeed. This shows that the difference between the left and right variation vanishes for the rotation and the variations around one axis. Then the tangent operator $\mathbf{T}(\boldsymbol{\psi})$ acts as the identity operator, see eq. (9.21).

Example. In this example, we calculate the variations of the rotation tensor in a slightly different way; directly using the composition formula of eq. (8.189) and the rotation tensor of eq. (8.99) for the semi-tangential parametrization.

Assume that $\tilde{\boldsymbol{\psi}}, \tilde{\boldsymbol{\theta}}_A \in T_I\mathrm{SO}(3),$ and their axial vectors are: $\boldsymbol{\psi} = [9, 5, -1]^T$ and $\boldsymbol{\theta}_A = [-0.8, -0.1, 0.4]^T.$ The variations are defined as follows:

1. for the additive composition, we use $\boldsymbol{\psi}_A = \boldsymbol{\psi} + \epsilon\boldsymbol{\theta}_A,$ and calculate

$$\delta_{\tilde{\theta}_A}\mathbf{R}(\boldsymbol{\psi}) = \frac{\mathrm{d}}{\mathrm{d}\epsilon}[\mathbf{R}(\boldsymbol{\psi}_A)]_{\epsilon=0} = \begin{bmatrix} -0.0388889 & 0.0296296 & 0.0685185 \\ 0.0388889 & 0.0537037 & 0.0148148 \\ 0.0444444 & 0.0351852 & -0.00925926 \end{bmatrix}.$$

2. for the left composition, we use $\boldsymbol{\psi}_B = \frac{1}{1-\boldsymbol{\psi}\cdot\epsilon\boldsymbol{\theta}_B}(\boldsymbol{\psi} + \epsilon\boldsymbol{\theta}_B + \epsilon\boldsymbol{\theta}_B \times \boldsymbol{\psi}),$ and calculate

$$\delta_{\tilde{\theta}_B}\mathbf{R}(\boldsymbol{\psi}) = \frac{\mathrm{d}}{\mathrm{d}\epsilon}[\mathbf{R}(\boldsymbol{\psi}_B)]_{\epsilon=0} = \begin{bmatrix} -0.0388889 & 0.0296296 & 0.0685185 \\ 0.0388889 & 0.0537037 & 0.0148148 \\ 0.0444444 & 0.0351852 & -0.00925926 \end{bmatrix},$$

   where $\boldsymbol{\theta}_B = \mathbf{T}(\boldsymbol{\psi})\ \boldsymbol{\theta}_A = [0.0101852, -0.0268519, 0.0324074]^T.$ We checked that $\delta_{\tilde{\theta}_B}\mathbf{R} = (2\tilde{\boldsymbol{\theta}}_B)\ \mathbf{R}(\boldsymbol{\psi})$ yields exactly the same matrix.
3. for the right composition, we use $\boldsymbol{\psi}_B = \frac{1}{1-\boldsymbol{\psi}\cdot\epsilon\boldsymbol{\Theta}_B}(\boldsymbol{\psi}+\epsilon\boldsymbol{\Theta}_B-\epsilon\boldsymbol{\Theta}_B\times\boldsymbol{\psi}),$ and calculate

$$\delta_{\tilde{\Theta}_B}\mathbf{R}(\boldsymbol{\psi}) = \frac{\mathrm{d}}{\mathrm{d}\epsilon}[\mathbf{R}(\boldsymbol{\psi}_B)]_{\epsilon=0} = \begin{bmatrix} -0.0388889 & 0.0296296 & 0.0685185 \\ 0.0388889 & 0.0537037 & 0.0148148 \\ 0.0444444 & 0.0351852 & -0.00925926 \end{bmatrix},$$

   where $\boldsymbol{\Theta}_B = \mathbf{T}^T(\boldsymbol{\psi})\ \boldsymbol{\theta}_A = [-0.025, 0.025, -0.025]^T.$ We check that $\delta_{\tilde{\Theta}_B}\mathbf{R} = \mathbf{R}(\boldsymbol{\psi})\ (2\tilde{\boldsymbol{\Theta}}_B)$ yields exactly the same matrix.

The above results confirm that, as derived in eq. (9.58), the variations are equal indeed.

Now, we calculate the rotation matrices $\mathbf{R}$ for $\boldsymbol{\psi}_A$ and $\boldsymbol{\psi}_B$ obtained by taking $\epsilon = 1,$ i.e. for the finite increment of rotation vectors. Note that for $\boldsymbol{\psi} = \mathbf{0}$ we obtain $\boldsymbol{\psi}_A = \boldsymbol{\psi}_B,$ because then $\boldsymbol{\psi}_A = \boldsymbol{\theta}_A$ and $\mathbf{T} = \mathbf{I}$ so $\boldsymbol{\theta}_B = \boldsymbol{\theta}_A$ and $\boldsymbol{\psi}_B = \boldsymbol{\theta}_B,$ for which we finally obtain

$\boldsymbol{\psi}_B = \boldsymbol{\theta}_A = \boldsymbol{\psi}_A$. However, for $\boldsymbol{\psi} \neq \mathbf{0}$, a difference between $\boldsymbol{\psi}_A$ and $\boldsymbol{\psi}_B$ exists so the rotation matrices are different, i.e.

$$\mathbf{R}(\boldsymbol{\psi}_A) = \begin{bmatrix} 0.473707 & 0.880682 & -0.000431 \\ 0.854767 & -0.459886 & -0.240579 \\ -0.212072 & 0.113595 & -0.970630 \end{bmatrix},$$

$$\mathbf{R}(\boldsymbol{\psi}_B) = \begin{bmatrix} 0.477253 & 0.878746 & -0.005914 \\ 0.851921 & -0.464315 & -0.242162 \\ -0.215545 & 0.110533 & -0.970218 \end{bmatrix}.$$

For both multiplicative composition rules, we obtain the same $\mathbf{R}(\boldsymbol{\psi}_B)$, which is in agreement with eq. (8.177).

9.2.4 Second variation of rotation tensor

Definition of second variation. To define the second variation, we must extend the notation used earlier.

For instance, for the additive composition of rotational parameters, we used $\boldsymbol{\psi}_\epsilon = \boldsymbol{\psi} + \epsilon\boldsymbol{\theta}_A \in T_I SO(3)$ to define the first variation in eq. (9.42). Now, we need two perturbed vectors

$$\boldsymbol{\psi}^- = \boldsymbol{\psi} + \epsilon\boldsymbol{\theta}^- \in T_I SO(3), \qquad \boldsymbol{\psi}^+ = \boldsymbol{\psi} + \epsilon\boldsymbol{\theta}^+ \in T_I SO(3), \tag{9.73}$$

so we use two superscripts, "–" and "+", and omit the subscript "ϵ", to simplify the notation. (Note that we could also denote $\boldsymbol{\theta}^- \doteq \delta\boldsymbol{\psi}$ and $\boldsymbol{\theta}^+ \doteq \Delta\boldsymbol{\psi}$, using the notation typical in mechanics.) We define two variations of some function f as the following directional derivatives:

$$\delta f \doteq \frac{\mathrm{d}}{\mathrm{d}\epsilon} f(\boldsymbol{\psi} + \epsilon\boldsymbol{\theta}^-)\Big|_{\epsilon=0}, \qquad \chi f \doteq \frac{\mathrm{d}}{\mathrm{d}\epsilon} f(\boldsymbol{\psi} + \epsilon\boldsymbol{\theta}^+)\Big|_{\epsilon=0}, \tag{9.74}$$

where "δ" and "χ" are associated with the directions $\boldsymbol{\theta}^-$ and $\boldsymbol{\theta}^+$, respectively. The second variation is defined as the directional derivative of the first variation,

$$\chi(\delta f) \doteq \frac{\mathrm{d}}{\mathrm{d}\epsilon}\, \delta f(\boldsymbol{\psi} + \epsilon\boldsymbol{\theta}^+)\Big|_{\epsilon=0}. \tag{9.75}$$

Analogous expressions will be used for multiplicative composition of rotations.

Below, the second variations are derived for the canonical rotation vector; for the semi-tangential vector, the procedure is analogous and the obtained results are provided in eqs. (9.87) and (9.88).

A. Second variation of rotation tensor for additive composition

For the additive composition of the rotation parameters (in the notation introduced above), the first variation is defined as

$$\delta\mathbf{R} \doteq D\mathbf{R}(\boldsymbol{\psi}) \cdot \tilde{\boldsymbol{\theta}}^- = \frac{\mathrm{d}}{\mathrm{d}\epsilon}[\mathbf{R}(\boldsymbol{\psi}^-)]_{\epsilon=0}, \tag{9.76}$$

while the second variation is defined as

$$\chi\delta\mathbf{R} \doteq D\,[\delta\mathbf{R}] \cdot \tilde{\boldsymbol{\theta}}^+ = \frac{\mathrm{d}}{\mathrm{d}\epsilon}[\delta\mathbf{R}(\boldsymbol{\psi}^+)]_{\epsilon=0}. \tag{9.77}$$

The above directional derivatives can be calculated using automatic differentiation of a symbolic manipulation program. The concise forms can be also derived using the multiplicative composition of rotation tensors, as shown below.

B. Second variation of rotation tensor for multiplicative composition

Recall eq. (9.57) linking the variations for the additive composition and the multiplicative (left and right) compositions of canonical rotation parameters, which can be rewritten as follows:

$$\underbrace{\delta\mathbf{R}}_{\text{additive}} = \underbrace{\{[\mathbf{T}(\boldsymbol{\psi})\,\boldsymbol{\theta}^-] \times \mathbf{I}\}\,\mathbf{R}(\boldsymbol{\psi})}_{\text{left, multiplicative}} = \underbrace{\mathbf{R}(\boldsymbol{\psi})\,\{[\mathbf{T}^T(\boldsymbol{\psi})\,\boldsymbol{\theta}^-] \times \mathbf{I}\}}_{\text{right, multiplicative}}, \tag{9.78}$$

where the tangent operator $\mathbf{T}$ is defined in eq. (9.17). Below, we only consider the canonical parametrization for which $\mathbf{T}$ has the form given in eq. (9.18).

Left multiplicative rule. The second differential of $\mathbf{R}$ is defined as the directional derivative of the respective first variation of eq. (9.78) in direction $\boldsymbol{\theta}^+$,

$$\chi(\delta\,\mathbf{R}) \doteq \frac{\mathrm{d}}{\mathrm{d}\epsilon}\left\{[\mathbf{T}(\boldsymbol{\psi} + \epsilon\boldsymbol{\theta}^+)\ \boldsymbol{\theta}^-] \times \mathbf{I}\right\}\mathbf{R}(\boldsymbol{\psi} + \epsilon\boldsymbol{\theta}^+)\Big|_{\epsilon=0}. \tag{9.79}$$

The derivative of a cross-product of a vector $\mathbf{a}$ and a tensor $\mathbf{A}$ with respect to the scalar ϵ is $(\mathbf{a} \times \mathbf{A})' = \mathbf{a}' \times \mathbf{A} + \mathbf{a} \times \mathbf{A}'$ and, hence,

$$\chi(\delta\,\mathbf{R}) = \{(\chi\mathbf{T}\,\boldsymbol{\theta}^-) \times \mathbf{I}\}\,\mathbf{R} \ + \ \{(\mathbf{T}\,\boldsymbol{\theta}^-) \times \mathbf{I}\}\,\chi\mathbf{R}. \tag{9.80}$$

Using $\chi\mathbf{R} = [(\mathbf{T}\boldsymbol{\theta}^+) \times \mathbf{I}]\,\mathbf{R}$, this becomes

$$\chi(\delta\,\mathbf{R}) = \big\{[(\chi\mathbf{T}\,\boldsymbol{\theta}^-)\times\mathbf{I}] \;+\; [(\mathbf{T}\,\boldsymbol{\theta}^-)\times\mathbf{I}][(\mathbf{T}\boldsymbol{\theta}^+)\times\mathbf{I}]\big\}\;\mathbf{R}, \tag{9.81}$$

where $\mathbf{R}$ is factored out of the braces.

The second component can be directly evaluated. Regarding the first component, the differential $\chi\mathbf{T}$ is defined in eq. (9.40) and we can calculate the product

$$\begin{aligned}\chi\mathbf{T}(\boldsymbol{\psi},\boldsymbol{\theta}^+)\,\boldsymbol{\theta}^- &= a_1\,(\mathbf{e}\cdot\boldsymbol{\theta}^+)\,\boldsymbol{\theta}^- + a_2\,(\mathbf{e}\cdot\boldsymbol{\theta}^-)\,\boldsymbol{\theta}^+ + a_2\,(\boldsymbol{\theta}^+\cdot\boldsymbol{\theta}^-)\,\mathbf{e}\\ &\quad + a_3\,(\mathbf{e}\cdot\boldsymbol{\theta}^+)(\mathbf{e}\cdot\boldsymbol{\theta}^-)\,\mathbf{e} + a_4\,(\mathbf{e}\cdot\boldsymbol{\theta}^+)\,\tilde{\boldsymbol{\psi}}\,\boldsymbol{\theta}^- + a_5\,(\boldsymbol{\theta}^+\times\boldsymbol{\theta}^-),\end{aligned} \tag{9.82}$$

which is a vector, so the term $(\chi\mathbf{T}\,\boldsymbol{\theta}^-)\times\mathbf{I}$ is the associated skew-symmetric tensor. We see that only two terms (third and fourth) are symmetric with respect to $\boldsymbol{\theta}^-$ and $\boldsymbol{\theta}^+$.

Right multiplicative rule. The second differential of $\mathbf{R}$ is defined as the directional derivative of the respective first variation of eq. (9.78) in the direction $\boldsymbol{\theta}^+$,

$$\chi(\delta\,\mathbf{R}) \doteq \frac{\mathrm{d}}{\mathrm{d}\epsilon}\,\big\{\mathbf{R}(\boldsymbol{\psi}+\epsilon\boldsymbol{\theta}^+)\,[\mathbf{T}^T(\boldsymbol{\psi}+\epsilon\boldsymbol{\theta}^+)\;\boldsymbol{\theta}^-\times\mathbf{I}]\big\}\bigg|_{\epsilon=0}. \tag{9.83}$$

Then we obtain

$$\chi(\delta\,\mathbf{R}) = \chi\mathbf{R}\,[(\mathbf{T}^T\boldsymbol{\theta}^-)\times\mathbf{I}] \;+\; \mathbf{R}\,[(\chi\mathbf{T}^T\boldsymbol{\theta}^-)\times\mathbf{I}], \tag{9.84}$$

which, using $\chi\mathbf{R} = \mathbf{R}\,[(\mathbf{T}^T\boldsymbol{\theta}^+)\times\mathbf{I}]$, becomes

$$\chi(\delta\,\mathbf{R}) = \mathbf{R}\;\big\{[(\chi\mathbf{T}^T\boldsymbol{\theta}^-)\times\mathbf{I}] \;+\; [(\mathbf{T}^T\boldsymbol{\theta}^+)\times\mathbf{I}][(\mathbf{T}^T\boldsymbol{\theta}^-)\times\mathbf{I}]\big\}, \tag{9.85}$$

where $\mathbf{R}$ pre-multiplies the term in braces, and in the last term the position of $\boldsymbol{\theta}^+$ and $\boldsymbol{\theta}^-$ is interchanged, comparing to eq. (9.81) for the left composition.

The second component can be directly evaluated. In the first component, the differential $\chi\mathbf{T}$ is defined in eq. (9.40), and its transposition changes the sign of skew-symmetric terms at a_4 and a_5. Then the product becomes

$$\begin{aligned}\chi\mathbf{T}^T(\boldsymbol{\psi},\boldsymbol{\theta}^+)\,\boldsymbol{\theta}^- &= a_1\,(\mathbf{e}\cdot\boldsymbol{\theta}^+)\,\boldsymbol{\theta}^- + a_2\,(\mathbf{e}\cdot\boldsymbol{\theta}^-)\,\boldsymbol{\theta}^+ + a_2\,(\boldsymbol{\theta}^+\cdot\boldsymbol{\theta}^-)\,\mathbf{e}\\ &\quad + a_3\,(\mathbf{e}\cdot\boldsymbol{\theta}^+)(\mathbf{e}\cdot\boldsymbol{\theta}^-)\,\mathbf{e} - a_4\,(\mathbf{e}\cdot\boldsymbol{\theta}^+)\,\tilde{\boldsymbol{\psi}}\,\boldsymbol{\theta}^- - a_5\,(\boldsymbol{\theta}^+\times\boldsymbol{\theta}^-),\end{aligned} \tag{9.86}$$

where only the third and fourth terms are symmetric with respect to $\boldsymbol{\theta}^-$ and $\boldsymbol{\theta}^+$.

Second variations for semi-tangential rotation vector. The second differential of $\mathbf{R}$ is defined as the directional derivative of the respective first variation of eq. (9.60) in direction $\boldsymbol{\theta}^+$. Then, for the left composition of rotations, we obtain

$$\chi(\delta\,\mathbf{R}) = \left\{2\,[(\chi\mathbf{T}\,\boldsymbol{\theta}^-)\times\mathbf{I}] \;+\; 4\,[(\mathbf{T}\,\boldsymbol{\theta}^-)\times\mathbf{I}][(\mathbf{T}\boldsymbol{\theta}^+)\times\mathbf{I}]\right\}\,\mathbf{R}, \qquad (9.87)$$

while for the right composition of rotations, we obtain

$$\chi(\delta\,\mathbf{R}) = \mathbf{R}\,\left\{2\,[(\chi\mathbf{T}^T\boldsymbol{\theta}^-)\times\mathbf{I}] \;+\; 4\,[(\mathbf{T}^T\boldsymbol{\theta}^+)\times\mathbf{I}][(\mathbf{T}^T\boldsymbol{\theta}^-)\times\mathbf{I}]\right\}. \qquad (9.88)$$

Note that the multipliers 2 and 4 have appeared in these formulas, in comparison with eqs. (9.81) and (9.85).

Special case: co-axial rotation vectors. Consider the case when $\boldsymbol{\psi}, \boldsymbol{\theta}^+, \boldsymbol{\theta}^-$ are co-axial vectors, i.e. the rotations are performed about one axis, $\mathbf{e}$. Let $\boldsymbol{\psi} = \psi\,\mathbf{e}$, $\boldsymbol{\theta}^- = \alpha\,\mathbf{e}$, and $\boldsymbol{\theta}^+ = \beta\,\mathbf{e}$, where ψ, α, β denote the angles of rotation. Then, by the property of eq. (9.21), we have

$$\mathbf{T}(\boldsymbol{\psi})\,\boldsymbol{\theta}^- = \alpha\mathbf{e}, \qquad \mathbf{T}(\boldsymbol{\psi})\,\boldsymbol{\theta}^+ = \beta\mathbf{e}, \qquad \chi\mathbf{T}\,\boldsymbol{\theta}^- = \alpha\beta\,A\,\mathbf{e}, \qquad (9.89)$$

where $A \doteq (-2b_1 + a_3 + a_2 + b_2 + b_3) = -[2(\cos\omega - 1) + \omega]/\omega^2$, and $\omega \doteq \|\boldsymbol{\psi}\| = \sqrt{\psi^2}$. The plot of A is presented in Fig. 9.4. For $\omega \to \infty$, A tends to zero.

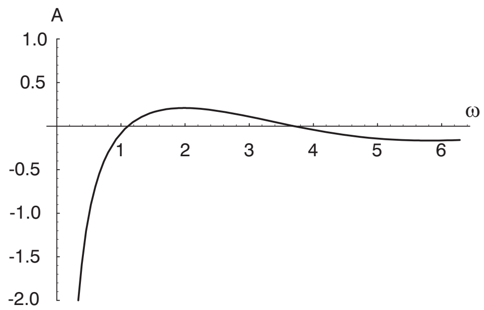

Fig. 9.4 Coefficient A as a function of ω.

The first differential of $\mathbf{R}$ of eq. (9.78) becomes

$$\delta\mathbf{R} = \left\{[\mathbf{T}(\boldsymbol{\psi})\,\boldsymbol{\theta}^-]\times\mathbf{I}\right\}\,\mathbf{R}(\boldsymbol{\psi}) = \alpha\,(\mathbf{e}\times\mathbf{I})\;\mathbf{R}(\boldsymbol{\psi}), \qquad (9.90)$$

while the second differential of eq. (9.81) becomes

$$\chi(\delta\,\mathbf{R}) = \alpha\beta\ (A\,\mathbf{e}\times\mathbf{I}\ +\ \mathbf{e}\otimes\mathbf{e}-\mathbf{I})\ \mathbf{R}. \tag{9.91}$$

Next, we can use the relations $\mathbf{S} \doteq \mathbf{e}\times\mathbf{I}$ and $\mathbf{S}^2 = \mathbf{e}\otimes\mathbf{e}-\mathbf{I}$ from Table 8.1, and the rotation tensor in the form of eq. (8.9), $\mathbf{R} \doteq \mathbf{I} + s\,\mathbf{S} + (1-c)\,\mathbf{S}^2$, where $s \doteq \sin\omega$ and $c \doteq \cos\omega$. Then the differentials of the rotation tensors are as follows:

$$\delta\mathbf{R} = \alpha\mathbf{S}\,\mathbf{R}(\boldsymbol{\psi}) = \alpha[\mathbf{S} + s\,\mathbf{S}^2 + (1-c)\,\mathbf{S}^3] = \alpha(c\,\mathbf{S} + s\,\mathbf{S}^2), \tag{9.92}$$

$$\chi(\delta\,\mathbf{R}) = \alpha\beta\ \left(A\,\mathbf{S}\ +\ \mathbf{S}^2\right)\,\mathbf{R} = \alpha\beta\left[\,(A\,c-s)\,\mathbf{S} + (A\,s+c)\,\mathbf{S}^2\right]. \tag{9.93}$$

For simplicity assume that the rotations are performed around the reference axis $\mathbf{i}_3$, i.e. $\mathbf{e} \doteq \mathbf{i}_3$. Then

$$\mathbf{S} = \mathbf{i}_2\otimes\mathbf{i}_1 - \mathbf{i}_1\otimes\mathbf{i}_2, \qquad \mathbf{S}^2 = -(\mathbf{i}_1\otimes\mathbf{i}_1 + \mathbf{i}_2\otimes\mathbf{i}_2),$$

see Table 8.1, and representations of the tensors are

$$\mathbf{R} = \mathbf{I} + s\,\mathbf{S} + (1-c)\,\mathbf{S}^2 = \begin{bmatrix} c & -s \\ s & c \end{bmatrix}, \tag{9.94}$$

$$\delta\mathbf{R} = \alpha(c\,\mathbf{S} + s\,\mathbf{S}^2) = \alpha\ \begin{bmatrix} -s & -c \\ c & -s \end{bmatrix}, \tag{9.95}$$

$$\begin{aligned}\chi(\delta\,\mathbf{R}) &= \alpha\beta\left[\,(A\,c-s)\,\mathbf{S} + (A\,s+c)\,\mathbf{S}^2\right] \\ &= \alpha\beta\begin{bmatrix} -(A\,s+c) & -(A\,c-s) \\ (A\,c-s) & -(A\,s+c) \end{bmatrix}. \end{aligned} \tag{9.96}$$

Finally, we note that for the co-axial rotation vectors, the difference between the left and right composition rules vanishes.

9.3 Algorithmic schemes for finite rotations

In this section we consider algorithmic schemes of treating finite rotations for a static (time-independent) problem and assume that the Newton method is used to solve the non-linear equilibrium equations.

The tangent matrix and residual for the Newton method can be obtained from any of the three forms of variations which were presented earlier as follows:

1. For the canonical parametrization: the first variation in eq. (9.57) and the second variation in eqs. (9.77), (9.81), and (9.85).

2. For the semi-tangential parametrization: the first variation in eq. (9.60) and the second variation in eqs. (9.77), (9.87), and (9.88).

The tangent matrix and residual obtained for these three forms are fully equivalent.

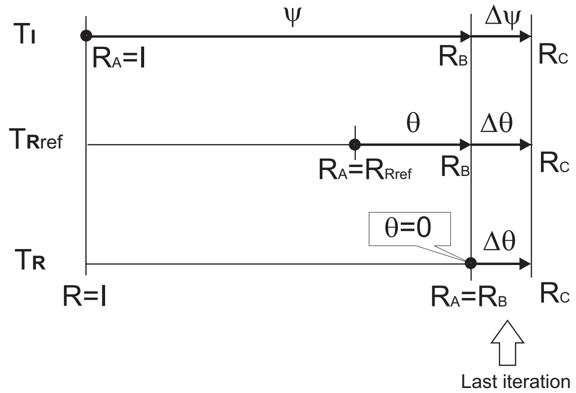

Fig. 9.5 Three schemes of treating finite rotations.

In the algorithmic treatment of rotations, we have to make several choices, regarding (a) the rotation vector used for the increment of rotations (e.g. canonical or semi-tangential vector), (b) parameters used to store nodal rotations (e.g. quaternions or rotation matrices), and (c) an approximation of nodal rotation parameters over the element.

To select the best algorithmic procedure, we have to consider the theoretical properties of each combination of choices, implement them, and subject them to rigorous testing. This is not only laborious but also requires accounting for certain limitations. For instance, in testing of rotations, we must avoid too complex examples to be able to run them automatically without the user's intervention. Non-linear solutions can be very complex and possess extremum and turning points, as well as bifurcation points. To obtain some solutions, not only is an arc-length procedure required, but also additional advanced capabilities, enabling localization of bifurcation points and branch switching. Such capabilities require the user's assistance and, for this reason, are not currently available in commercial FE codes. When testing schemes for rotations we should avoid examples which require them.

Below, we describe three algorithmic schemes of treating finite rotations, formulated in various tangent planes to SO(3):

Scheme 1 is formulated in the initial tangent plane at $\mathbf{R}_A = \mathbf{I}$, i.e. in T_I, and corresponds to the Total Lagrangian description. The global rotation vector $\boldsymbol{\psi}$ is used and updated throughout the whole solution process.

Scheme 2 is formulated in the tangent plane at $\mathbf{R}_A = \mathbf{R}_{\text{ref}}$, i.e. in $T_{R_{\text{ref}}}$, where $\mathbf{R}_{\text{ref}}$ is the last converged solution. This scheme corresponds to the Updated Lagrangian description. The rotation vector $\boldsymbol{\theta}$ is used and updated for each step (increment).

Scheme 3 is formulated in the tangent plane at $\mathbf{R}_A = \mathbf{R}_B$, i.e. in T_R, where $\mathbf{R}_B$ is the last available solution, in general, non-converged. This scheme corresponds to the Eulerian description. The rotation vector $\boldsymbol{\theta} = \mathbf{0}$ throughout the whole solution process.

All these schemes are presented in Fig. 9.5 and the increment of a rotation vector is used in all of them for an iteration of the Newton method. Note that the rotation vector involves only three parameters and, hence, there is no need to append orthogonality constraints, which is convenient. The increment of a rotation vector can also belong to various tangent planes, so we use either $\Delta\boldsymbol{\psi}$ or $\Delta\boldsymbol{\theta}$. Additional questions must also be considered, such as

1. how to update the rotation vector $\boldsymbol{\psi}$ used by Scheme 1 and $\boldsymbol{\theta}$ used by Scheme 2. We can use either a multiplicative update scheme or an additive update scheme.
   In the multiplicative update, we can use either the rotation matrices or quaternions. The quaternions give the advantage that they can be easily renormalized, so they always yield orthogonal rotation matrices. It is complicated to recover the orthogonality for the rotation matrices.
2. How to update the rotation matrix $\mathbf{R}_A$, which is used by Schemes 2 and 3. If, instead of the rotation matrices, we use quaternions, then the update can be achieved via the composition of quaternions given by eq. (8.185).

For both updates, the increment of the rotation vector must be converted to a quaternion and composed with the known quaternion; either for the previous step (in Scheme 2) or for the previous iteration (in Scheme 3).

9.3.1 Scheme 1: formulation in $T_I\mathrm{SO}(3)$

In this scheme we use as the rotational unknown, the rotation vector $\boldsymbol{\psi}$ related to $\mathbf{R}_A = \mathbf{I}$, i.e. $\tilde{\boldsymbol{\psi}} \in T_I\mathrm{SO}(3)$, where T_I is the initial tangent plane, see Fig. 9.5. The total rotation is represented by $\mathbf{R}_B \doteq \mathbf{R}(\boldsymbol{\psi})$.

The additive update procedure for the rotation vector and its increment belonging to the initial tangent plane, i.e. $\tilde{\boldsymbol{\psi}}, \Delta\tilde{\boldsymbol{\psi}} \in T_I\mathrm{SO}(3)$, is presented in Table 9.2.

Table 9.2 Scheme 1. Additive update. $\tilde{\boldsymbol{\psi}}, \Delta\tilde{\boldsymbol{\psi}} \in T_I\mathrm{SO}(3)$.

Initialize: $\boldsymbol{\psi} = \mathbf{0}$	$\longleftarrow$	total
Step		
Newton loop		
Form equilibrium equations using $\boldsymbol{\psi}$, solve for $\Delta\boldsymbol{\psi}$		
Update $\boldsymbol{\psi} = \boldsymbol{\psi} + \Delta\boldsymbol{\psi}$	$\longleftarrow$	total (additive)
End of Newton loop		

The multiplicative update of rotations is exact, see Sect. 8.3, but the additive update of Scheme 1 also yields very accurate results for shells, even in examples involving finite rotations. This can be explained as follows:

1. The additive update is exact if $\boldsymbol{\psi}$ and $\Delta\boldsymbol{\psi}$ are parallel and have the same sense, i.e.
$$\mathbf{R}_C = \underbrace{\mathbf{R}(\Delta\boldsymbol{\psi})\ \mathbf{R}(\boldsymbol{\psi})}_{\text{left}} = \mathbf{R}(\boldsymbol{\psi} + \Delta\boldsymbol{\psi}), \tag{9.97}$$
see the proof of eq. (8.195). Such, or almost such, rotations and their increments are characteristic for the most common one-parameter external loads, i.e. with the magnitude varied by one parameter.
2. Even if the formula $\boldsymbol{\psi} + \Delta\boldsymbol{\psi}$ is not exact, still the operation $(\boldsymbol{\psi} + \Delta\boldsymbol{\psi}) \rightarrow \mathbf{R}$ is exact.
3. In problems involving large strains and non-linear materials, the rotations are not the only source of non-linearity and, hence, we do not have to be too exact when updating rotational parameters, as long as the Newton scheme converges.

However, we must be aware that there are limits of this scheme and, e.g. in the twisted ring example of Sect. 9.3.5, it yields a wrong solution at the rotations close to 2π.

9.3.2 Scheme 2: formulation in $\mathrm{T}_{R_{\mathrm{ref}}}\mathrm{SO}(3)$

In this scheme, we use as the rotational unknown, the rotation vector $\boldsymbol{\theta}$ (or $\boldsymbol{\Theta}$) related to $\mathbf{R}_{\mathrm{ref}} \doteq \mathbf{R}_A$ where $\mathbf{R}_A$ is the last converged solution.

Hence, $\tilde{\boldsymbol{\theta}}\,\mathbf{R}_A$ (or $\mathbf{R}_A\,\tilde{\boldsymbol{\Theta}}$) $\in T_{R_{\text{ref}}}\text{SO}(3)$, where $T_{R_{\text{ref}}}$ is the reference tangent plane, see Fig. 9.5.

The total rotation $\mathbf{R}_C$ is related to the known rotation $\mathbf{R}_B$ with the help of the rotation for the step by either the left or the right composition rule as follows:

$$\mathbf{R}_C = \underbrace{\mathbf{R}(\Delta\boldsymbol{\theta})\;\mathbf{R}(\boldsymbol{\theta})}_{\text{left, for step}}\;\mathbf{R}_B, \qquad \mathbf{R}_C = \mathbf{R}_B\;\underbrace{\mathbf{R}(\boldsymbol{\Theta})\;\mathbf{R}(\Delta\boldsymbol{\Theta})}_{\text{right, for step}}. \tag{9.98}$$

The notation used above is similar to that in eqs. (9.1) and (9.28).

For this formulation, we use two schemes based on quaternions which are presented below; the multiplicative update in Table 9.3 and the multiplicative/additive update in Table 9.4. They have the following features:

1. In both schemes, the total quaternion is used. In the first scheme, the total quaternion $\mathbf{X}$ is updated in each iteration,

$$\mathbf{R}_B = \mathbf{R}(\Delta\boldsymbol{\theta})\;\underbrace{\mathbf{R}(\boldsymbol{\theta})\;\mathbf{R}_A}_{\mathbf{X}}, \qquad \mathbf{R}_B = \underbrace{\mathbf{R}_A\;\mathbf{R}(\boldsymbol{\Theta})}_{\mathbf{X}}\;\mathbf{R}(\Delta\boldsymbol{\Theta}), \tag{9.99}$$

   while in the second scheme, the total quaternion $\mathbf{X}_n$ is updated when the Newton iterations have converged,

$$\mathbf{R}_B = \mathbf{R}(\Delta\boldsymbol{\theta})\;\mathbf{R}(\boldsymbol{\theta})\;\underbrace{\mathbf{R}_A}_{\mathbf{X}_n}, \qquad \mathbf{R}_B = \underbrace{\mathbf{R}_A}_{\mathbf{X}_n}\;\mathbf{R}(\boldsymbol{\Theta})\;\mathbf{R}(\Delta\boldsymbol{\Theta}). \tag{9.100}$$

   In both schemes, the updates of the total quaternion are multiplicative, via a composition of quaternions, as in eq. (8.185). The calculations for the step are different in each scheme.

2. In the multiplicative scheme, the increment of the rotation vector $\Delta\boldsymbol{\Theta}$ is converted to the quaternion $\Delta\mathbf{q}$ using eq. (8.96). The previous quaternion for the step $\mathbf{q}$ and the quaternion for the increment $\Delta\mathbf{q}$ are composed as in eq. (8.185) and then the rotation vector for the step $\boldsymbol{\Theta}$ is extracted from $\mathbf{q}$ by using eq. (8.94).
3. In the multiplicative/additive scheme, the increment of rotation vector $\Delta\boldsymbol{\Theta}$ is added to the rotation vector for the step $\boldsymbol{\Theta}$, converted to the quaternion for the step $\mathbf{q}$, and composed with the quaternion $\mathbf{X}_n$ for the previous converged solution. Note that $\mathbf{X}_n$ is updated only when the Newton iterations for the step have converged.

4. In both schemes, the rotation vector for the step, $\boldsymbol{\Theta}$ belongs to the tangent plane at the converged rotation for the previous increment, $\mathbf{R}^0_{n+1}\tilde{\boldsymbol{\Theta}} \in T_{R^0_{n+1}}\mathrm{SO}(3)$. However, the increments $\Delta\boldsymbol{\Theta}$ belong in the multiplicative scheme to $T_{R^i_{n+1}}\mathrm{SO}(3)$, which is the tangent plane at the last available rotation, not necessarily converged, and to $T_{R^0_{n+1}}\mathrm{SO}(3)$ in the multiplicative/additive scheme.
5. After the computations shown in Tables 9.3 and 9.4, the total rotation vector $\boldsymbol{\chi}$ is extracted from the total quaternion $\mathbf{X}$ by using eq. (8.94).

Note that the presented update schemes are extended is Sect. 9.4.3 for the rigid body dynamics, see Tables 9.6 and 9.8.

Table 9.3 Scheme 2. Multiplicative updates. $\mathbf{R}^i_{n+1}\Delta\tilde{\boldsymbol{\Theta}} \in T_{R^i_{n+1}}\mathrm{SO}(3)$.

Initialize $\mathbf{X}$	$\leftarrow$	total
Step		
$\boldsymbol{\Theta} = \mathbf{0}$, initialize $\mathbf{q}$		
Newton loop		
Form equilibrium equations using $(\mathbf{X}, \boldsymbol{\Theta})$, solve for $\Delta\boldsymbol{\Theta}$		
Update		
$\Delta\boldsymbol{\Theta} \to \Delta\mathbf{q} \to \mathbf{X} = \mathbf{X} \circ \Delta\mathbf{q}$	$\leftarrow$	total (multiplicative)
$\to \mathbf{q} = \mathbf{q} \circ \Delta\mathbf{q} \to \boldsymbol{\Theta}$	$\leftarrow$	for increment (multiplicative)
End of Newton loop		

Table 9.4 Scheme 2. Multiplicative/additive updates. $\mathbf{R}^0_{n+1}\Delta\tilde{\boldsymbol{\Theta}} \in T_{R^0_{n+1}}\mathrm{SO}(3)$.

Initialize $\mathbf{X}_n$	$\leftarrow$	total
Step		
$\boldsymbol{\Theta} = \mathbf{0}$		
Newton loop		
Form equilibrium equations using $(\mathbf{X}, \boldsymbol{\Theta})$, solve for $\Delta\boldsymbol{\Theta}$		
Update		
$\boldsymbol{\Theta} = \boldsymbol{\Theta} + \Delta\boldsymbol{\Theta}$	$\leftarrow$	for increment (additive)
$\boldsymbol{\Theta} \to \mathbf{q} \to \mathbf{X} = \mathbf{X}_n \circ \mathbf{q}$	$\leftarrow$	total (multiplicative)
End of Newton loop		
Update		
$\mathbf{X}_n = \mathbf{X}$	$\leftarrow$	total

9.3.3 Scheme 3: formulation in $\mathbf{T}_R\mathrm{SO}(3)$

In this scheme we use as the rotational unknown, the rotation vector $\boldsymbol{\theta}$ related to $\mathbf{R}_B$, where $\mathbf{R}_B$ is the last available solution, in general, non-converged. Hence, $\tilde{\boldsymbol{\theta}}\,\mathbf{R}_B$ (or $\mathbf{R}_B\,\tilde{\boldsymbol{\Theta}}$) $\in T_{R_B}\mathrm{SO}(3)$, where T_{R_B} is the current tangent plane, see Fig. 9.5.

We use the left composition rule and we assume $\boldsymbol{\psi} = \mathbf{0}$ in the scheme of Fig. 9.1, for which $\mathbf{R}_1(\boldsymbol{\psi}) = \mathbf{I}$ and $\mathbf{R}_B = \mathbf{R}_A$. Hence, $\mathbf{R}(\epsilon\boldsymbol{\theta}_A) = \mathbf{R}_2(\epsilon\boldsymbol{\theta}_B)$ and both forms of the perturbed rotation of eq. (9.1) become identical,

$$\mathbf{R}_C = \mathbf{R}_2(\epsilon\boldsymbol{\theta})\,\mathbf{R}_B, \tag{9.101}$$

where we denoted $\boldsymbol{\theta}$ instead of $\boldsymbol{\theta}_B$, and $\epsilon\tilde{\boldsymbol{\theta}}\,\mathbf{R}_B \in T_{R_B}\mathrm{SO}(3)$. Similarly, for the right composition of eq. (9.28), see Fig. 9.3, which yields

$$\mathbf{R}_C = \mathbf{R}_B\,\mathbf{R}_2(\epsilon\boldsymbol{\Theta}), \tag{9.102}$$

where we denoted $\boldsymbol{\Theta}$ instead of $\boldsymbol{\Theta}_B$, and $\mathbf{R}_B\,\epsilon\tilde{\boldsymbol{\Theta}} \in T_{R_B}\mathrm{SO}(3)$.

For this formulation, we use the multiplicative update scheme which is presented in Table 9.5, and has the following features:

1. Only one quaternion is used in this scheme. The quaternion $\mathbf{X}$ is used for the total rotation and is updated in every iteration,

$$\mathbf{R}_B = \underbrace{\mathbf{R}(\Delta\boldsymbol{\theta})}_{\Delta\mathbf{X}}\ \underbrace{\mathbf{R}(\boldsymbol{\theta})\ \mathbf{R}_A}_{\mathbf{X}}, \qquad \mathbf{R}_B = \underbrace{\mathbf{R}_A\ \mathbf{R}(\boldsymbol{\Theta})}_{\mathbf{X}}\ \underbrace{\mathbf{R}(\Delta\boldsymbol{\Theta})}_{\Delta\mathbf{X}}. \tag{9.103}$$

   The previous quaternion $\mathbf{X}$, and the quaternion for the iteration, $\Delta\mathbf{X}$, are composed multiplicatively, as in eq. (8.185).
2. The increment $\Delta\boldsymbol{\Theta}$ belongs to $T_{R^i_{n+1}}\mathrm{SO}(3)$, which is the tangent plane at the last available rotation, not necessarily converged. The increment $\Delta\boldsymbol{\Theta}$ is converted to the quaternion $\Delta\mathbf{X}$ using eq. (8.96).

Table 9.5 Scheme 3. Multiplicative update. $\mathbf{R}^i_{n+1}\Delta\tilde{\boldsymbol{\Theta}} \in T_{R^i_{n+1}}\mathrm{SO}(3)$.

Initialize $\mathbf{X}$	$\leftarrow$	total
Step		
Newton loop		
Form equilibrium equations using $(\mathbf{X}, \boldsymbol{\Theta} = \mathbf{0})$, solve for $\Delta\boldsymbol{\Theta}$		
Update		
$\Delta\boldsymbol{\Theta} \rightarrow \Delta\mathbf{X} \rightarrow \mathbf{X} = \mathbf{X} \circ \Delta\mathbf{X}$	$\leftarrow$	total (multiplicative)
End of Newton loop		

9.3.4 Symmetry of tangent operator for structures with rotational dofs

The question of symmetry of the tangent operator (stiffness matrix) for the Newton method is very important in numerical implementations and, for structures with rotational dofs, was considered, e.g., in [220, 44, 206, 40, 148].

Consider a conservative system, e.g. a shell or a beam made of a hyperelastic material and deformation-independent loads, for which the potential energy exists. The potential energy of the whole body is $\Pi = \int_V \pi \, \mathrm{d}V$, where π is the potential energy density. In general, π depends on displacements and rotations but, for the sake of simplicity, the displacements are disregarded below.

Below, the notation is the same as in Sect. 9.1, where we considered increments of rotation vectors in two tangent planes. The variations are defined as in Sect. 9.2, see eqs. (9.74) and (9.75). If we designate $\boldsymbol{\theta}^- \doteq \delta\boldsymbol{\psi}$ and $\boldsymbol{\theta}^+ \doteq \Delta\boldsymbol{\psi}$ in these equations, then this notation becomes suitable for incremental formulations.

Consider the potential energy density $\pi(\mathbf{R})$ at some $\mathbf{R} \in \mathrm{SO}(3)$. The first and second differentials of the potential energy are

$$\delta\pi = \frac{\partial \pi}{\partial \mathbf{R}} \cdot \delta\mathbf{R}, \qquad \chi(\delta\pi) = \chi\left(\frac{\partial \pi}{\partial \mathbf{R}}\right) \cdot \delta\mathbf{R} + \frac{\partial \pi}{\partial \mathbf{R}} \cdot \chi(\delta\mathbf{R}). \quad (9.104)$$

The second differential $\chi(\delta\pi)$ yields the tangent operator (stiffness matrix), therefore its symmetry is of interest and is examined below.

1. For the first component of $\chi(\delta\pi)$ of eq. (9.104), we have

$$\chi(\frac{\partial \pi}{\partial \mathbf{R}})\cdot\delta\mathbf{R} = \left(\left[\frac{\partial^2 \pi}{\partial \mathbf{R}\partial \mathbf{R}}\right] \chi\mathbf{R}\right)\cdot\delta\mathbf{R} = \left(\left[\frac{\partial^2 \pi}{\partial \mathbf{R}\partial \mathbf{R}}\right]^T \delta\mathbf{R}\right)\cdot\chi\mathbf{R}, \quad (9.105)$$

   where the first differentials of the rotation tensor, e.g. for the left composition rule and the canonical parametrization, by eq. (9.78) are

$$\delta\mathbf{R} = (\mathbf{T}\boldsymbol{\theta}^-) \times \mathbf{R}, \qquad \chi\mathbf{R} = (\mathbf{T}\boldsymbol{\theta}^+) \times \mathbf{R}. \quad (9.106)$$

   The last form of eq. (9.105) is obtained by the identity (K8) from [33], p. 62, and the term in brackets is a fourth-rank tensor. Symmetry of this term implies symmetry of the whole component w.r.t. $\boldsymbol{\theta}^-$ and $\boldsymbol{\theta}^+$.

2. In the second component of $\chi(\delta\pi)$ of eq. (9.104), we have a scalar product of $\partial\pi/\partial\mathbf{R}$ and the second differential of the rotation tensor, $\chi(\delta\mathbf{R})$. At the equilibrium configuration $\partial\pi/\partial\mathbf{R} = \mathbf{0}$, so the whole component vanishes, but otherwise its contribution is non-trivial. The second differential $\chi(\delta\mathbf{R})$, e.g. for the left composition rule and the canonical parametrization, is defined by eq. (9.81).

We see that the second differential of π has a complicated form and non-symmetric components and it is not easy to resolve the question of symmetry of the corresponding tangent matrix by inspection of the above formulas. Hence, it is advisable to verify numerically whether the tangent matrix of a newly developed finite element is symmetric.

9.3.5 Example: twisted ring by 3D beam element

The twisted ring example is highly non-linear and demanding, due to the presence of finite rotations. It is described in detail and computed using the shell elements in Sect. 15.3.15. Here, we use our two-node 3D beam element; it is relatively simple and, therefore, convenient to test various schemes of treating finite rotations. Below, the results obtained for the canonical rotation vector are presented.

The ring is twisted by a moment applied at one point and fixed at the opposite point, both on the same axis. The whole ring is computed using the arc-length method for the initial $M_x^{\mathrm{ref}} = 50$. Below, we report the rotation r_x and the displacement u_x obtained by the schemes of the preceding sections at point A of Fig. 15.42.

Two solutions by Scheme 1 are shown in Fig. 9.6 for the mesh with 124 and 1000 elements. The curves coincide in the almost whole range for both meshes, but differ when the rotation r_x approaches 2π. It seems that at this value the curves for the displacement and the rotation have vertical asymptotes, which are not physically correct. Note that the curves for the 1000-element mesh are closer to them than the curves for the 124-element mesh. Other examples of erroneous behavior of Scheme 1 at rotations equal to 2π are given in [107].

The solutions from the two schemes, Schemes 1 and 2, are shown in Fig. 9.7, and are obtained for the 124-element mesh. Scheme 1 yields rotations for up to $r_x = 2\pi$ but Scheme 2 allows to perform several turns and we plotted the rotation for up to $r_x \approx 30$. Note that in Scheme 2 we do not use the total rotation vector $\boldsymbol{\psi}$ but, to visualize the

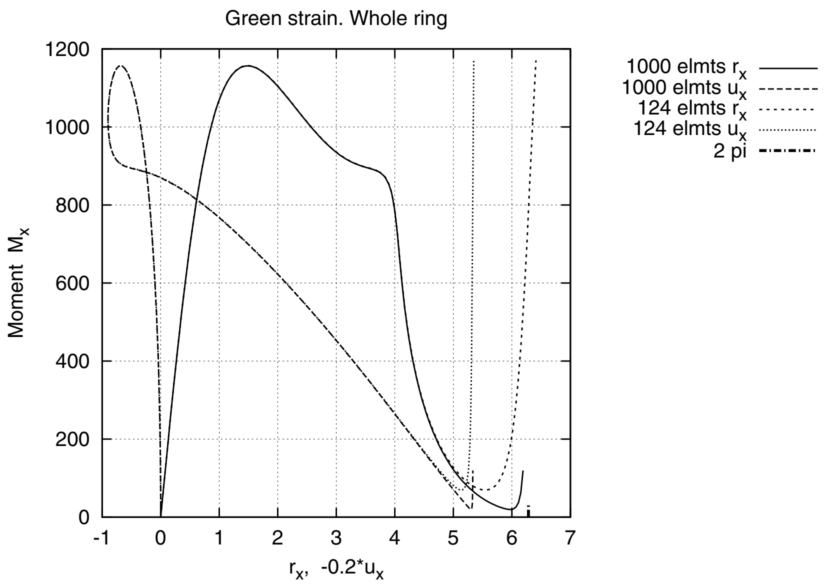

Fig. 9.6 Twisted ring: vertical asymptote at $r_x = 2\pi$ for Scheme 1. $E = 2.1 \cdot 10^6$, $\nu = 0.3$, $w = 1$, $h = 1/3$, $r = 20$.

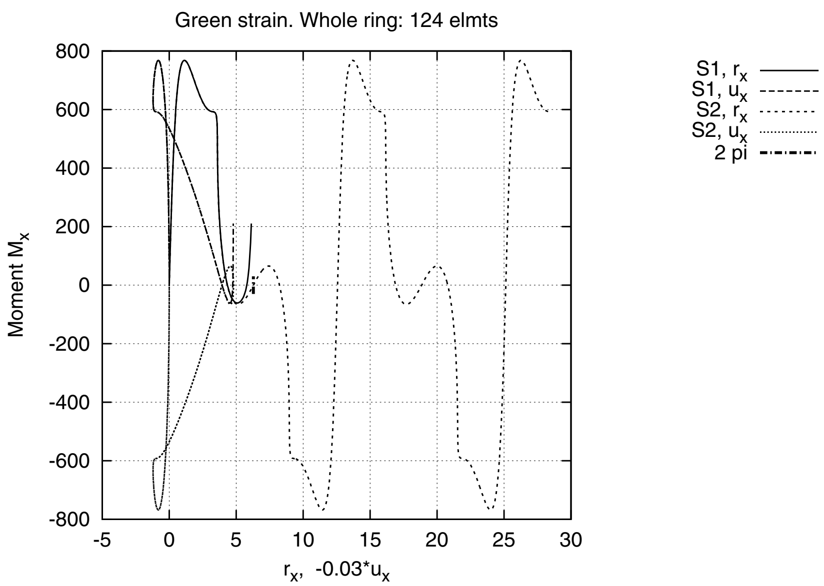

Fig. 9.7 Twisted ring: Scheme 1 and Scheme 2. $E = 2 \cdot 10^5$, $\nu = 0.3$, $w = 6$, $h = 0.6$, $r = 120$.

rotations, we summed up the increments $\Delta\psi$, and the result is plotted in Fig. 9.7. The displacements u_x for both schemes coincide and the same closed curve is obtained for multiple turns.

9.4 Angular velocity and acceleration

9.4.1 Basic definitions

In this section, we present basic notions and relations pertaining to rotations in dynamics, i.e. involving time derivatives of rotational tensors and parameters. Very important is the difference between the angular velocity and acceleration and the time derivatives of rotation vectors.

Instantaneous angular motion. Consider instantaneous angular motion of a rigid body about a fixed point, 0, shown in Fig. 9.8.

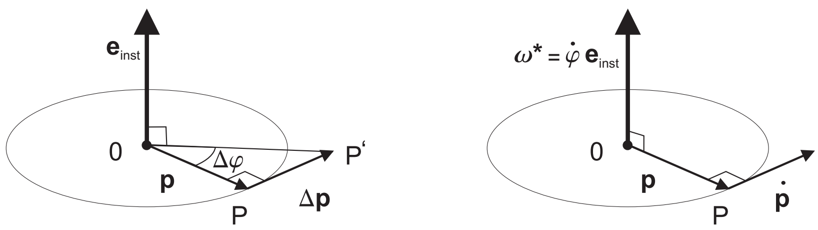

Fig. 9.8 Instantaneous angular motion about an axis $\mathbf{e}_{\text{inst}}$.

The position vector $\mathbf{p}_0$ of an arbitrary point P in the initial configuration is mapped smoothly into a new vector $\mathbf{p}$: $\mathbf{p}(t) = \mathbf{R}(t)\,\mathbf{p}_0$, where $\mathbf{R} \in \text{SO}(3)$ and time $t \in [0, t_{\text{max}}]$. By differentiation of both sides of this relation w.r.t. time t, we obtain

$$\dot{\mathbf{p}}(t) = \dot{\mathbf{R}}(t)\,\mathbf{p}_0 = \dot{\mathbf{R}}(t)\,\mathbf{R}^T(t)\,\mathbf{p}(t), \tag{9.107}$$

where $\dot{(\cdot)} \doteq \text{d}(\cdot)/\text{d}t$ denotes the time derivative and $\dot{\mathbf{p}}(t)$ is the velocity of point P. Note that $\mathbf{p}_0$ was eliminated so all terms are at one time instant, t.

Eulerian (spatial, or left) angular velocity. The Eulerian (spatial, or left) angular velocity tensor and its axial vector are defined as

$$\tilde{\boldsymbol{\omega}}^* \doteq \dot{\mathbf{R}}\,\mathbf{R}^T \in \text{so}(3), \qquad \boldsymbol{\omega}^* \doteq \tfrac{1}{2}(\mathbf{I} \times \tilde{\boldsymbol{\omega}}^*). \tag{9.108}$$

Note that $\tilde{\boldsymbol{\omega}}^*$ is a skew-symmetric tensor, which can be shown as follows: From the time differentiation of the orthogonality condition $\mathbf{R}\mathbf{R}^T = \mathbf{I}$, we obtain $\dot{\mathbf{R}}\mathbf{R}^T + \mathbf{R}\dot{\mathbf{R}}^T = \mathbf{0}$, which, by eq. (9.108), is equivalent to $\tilde{\boldsymbol{\omega}}^* = -(\tilde{\boldsymbol{\omega}}^*)^T$, which is the definition of skew-symmetry.

Using $\tilde{\boldsymbol{\omega}}^*$, eq. (9.107) can be rewritten in two characteristic ways:

1. $\dot{\mathbf{p}} = \boldsymbol{\omega}^* \times \mathbf{p}$, from which we see that the velocity $\dot{\mathbf{p}}$ is perpendicular to the angular velocity vector $\boldsymbol{\omega}^*$ and to the position vector $\mathbf{p}$, see Fig. 9.8b.
2. $\dot{\mathbf{R}} - \tilde{\boldsymbol{\omega}}^*\mathbf{R} = \mathbf{0}$, obtained by using $\mathbf{p}(t) = \mathbf{R}(t)\,\mathbf{p}_0$. Given the $\tilde{\boldsymbol{\omega}}^*$, this is the ODE generating rotations $\mathbf{R}$, for the initial condition $\mathbf{R}(t=0) = \mathbf{R}_0$.

Direction of $\boldsymbol{\omega}^*$. The direction of the angular velocity vector $\boldsymbol{\omega}^*$ can be established as follows. Denote the instantaneous axis of rotation by $\mathbf{e}_{\rm inst}$, and the rotation angle by $\Delta\psi$. Then we can write a simple geometrical formula,

$$\Delta\mathbf{p} = (\Delta\psi\, \mathbf{e}_{\rm inst}) \times \mathbf{p}, \tag{9.109}$$

see Fig. 9.8a. Dividing by Δt, and taking the limit $\Delta t \to 0$, we obtain

$$\dot{\mathbf{p}} = (\dot{\psi}\, \mathbf{e}_{\rm inst}) \times \mathbf{p}, \tag{9.110}$$

where $\dot{\mathbf{p}} \doteq \lim_{\Delta t \to 0}(\Delta\mathbf{p}/\Delta t)$ and $\dot{\psi} \doteq \lim_{\Delta t \to 0}(\Delta\psi/\Delta t)$. By comparison with the earlier derived formula, $\dot{\mathbf{p}} = \boldsymbol{\omega}^* \times \mathbf{p}$, we see that

$$\boldsymbol{\omega}^* = \dot{\psi}\, \mathbf{e}_{\rm inst}, \tag{9.111}$$

i.e. $\boldsymbol{\omega}^*$ has direction of the instantaneous axis $\mathbf{e}_{\rm inst}$, see Fig. 9.8b. We stress that $\mathbf{e}_{\rm inst}$ is instantaneous, i.e. is valid only for an infinitesimal Δt, and is usually different from the axis of rotation $\mathbf{e}$ for a finite time period !

Remark. The above relations are typical for the rigid-body mechanics, but can be also used for shells. We can just replace the position vector $\mathbf{p}$ by the current director $\mathbf{a}_3$, to obtain the relation $\dot{\mathbf{a}}_3 = \boldsymbol{\omega}^* \times \mathbf{a}_3$, see the study on shell intersections in [207].

Lagrangian (material, or right) angular velocity. The Lagrangian (material, or right) angular velocity tensor and its axial vector are defined as

$$\tilde{\boldsymbol{\omega}} \doteq \mathbf{R}^T \dot{\mathbf{R}} \in \mathrm{so}(3), \qquad \boldsymbol{\omega} \doteq \tfrac{1}{2}(\mathbf{I} \times \tilde{\boldsymbol{\omega}}). \tag{9.112}$$

They can be obtained by back-rotation of the left angular velocity, i.e.

$$\tilde{\boldsymbol{\omega}} = \mathbf{R}^T \tilde{\boldsymbol{\omega}}^* \mathbf{R}, \qquad \boldsymbol{\omega} = \mathbf{R}^T \boldsymbol{\omega}^*. \tag{9.113}$$

Using the above relation, the equation generating rotations becomes

$$\dot{\mathbf{R}} - \tilde{\boldsymbol{\omega}}^* \mathbf{R} = \dot{\mathbf{R}} - (\mathbf{R}\tilde{\boldsymbol{\omega}}\mathbf{R}^T)\mathbf{R} = \dot{\mathbf{R}} - \mathbf{R}\tilde{\boldsymbol{\omega}} = \mathbf{0}, \tag{9.114}$$

where $\tilde{\boldsymbol{\omega}}$ multiplies $\mathbf{R}$ from the right.

Angular acceleration. The angular acceleration vectors are defined as time derivatives of the left and right velocity vectors

$$\mathbf{a}_a^* \doteq \dot{\boldsymbol{\omega}}^*, \qquad \mathbf{a}_a \doteq \dot{\boldsymbol{\omega}}, \tag{9.115}$$

where $\mathbf{a}_a^*$ is the Eulerian (spatial, or left) angular acceleration and $\mathbf{a}_a$ is the Lagrangian (material, or right) angular acceleration.

To find the relation between these accelerations and time derivatives of the rotation tensor, we have to introduce skew-symmetric tensors associated with the accelerations and use the time-differentiated eqs. (9.108) and (9.112). More useful, however, are vectorial formulas obtained for particular parametrizations of rotations.

9.4.2 Angular velocity and acceleration for parametrizations

Below, we derive the relations between the earlier-defined angular velocity and acceleration vectors and the time derivatives of the rotation vector for the semi-tangential and canonical parametrization.

A. Left angular velocity

a. For the semi-tangential parametrization, we rewrite the variation for the left composition rule of eq. (9.60) as follows:

$$\underbrace{\delta_{\tilde{\theta}_A} \mathbf{R}(\boldsymbol{\psi})}_{\text{additive}} = \underbrace{\{[2\,\mathbf{T}(\boldsymbol{\psi})\,\boldsymbol{\theta}_A] \times \mathbf{I}\}\,\mathbf{R}(\boldsymbol{\psi})}_{\text{left, multiplicative}} \tag{9.116}$$

in which the variation on both sides are calculated in the direction $\tilde{\boldsymbol{\theta}}_A \in T_I\mathrm{SO}(3)$. We can link the variations to the time derivatives by using $\delta \mathbf{R} = \dot{\mathbf{R}}\, \delta t$ and $\boldsymbol{\theta}_A = \dot{\boldsymbol{\psi}}\, \delta t$, from which the above equation becomes

$$\dot{\mathbf{R}}(\boldsymbol{\psi}) = \{[2\, \mathbf{T}(\boldsymbol{\psi})\, \dot{\boldsymbol{\psi}}] \times \mathbf{I}\}\, \mathbf{R}(\boldsymbol{\psi}). \tag{9.117}$$

By the post-multiplication by $\mathbf{R}^T$, we obtain

$$\underbrace{\dot{\mathbf{R}}(\boldsymbol{\psi})\, \mathbf{R}^T(\boldsymbol{\psi})}_{=\tilde{\boldsymbol{\omega}}^*} = [2\, \mathbf{T}(\boldsymbol{\psi})\, \dot{\boldsymbol{\psi}}] \times \mathbf{I}, \tag{9.118}$$

where $\tilde{\boldsymbol{\omega}}^* = \boldsymbol{\omega}^* \times \mathbf{I}$ is the skew-symmetric tensor of the left angular velocity of eq. (9.108). Hence, in terms of the axial vectors, we have

$$\boldsymbol{\omega}^* = \mathbf{T}(\boldsymbol{\psi})\, \dot{\boldsymbol{\psi}} = \frac{2}{1 + \boldsymbol{\psi} \cdot \boldsymbol{\psi}} (\dot{\boldsymbol{\psi}} + \boldsymbol{\psi} \times \dot{\boldsymbol{\psi}}), \tag{9.119}$$

where $\mathbf{T}$ of eq. (9.10) was used.

b. For the canonical parametrization, we begin from eq. (9.57):

$$\underbrace{\delta \mathbf{R}(\boldsymbol{\psi})}_{\text{additive}} = \underbrace{\{[\mathbf{T}(\boldsymbol{\psi})\, \boldsymbol{\theta}_A] \times \mathbf{I}\}\, \mathbf{R}(\boldsymbol{\psi})}_{\text{left, multiplicative}}, \tag{9.120}$$

and, in the same way as for the semi-tangential parametrization, we obtain

$$\boldsymbol{\omega}^* = \mathbf{T}(\boldsymbol{\psi})\, \dot{\boldsymbol{\psi}} = c_1\, \dot{\boldsymbol{\psi}} + A\, \boldsymbol{\psi} + c_2\, \boldsymbol{\psi} \times \dot{\boldsymbol{\psi}}, \tag{9.121}$$

where $A \doteq (1 - c_1)\, (\boldsymbol{\psi} \cdot \dot{\boldsymbol{\psi}})/(\boldsymbol{\psi} \cdot \boldsymbol{\psi})$, and $\mathbf{T}$ of eq. (9.18) was used.

Note that eqs. (9.119) and (9.121) link the left angular velocity vector $\boldsymbol{\omega}^*$ and the time derivative of the rotation vector $\boldsymbol{\psi}$.

B. Right angular velocity

a. For the semi-tangential parametrization, we rewrite the variation for the right composition rule of eq. (9.60) as follows:

$$\underbrace{\delta_{\tilde{\theta}_A} \mathbf{R}(\boldsymbol{\psi})}_{\text{additive}} = \underbrace{\mathbf{R}(\boldsymbol{\psi})\ \left\{ \left[2\, \mathbf{T}^T(\boldsymbol{\psi})\, \boldsymbol{\theta}_A\right] \times \mathbf{I} \right\}}_{\text{right, multiplicative}}. \tag{9.122}$$

Using $\delta \mathbf{R} = \dot{\mathbf{R}}\, \delta t$ and $\boldsymbol{\theta}_A = \dot{\boldsymbol{\psi}}\, \delta t$, we obtain

$$\dot{\mathbf{R}}(\boldsymbol{\psi}) = \mathbf{R}(\boldsymbol{\psi})\ \left\{ \left[2\, \mathbf{T}^T(\boldsymbol{\psi})\, \dot{\boldsymbol{\psi}}\right] \times \mathbf{I} \right\}. \tag{9.123}$$

By the left multiplication by $\mathbf{R}^T$, we obtain

$$\underbrace{\mathbf{R}^T(\boldsymbol{\psi})\,\dot{\mathbf{R}}(\boldsymbol{\psi})}_{=\tilde{\boldsymbol{\omega}}} = \left[2\,\mathbf{T}^T(\boldsymbol{\psi})\,\dot{\boldsymbol{\psi}}\right] \times \mathbf{I}, \tag{9.124}$$

where $\tilde{\boldsymbol{\omega}} = \boldsymbol{\omega} \times \mathbf{I}$ is the skew-symmetric tensor of the right angular velocity of eq. (9.112). Hence, for the axial vectors we have

$$\boldsymbol{\omega} = 2\,\mathbf{T}^T(\boldsymbol{\psi})\ \dot{\boldsymbol{\psi}} = \frac{2}{1+\boldsymbol{\psi}\cdot\boldsymbol{\psi}}(\dot{\boldsymbol{\psi}} - \boldsymbol{\psi} \times \dot{\boldsymbol{\psi}}), \tag{9.125}$$

where $\mathbf{T}$ of eq. (9.10) was used.

b. For the canonical parametrization, we rewrite the variation for the right composition rule of eq. (9.57) as

$$\underbrace{\delta\mathbf{R}(\boldsymbol{\psi})}_{\text{additive}} = \underbrace{\mathbf{R}(\boldsymbol{\psi})\ \left\{\left[\mathbf{T}^T(\boldsymbol{\psi})\,\boldsymbol{\theta}_A\right] \times \mathbf{I}\right\}}_{\text{right, multiplicative}} \tag{9.126}$$

and, in the same way as for the semi-tangential parametrization, we obtain

$$\boldsymbol{\omega} = \mathbf{T}^T(\boldsymbol{\psi})\ \dot{\boldsymbol{\psi}} = c_1\,\dot{\boldsymbol{\psi}} + A\,\boldsymbol{\psi} - c_2\,\boldsymbol{\psi} \times \dot{\boldsymbol{\psi}}, \tag{9.127}$$

where $A \doteq (1-c_1)\,(\boldsymbol{\psi}\cdot\dot{\boldsymbol{\psi}})/(\boldsymbol{\psi}\cdot\boldsymbol{\psi})$, and $\mathbf{T}$ of eq. (9.18) was used.

Note that eqs. (9.125) and (9.127) link the right angular velocity vector $\boldsymbol{\omega}^*$ and the time derivative of the rotation vector $\boldsymbol{\psi}$.

Remark 1. Recall the properties of $\mathbf{T}$ for the canonical rotation vector of Sect. 9.1, where we found that if $\boldsymbol{\psi}$ and $\boldsymbol{\theta}_A$ are coaxial, then $\mathbf{T}(\boldsymbol{\psi})$ acts as the identity operator. (For the semi-tangential vector, $\mathbf{T}(\boldsymbol{\psi})$ shortens $\boldsymbol{\theta}_A$.) The same property holds if we replace $\mathbf{T}$ by $\mathbf{T}^T$, and $\boldsymbol{\theta}_A$ by $\dot{\boldsymbol{\psi}}$. If $\boldsymbol{\psi}$ and $\dot{\boldsymbol{\psi}}$, are coaxial, then $\mathbf{e}_{\text{inst}} = \mathbf{e}$, i.e. the instantaneous axis of rotation $\mathbf{e}_{\text{inst}}$ coincides with the axis of rotation $\mathbf{e}$ for a finite time period. Hence, for the angular motion about a fixed axis, we have $\boldsymbol{\omega} = \dot{\boldsymbol{\psi}}$.

Remark 2. Let us rewrite eq. (9.121), linking the left angular velocity $\boldsymbol{\omega}^*$ and the time derivative of the canonical rotation vector $\boldsymbol{\psi}$, in the form

$$\dot{\boldsymbol{\psi}} - \mathbf{T}^{-1}(\boldsymbol{\psi})\,\boldsymbol{\omega}^* = \mathbf{0}. \tag{9.128}$$

If $\boldsymbol{\omega}^*$ is known, then this is the ODE which generates $\boldsymbol{\psi}$, given the initial condition $\boldsymbol{\psi}(t=0)=\boldsymbol{\psi}_0$. This equation is an analogue of the equation generating rotations $\mathbf{R}\in \mathrm{SO}(3)$,

$$\dot{\mathbf{R}}-\tilde{\boldsymbol{\omega}}^*\mathbf{R}=\mathbf{0}, \tag{9.129}$$

where the skew-symmetric $\tilde{\boldsymbol{\omega}}^*\in \mathrm{so}(3)$ is known. Note that $\boldsymbol{\omega}^*$ of eq. (9.128) is the axial vector of $\tilde{\boldsymbol{\omega}}^*$ of eq. (9.129).

Update of angular velocity. Consider the right angular velocities at two time instants, t_n and t_{n+1}, which, by eq. (9.112), are defined as

$$\tilde{\boldsymbol{\omega}}_{n+1}\doteq\mathbf{R}_{n+1}^T\dot{\mathbf{R}}_{n+1}, \qquad \tilde{\boldsymbol{\omega}}_n\doteq\mathbf{R}_n^T\dot{\mathbf{R}}_n. \tag{9.130}$$

Using the incremental rotation $\Delta\mathbf{R}$, we have

$$\mathbf{R}_{n+1}=\mathbf{R}_n\Delta\mathbf{R}, \qquad \dot{\mathbf{R}}_{n+1}=\dot{\mathbf{R}}_n\Delta\mathbf{R}+\mathbf{R}_n\dot{\overbrace{\Delta\mathbf{R}}} \tag{9.131}$$

and, using them in eq. $(9.130)_1$, we obtain

$$\tilde{\boldsymbol{\omega}}_{n+1}=\Delta\mathbf{R}^T\,\tilde{\boldsymbol{\omega}}_n\,\Delta\mathbf{R}+\Delta\tilde{\mathbf{w}}, \tag{9.132}$$

where $\Delta\tilde{\mathbf{w}}\doteq\Delta\mathbf{R}^T\,\dot{\overbrace{\Delta\mathbf{R}}}\in \mathrm{so}(3)$ is the (right) angular velocity tensor for the incremental rotation. In terms of the axial vectors, we can write

$$\boldsymbol{\omega}_{n+1}=\Delta\mathbf{R}^T\boldsymbol{\omega}_n+\Delta\mathbf{w}, \tag{9.133}$$

in which $\Delta\mathbf{R}$ and $\Delta\mathbf{w}$ are associated with the increment.

The above formula can be simplified for small increments of the rotation vector and its time derivatives. For $\Delta\mathbf{R}\approx\mathbf{I}+\Delta\tilde{\boldsymbol{\psi}}$, we have $\dot{\overbrace{\Delta\mathbf{R}}}=\Delta\dot{\tilde{\boldsymbol{\psi}}}$ and $\Delta\tilde{\mathbf{w}}=(\mathbf{I}-\Delta\tilde{\boldsymbol{\psi}})\Delta\dot{\tilde{\boldsymbol{\psi}}}$, which yield

$$\tilde{\boldsymbol{\omega}}_{n+1}\;\approx\;(\mathbf{I}-\Delta\tilde{\boldsymbol{\psi}})(\tilde{\boldsymbol{\omega}}_n+\Delta\dot{\tilde{\boldsymbol{\psi}}})\;\approx\;\tilde{\boldsymbol{\omega}}_n+\Delta\dot{\tilde{\boldsymbol{\psi}}}. \tag{9.134}$$

Generally, the update of the angular velocity should be consistent with the time-stepping algorithm.

C. Angular acceleration, left and right

a. For the semi-tangential parametrization, eqs. (9.119) and (9.125) link the angular velocity vectors $\boldsymbol{\omega}^*$ and $\boldsymbol{\omega}$ and the time derivative of the rotation vector $\boldsymbol{\psi}$. By time differentiation of them, we obtain

$$\mathbf{a}_a^* \doteq \dot{\boldsymbol{\omega}}^* = 2\,\mathbf{T}(\boldsymbol{\psi})\,\ddot{\boldsymbol{\psi}} + 2\,\dot{\mathbf{T}}(\boldsymbol{\psi})\,\dot{\boldsymbol{\psi}}, \quad \mathbf{a}_a \doteq \dot{\boldsymbol{\omega}} = 2\,\mathbf{T}^T(\boldsymbol{\psi})\,\ddot{\boldsymbol{\psi}} + 2\,\dot{\mathbf{T}}^T(\boldsymbol{\psi})\,\dot{\boldsymbol{\psi}}. \tag{9.135}$$

For $\mathbf{T}$ given by eq. (9.10), we obtain

$$\dot{\mathbf{T}}(\boldsymbol{\psi}) = a_1(\mathbf{I} + \tilde{\boldsymbol{\psi}}) + \frac{1}{1 + \boldsymbol{\psi} \cdot \boldsymbol{\psi}} \dot{\tilde{\boldsymbol{\psi}}}, \tag{9.136}$$

where $a_1 \doteq -2(\dot{\boldsymbol{\psi}} \cdot \boldsymbol{\psi})/(1 + \boldsymbol{\psi} \cdot \boldsymbol{\psi})^2$. Note that $\dot{\mathbf{T}}$ is analogous to $\chi\mathbf{T}$ of eq. (9.39).

b. For the canonical parametrization, eqs. (9.121) and (9.127) link the angular velocity vectors $\boldsymbol{\omega}^*$ and $\boldsymbol{\omega}$ and the time derivative of the rotation vector $\boldsymbol{\psi}$. By time differentiation of them, we obtain

$$\mathbf{a}_a^* \doteq \dot{\boldsymbol{\omega}}^* = \mathbf{T}(\boldsymbol{\psi})\,\ddot{\boldsymbol{\psi}} + \dot{\mathbf{T}}(\boldsymbol{\psi})\,\dot{\boldsymbol{\psi}}, \qquad \mathbf{a}_a \doteq \dot{\boldsymbol{\omega}} = \mathbf{T}^T(\boldsymbol{\psi})\,\ddot{\boldsymbol{\psi}} + \dot{\mathbf{T}}^T(\boldsymbol{\psi})\,\dot{\boldsymbol{\psi}}. \tag{9.137}$$

For $\mathbf{T}$ given by eq. (9.18), we obtain

$$\begin{aligned}\dot{\mathbf{T}}(\boldsymbol{\psi}) &= a_1\,(\dot{\boldsymbol{\psi}} \cdot \mathbf{e})\,\mathbf{I} + a_2\,(\dot{\boldsymbol{\psi}} \otimes \mathbf{e} + \mathbf{e} \otimes \dot{\boldsymbol{\psi}}) \\ &\quad + a_3\,(\dot{\boldsymbol{\psi}} \cdot \mathbf{e})\,(\mathbf{e} \otimes \mathbf{e}) + a_4\,(\dot{\boldsymbol{\psi}} \cdot \mathbf{e})\,\tilde{\boldsymbol{\psi}} + a_5\,(\dot{\boldsymbol{\psi}} \times \mathbf{I}),\end{aligned} \tag{9.138}$$

where the scalar coefficients are defined by eq. (9.41). Note that $\dot{\mathbf{T}}$ is analogous to $\chi\mathbf{T}$ of eq. (9.40). For $\boldsymbol{\psi} \to \mathbf{0}$: $\dot{\mathbf{T}}^T(\boldsymbol{\psi}) \to -\frac{1}{2}(\dot{\boldsymbol{\psi}} \times \mathbf{I})$ and $\dot{\boldsymbol{\omega}} \to \ddot{\boldsymbol{\psi}}$, as $\dot{\boldsymbol{\psi}} \times \dot{\boldsymbol{\psi}} = \mathbf{0}$.

Finally, we note that using the above-derived relations between the angular velocities and accelerations and the time derivatives of rotation vectors, we can formulate various algorithms of dynamics in terms of $\{\boldsymbol{\psi}, \dot{\boldsymbol{\psi}}, \ddot{\boldsymbol{\psi}}\}$, as in [250].

9.4.3 Examples of updates for rigid body motion

The updates of rotational parameters can be conveniently presented for the equations of angular motion of a rigid body, which are relatively simple. We base on the algorithm ALGO-C1 of [221], which conserves the angular momentum and the kinetic energy and develop our algorithms as modifications of ALGO-C1.

In the formulation presented below, the right composition rule of rotations is used, i.e. $\boldsymbol{\Lambda}_{n+1} = \boldsymbol{\Lambda}_n \exp \tilde{\boldsymbol{\Theta}}$, where $\boldsymbol{\Lambda} \in \mathrm{SO}(3)$ is the rotation tensor and $\boldsymbol{\Theta}$ is the canonical rotation vector for the time step. This vector belongs to the tangent plane at the converged rotation for the previous time step, i.e. $\boldsymbol{\Lambda}^0_{n+1}\tilde{\boldsymbol{\Theta}} \in T_{\Lambda^0_{n+1}}\mathrm{SO}(3)$, where $\boldsymbol{\Lambda}^0_{n+1} = \boldsymbol{\Lambda}^{\mathrm{conv}}_n$. Hence, we use the formulation in $T_{R_{\mathrm{ref}}}\mathrm{SO}(3)$ of Sect. 9.3.

The notation used below is similar to that in [221]. Hence, $\mathbf{W}$ is the material (right) angular velocity vector (equal to $\boldsymbol{\omega}$ of eq. (9.112)) and $\mathbf{A} \doteq \dot{\mathbf{W}}$ is the angular acceleration (equal to $\mathbf{a}$ of eq. (9.115)). The spatial angular momentum is $\boldsymbol{\pi}(t) \doteq \boldsymbol{\Lambda}(t)\, \mathbb{J}\, \mathbf{W}(t)$ and the kinetic energy of the angular motion is $E_k(t) \doteq \frac{1}{2}\mathbf{W}(t) \cdot [\mathbb{J}\mathbf{W}(t)]$, both relative to the center of mass, where $\mathbb{J}$ is the material (time-independent) inertia tensor.

The basic idea underlying the ALGO-C1 algorithm follows that proposed earlier for the dynamics with translational dofs in [270]. The second Newton law for the angular motion, $\mathrm{d}\boldsymbol{\pi}/\mathrm{d}t = \mathbf{m}$, where $\mathbf{m}$ is the external torque, is integrated w.r.t. time in the interval $[t_n, t_{n+1}]$, which yields

$$\boldsymbol{\pi}_{n+1} - \boldsymbol{\pi}_n = \int_{t_n}^{t_{n+1}} \mathbf{m}(t)\, \mathrm{d}t. \tag{9.139}$$

This eliminates acceleration from the governing equations; still, however, it can be recovered using angular velocities. Finally, the equation of motion is

$$\boldsymbol{\Lambda}_{n+1}\, \mathbb{J}\, \mathbf{W}_{n+1} - \boldsymbol{\Lambda}_n\, \mathbb{J}\, \mathbf{W}_n - h\mathbf{m}_{n+\alpha} = \mathbf{0}, \tag{9.140}$$

where $h \doteq t_{n+1} - t_n$, and $\alpha \in [0, 1]$. The Newmark algorithm for the rotational parameters used in [221] is as follows:

$$\boldsymbol{\Theta} = h\mathbf{W}_n + h^2 \left[\left(\frac{1}{2} - \beta \right) \mathbf{A}_n + \beta \mathbf{A}_{n+1} \right], \qquad \beta \in \left[0, \frac{1}{2}\right], \tag{9.141}$$

$$\mathbf{W}_{n+1} = \mathbf{W}_n + h[(1-\gamma)\mathbf{A}_n + \gamma \mathbf{A}_{n+1}], \qquad \gamma \in [0, 1], \tag{9.142}$$

and involves $\{\boldsymbol{\Theta}, \mathbf{W}, \dot{\mathbf{W}}\}$. Note that $\{\boldsymbol{\Theta}, \dot{\boldsymbol{\Theta}}, \ddot{\boldsymbol{\Theta}}\}$ are used, e.g., in [44, 250]. In [146], the latter set of variables is treated as more correct, but our experience indicates that its use diminishes the radius of convergence of the Newton method and the time steps must be smaller.

The motion is free when either the integral in eq. (9.139) is equal to zero or $\mathbf{m}_{n+\alpha} = \mathbf{0}$ in eq. (9.140) and then $\boldsymbol{\pi}_{n+1} = \boldsymbol{\pi}_n$, i.e. the angular momentum is preserved. It is shown in [221] that the kinetic energy E_k is conserved for any $\gamma = 2\beta$.

The algorithms which are defined below have the following features:

1. In all presented algorithms, the converged results for the step are combined in the same way with the results for previous time steps. It is done via a composition of two quaternions: the total quaternion $\mathbf{X}$, and the quaternion for time step $\mathbf{q}$. Hence, the difference between the algorithms is confined to the computations within the time step.
2. The canonical rotation vector for the time step $\boldsymbol{\Theta}$ belongs to the tangent plane at the converged rotation for the previous time step, i.e. $\boldsymbol{\Lambda}^0_{n+1}\tilde{\boldsymbol{\Theta}} \in T_{\Lambda^0_{n+1}}\mathrm{SO}(3)$. However, its increments $\Delta\boldsymbol{\Theta}$ can belong either to the same plane or to $T_{\Lambda^i_{n+1}}\mathrm{SO}(3)$, which is the tangent plane at the last available rotation, not necessarily converged. This constitutes the difference between Algorithm 1 and Algorithms 2 and 3.
3. The update of the angular velocity is as follows:
$$\mathbf{W}^{i+1}_{n+1} = \mathbf{W}^{i}_{n+1} + \frac{\gamma}{\beta h}\left[\boldsymbol{\Theta}^{(i+1)} - \boldsymbol{\Theta}^{(i)}\right], \tag{9.143}$$
where i and $i+1$ designated iterations. In Algorithm 1 of Table 9.6, $\boldsymbol{\Theta}^{(i+1)}$ is recovered from the updated quaternion $\mathbf{q}$ for the time step, while in the algorithms of Tables 9.7 and 9.8, $\boldsymbol{\Theta}^{(i+1)}$ is obtained by the additive update. Hence, $\tilde{\boldsymbol{\Theta}}$ used in the update of angular velocity belongs to the initial tangent plane, i.e. $\boldsymbol{\Lambda}^0_{n+1}\tilde{\boldsymbol{\Theta}} \in T_{\Lambda^0_{n+1}}\mathrm{SO}(3)$, in all algorithms.
4. After the computations shown in Tables 9.6, 9.7 and 9.8, the total rotation vector $\boldsymbol{\chi}$ is extracted from the total quaternion $\mathbf{X}$ and the angular acceleration $\mathbf{A}$ is computed from the angular velocity $\mathbf{W}$.

Algorithm 1. Multiplicative updates. In this algorithm $\Delta\tilde{\boldsymbol{\Theta}}$ belongs to the plane tangent at $\boldsymbol{\Lambda}^i_{n+1}$, which is the last available solution, not necessarily converged. This is basically the ALGO-C1 algorithm of [221].

We assume that the external torque $\mathbf{m}$ is independent of $\boldsymbol{\Theta}$. Then the tangent operator is

$$\mathbf{K}(\boldsymbol{\Lambda}_{n+1}, \boldsymbol{\Theta}) = \boldsymbol{\Lambda}_{n+1}\left[\frac{\gamma}{\beta h}\,\mathbb{J}\mathbf{T}(\boldsymbol{\Theta}) - (\widetilde{\mathbf{J}\mathbf{W}_{n+1}})\right], \tag{9.144}$$

where the operator $\mathbf{T}$, which is used here, is defined as in [221], i.e. it is equal to our $\mathbf{T}^{-T}$, where our $\mathbf{T}$ is given in eq. (9.18). To derive the above form of $\mathbf{K}$, the directional derivative of rotation $\boldsymbol{\Lambda}^i_{n+1}$ is calculated as

$$\frac{\mathrm{d}}{\mathrm{d}\epsilon}[\underbrace{\boldsymbol{\Lambda}_n \exp \tilde{\boldsymbol{\Theta}}^i}_{=\boldsymbol{\Lambda}^i_{n+1}} \exp(\epsilon \Delta\tilde{\boldsymbol{\Theta}})]_{\epsilon=0} = \boldsymbol{\Lambda}^i_{n+1}\Delta\tilde{\boldsymbol{\Theta}}, \tag{9.145}$$

where $\boldsymbol{\Lambda}^i_{n+1}\Delta\tilde{\boldsymbol{\Theta}} \in T_{\Lambda^i_{n+1}}\mathrm{SO}(3)$, i.e. the increment belongs to a different tangent plane than the total rotation vector $\tilde{\boldsymbol{\Theta}}$.

On the other hand, the directional derivative of angular velocity, $\mathbf{W}^i_{n+1} = (\gamma/\beta h)\,\boldsymbol{\Theta}^i + (\cdot)_n$, where $(\cdot)_n$ denotes the terms for t_n, is calculated as follows:

$$\frac{\mathrm{d}}{\mathrm{d}\epsilon}[\frac{\gamma}{\beta h}(\boldsymbol{\Theta}^i + \epsilon\Delta\tilde{\boldsymbol{\Theta}})]_{\epsilon=0} = \frac{\gamma}{\beta h}\Delta\tilde{\boldsymbol{\Theta}}, \tag{9.146}$$

where $\boldsymbol{\Lambda}^0_{n+1}\Delta\tilde{\boldsymbol{\Theta}} \in T_{\Lambda^0_{n+1}}\mathrm{SO}(3)$, i.e. it belongs to the same tangent plane as $\boldsymbol{\Lambda}^0_{n+1}\tilde{\boldsymbol{\Theta}}$. The transformation to the plane $T_{\Lambda^i}\mathrm{SO}(3)$ is

$$\underbrace{\Delta\boldsymbol{\Theta}}_{\in T_{\Lambda^i_{n+1}}} = \mathbf{T} \underbrace{\Delta\boldsymbol{\Theta}}_{\in T_{\Lambda^0_{n+1}}}. \tag{9.147}$$

The multiplicative updates of rotational parameters for the algorithm in $T_R\mathrm{SO}(3)$ are presented in Table 9.6. Note that two quaternions are used: $\mathbf{X}$ is the total quaternion, while $\mathbf{q}$ is the quaternion for the time step.

Algorithms 2 and 3. Multiplicative/additive updates. In these algorithms, $\Delta\tilde{\boldsymbol{\Theta}}$ belongs to the plane tangent at $\boldsymbol{\Lambda}^0_{n+1}$, which is the last converged solution for the previous time step, i.e. $\boldsymbol{\Lambda}^0_{n+1} = \boldsymbol{\Lambda}^{\mathrm{conv}}_n$. These algorithms are our modifications of ALGO-C1.

We assume that the external moment $\mathbf{m}$ is independent of $\boldsymbol{\Theta}$. Then the tangent operator is

$$\mathbf{K}(\boldsymbol{\Lambda}_{n+1}, \boldsymbol{\Theta}) = \boldsymbol{\Lambda}_{n+1}\left[\frac{\gamma}{\beta h}\mathbb{J} - (\widetilde{\mathbf{J}\mathbf{W}_{n+1}})\mathbf{T}^{-1}(\boldsymbol{\Theta})\right]. \tag{9.148}$$

This form of $\mathbf{K}$ is obtained when we use the inverse relation

$$\underbrace{\Delta\boldsymbol{\Theta}}_{\in T_{\Lambda^0_{n+1}}} = \mathbf{T}^{-1} \underbrace{\Delta\boldsymbol{\Theta}}_{\in T_{\Lambda^i_{n+1}}} \tag{9.149}$$

Table 9.6 Multiplicative updates of Algorithm 1. Quaternions.

Initialize		
$\mathbf{X}$	$\leftarrow$	total
Time step		
$\mathbf{W}$	$\leftarrow$	predict for step
$\mathbf{W} \to \boldsymbol{\Theta} \to \mathbf{q}$	$\leftarrow$	for step
$\mathbf{X} = \mathbf{X} \circ \mathbf{q} \to \boldsymbol{\Lambda}$	$\leftarrow$	total (multiplicative)
Newton loop		
Form governing equations using $\mathbf{K}(\boldsymbol{\Lambda}, \boldsymbol{\Theta})$	of eq. (9.144)	
Solve for $\Delta\boldsymbol{\Theta}$		
Update		
$\Delta\boldsymbol{\Theta} \to \Delta\mathbf{q} \to \mathbf{q} = \mathbf{q} \circ \Delta\mathbf{q} \to \boldsymbol{\Theta}$	$\leftarrow$	for step (multiplicative)
$\Delta\mathbf{q} \to \mathbf{X} = \mathbf{X} \circ \Delta\mathbf{q} \to \boldsymbol{\Lambda}$	$\leftarrow$	total (multiplicative)
$\boldsymbol{\Theta} \to \mathbf{W}$	$\leftarrow$	for step
End of Newton loop		

to transform $\Delta\tilde{\boldsymbol{\Theta}} = \Delta\boldsymbol{\Theta} \times \mathbf{I}$ in the directional derivative of rotation $\boldsymbol{\Lambda}^i_{n+1}$ of eq. (9.145), but when we leave the derivative of the angular velocity in eq. (9.146) unchanged. Here, $\boldsymbol{\Lambda}^0_{n+1}\Delta\tilde{\boldsymbol{\Theta}} \in T_{\Lambda^0_{n+1}}\mathrm{SO}(3)$.

The multiplicative/additive updates of rotational parameters are presented in two versions: Algorithm 2 uses the rotation matrices, see Table 9.7, while Algorithm 3 uses two quaternions, the total quaternion $\mathbf{X}$ and the quaternion for the time step $\mathbf{q}$, see Table 9.8.

The rotation matrix $\boldsymbol{\Lambda}_n$ in Table 9.7 and the total quaternion $\mathbf{X}$ in Table 9.8 are not updated until the Newton iterations for the time step have converged. The additive update of $\boldsymbol{\Theta}$ affects $\mathbf{T}$ and either the rotation matrix $\boldsymbol{\Lambda}^{(i)}$ or the quaternion $\mathbf{q}$ for the time step.

In both schemes, after the convergence of the Newton method, the total rotation vector $\boldsymbol{\chi}$ is recovered from the quaternion $\mathbf{X}$, which is essential to obtain $\boldsymbol{\chi}$ without jumps.

Example. Unstable rotations. In this example, unstable rotations about the axis of intermediate moment of inertia are simulated, see [221], and we compare different update schemes of rotation parameters.

The motion consists of three phases: (1) unstable rotations about the axis of intermediate moment of inertia, (2) small disturbance acts for a duration of one time step, and (3) free unstable motion. In the third phase, the kinetic energy and the angular momentum should be preserved. The

Table 9.7 Multiplicative/additive updates of Algorithm 2. Rotation matrices.

Initialize		
$\mathbf{X},\ \boldsymbol{\Lambda}$	$\leftarrow$	total
Time step		
$\mathbf{W}$	$\leftarrow$	predict for step
$\mathbf{W} \rightarrow \boldsymbol{\Theta} \rightarrow \boldsymbol{\Lambda}^{(0)}$	$\leftarrow$	for step
$\boldsymbol{\Lambda} = \boldsymbol{\Lambda}_n \boldsymbol{\Lambda}^{(0)}$	$\leftarrow$	total (multiplicative)
Newton loop		
Form governing equations using $\mathbf{K}(\boldsymbol{\Lambda}, \boldsymbol{\Theta})$ of eq. (9.148)		
Solve for $\Delta\boldsymbol{\Theta}$		
Update		
$\boldsymbol{\Theta} = \boldsymbol{\Theta} + \Delta\boldsymbol{\Theta}$	$\leftarrow$	for step (additive)
$\boldsymbol{\Theta} \rightarrow \boldsymbol{\Lambda}^{(i)}$	$\leftarrow$	for step
$\boldsymbol{\Lambda} = \boldsymbol{\Lambda}_n \boldsymbol{\Lambda}^{(i)}$	$\leftarrow$	total (multiplicative)
$\boldsymbol{\Theta} \rightarrow \mathbf{W}$	$\leftarrow$	for step
End of Newton loop		
Update		
$\boldsymbol{\Theta} \rightarrow \mathbf{q} \rightarrow \mathbf{X} = \mathbf{X} \circ \mathbf{q}$	$\leftarrow$	total (multiplicative)
$\boldsymbol{\Lambda}_n = \boldsymbol{\Lambda}$	$\leftarrow$	total

external torque $\mathbf{m}$ is defined as

$$\mathbf{m} = \begin{cases} C_1\,\mathbf{e}_1 & 0 \leq t \leq t_z \\ C_2\,\mathbf{e}_2 & t_z \leq t \leq t_z + h\,, \\ \mathbf{0} & t > t_z + h \end{cases} \qquad t_z + h = 2, \qquad C_1 = 20, \qquad h\,C_2 = 0.2,$$

the moment of inertia $\mathbb{J} = \mathrm{diag}[5, 10, 1]$, and the initial conditions $\boldsymbol{\chi}(0) = \mathbf{0}$, $\mathbf{W}(0) = \mathbf{0}$, $(\mathbf{A}(0) = \mathbf{0})$. The parameters for the Newmark algorithm are $\beta = 1/2$, $\gamma = 1$. The time step $h = 0.1$ is used to show large convergence radius of the algorithms used; nonetheless, it is too large to yield good accuracy of results.

The results for the multiplicative update (A1) and the multiplicative/additive updates (A1 and A2) are compared in Fig. 9.9 for $t_{\max}$ =10 sec. The results for A2 and A3 are identical. We see that all algorithms yield exactly the same solution and conserve the kinetic energy and the angular momentum during free motion. For a longer simulation, up to $t_{\max}$ =1000 sec, the results were also identical.

Table 9.8 Multiplicative/additive updates of Algorithm 3. Quaternions.

Initialize		
$\mathbf{X}_n$	$\leftarrow$	total
Time step		
$\mathbf{W}$	$\leftarrow$	predict for step
$\mathbf{W} \to \boldsymbol{\Theta} \to \mathbf{q}^{(0)}$	$\leftarrow$	for step ($\mathbf{q}^{(0)}$ - intermediate)
$\mathbf{X} = \mathbf{X}_n \circ \mathbf{q}^{(0)} \to \boldsymbol{\Lambda}$	$\leftarrow$	total (multiplicative)
Newton loop		
Form governing equations using $\mathbf{K}(\boldsymbol{\Lambda}, \boldsymbol{\Theta})$ of eq. (9.148)		
Solve for $\Delta\boldsymbol{\Theta}$		
Update		
$\boldsymbol{\Theta} = \boldsymbol{\Theta} + \Delta\boldsymbol{\Theta}$	$\leftarrow$	for step (additive)
$\boldsymbol{\Theta} \to \mathbf{q}^{(i)} \to \mathbf{X}_n \circ \mathbf{q}^{(i)} \to \boldsymbol{\Lambda}$	$\leftarrow$	total (multiplicative) ($\mathbf{X}$-not updated)
$\boldsymbol{\Theta} \to \mathbf{W}$	$\leftarrow$	for step
End of Newton loop		
Update		
$\boldsymbol{\Theta} \to \mathbf{q} \to \mathbf{X}_n = \mathbf{X}_n \circ \mathbf{q}$	$\leftarrow$	total (multiplicative)

The total number of iterations in the whole simulation is given in Table 9.9, and we see that the differences are minor, up to about 1.2% for the longer run.

Table 9.9 Number of iterations for particular updates. Unstable rotations. $h = 0.1$.

Algorithm	Updates	Table	Number of iterations in 10 sec	1000 sec
A1	multiplicative	9.6	359	41020
A2,A3	multiplicative/additive	9.7, 9.8	344	41485
(A1/A2) × 100%			104.4	98.9

Example. Fast spinning top. In this example, the motion of a symmetrical top in a uniform gravitational field is simulated, see [221] for more details. The top is not rotating freely so the energy and angular momentum are not to be conserved, but still we can compare the performance of the developed algorithms. The external torque is rendered by gravitation and is defined as follows:

$$\mathbf{m}_{n+\alpha} = -M g\, l\, (\boldsymbol{\Lambda}_{n+\alpha}\, \mathbf{e}_3) \times \mathbf{e}_3, \tag{9.150}$$

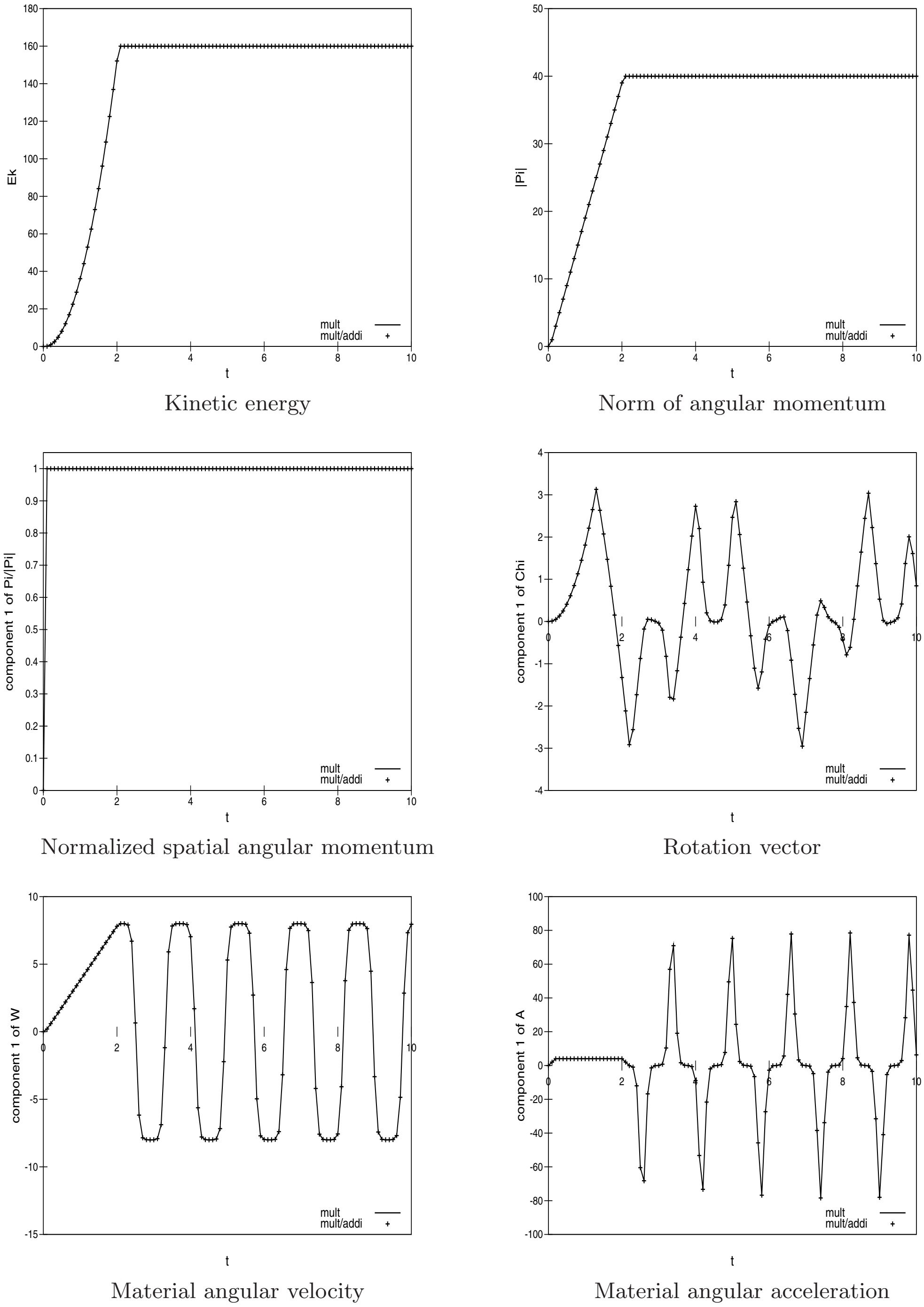

Fig. 9.9 Unstable rotations. Multiplicative and multiplicative/additive updates.

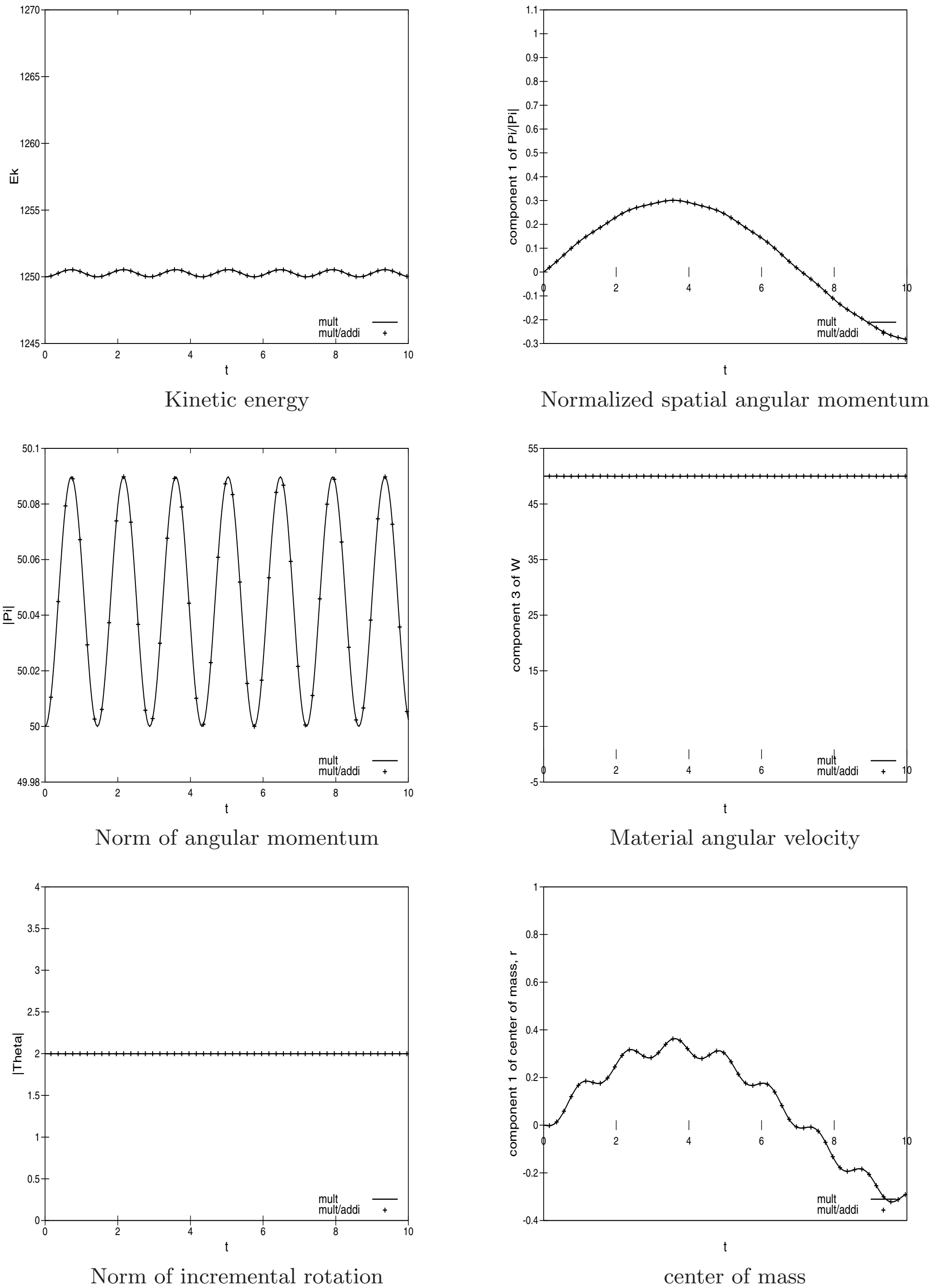

Fig. 9.10 Fast spinning top. Multiplicative and multiplicative/additive updates.

where $\boldsymbol{\Lambda}_{n+\alpha} = \boldsymbol{\Lambda}_n \exp(\alpha\tilde{\boldsymbol{\Theta}})$. Besides, M is mass, g is the gravitational acceleration, l is the distance from the center of mass to the fixed contact point, which is in the origin of the global frame $\{\mathbf{e}_i\}$. The basis vector $\mathbf{e}_3 \doteq \{0, 0, 1\}$.

The data is as follows: $Mg = 20$, $l = 1$, $\mathbb{J} = \text{diag}[5, 5, 1]$ and the initial conditions are $\boldsymbol{\chi}(0) = [\,0.3,\ 0,\ 0\,]^T$, $\mathbf{W}(0) = [\,0,\ 0,\ 50\,]^T$, $\mathbf{A}(0) = \mathbf{0}$, where $\boldsymbol{\chi}$ is the canonical rotation vector parameterizing $\boldsymbol{\Lambda}$. At $t = 0$, $\boldsymbol{\Lambda}(0) = \exp\tilde{\boldsymbol{\chi}}(0)$. Besides, $\alpha = 1/2$.

The torque $\mathbf{m}_{n+\alpha}$ depends on $\boldsymbol{\Theta}$ and contributes to the tangent operator in the following way:

$$\mathbf{K}_B(\boldsymbol{\Lambda}_{n+1}, \boldsymbol{\Theta}) = \mathbf{K}(\boldsymbol{\Lambda}_{n+1}, \boldsymbol{\Theta}) - h\,\mathbf{K}_{m\alpha}(\boldsymbol{\Theta}),$$

$$\mathbf{K}_{m\alpha}(\boldsymbol{\Theta}) = -Mg\,l\,\alpha\,\widetilde{\mathbf{e}}_3\,\boldsymbol{\Lambda}_{n+\alpha}\,\widetilde{\mathbf{e}}_3, \tag{9.151}$$

where $\mathbf{K}(\boldsymbol{\Lambda}_{n+1}, \boldsymbol{\Theta})$ is defined either by eq. (9.144) or by (9.148).

The results for the multiplicative update (A1) and the multiplicative/additive updates (A2 and A3) are compared in Fig. 9.10 for $t_{\max} = 10$ sec. The results for A2 and A3 are identical. For $h = 0.04$, all algorithms give identical results, and needed the same number of iterations (1000 iterations).

Finally, we can conclude, that for the incremental formulation with the iterative (Newton) solution within the time step, the additive update of rotation vectors provides the same accuracy and a similar effectiveness as the multiplicative update.