The Computations of Large Rotation Through an Index Two Nilpotent Equation

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Abstract: To characterize largely deformed spin-free reference configuration of materials, we have to construct an orthogonal transformation tensor $Q$ relative to the fixed frame, such that the tensorial equation $\dot{Q} = WQ$ holds for a given spin history $W$. This paper addresses some interesting issues about this equation. The Euler’s angles representation, and the (modified) Rodrigues parameters representation of the rotation group $SO(3)$ unavoidably suffer certain singularity, and at the same time the governing equations are nonlinear three-dimensional ODEs. A decomposition $Q = FQ_1$ is first derived here, which is amenable to a simpler treatment of $Q_1$ than $Q$, and the numerical calculation of $Q_1$ is obtained by transforming the governing equations in a space of $\mathbb{R}^3$, whose dimensions are two, and the singularity-free interval is largely extended. Then, we develop a novel method to express $Q_1$ in terms of a noncanonical orthogonal matrix, the governing equation of which is a linear ODEs system with its state matrix being nilpotent with index two. We examine six methods on the computation of $Q$ from the theoretical and computational aspects, and conclude that the new methods can be applied to the calculations of large rotations.

keyword: Large rotation, Nilpotent matrix, Singularity-free, Lie algebra, Noncanonical orthogonal matrix.

1 Introduction

The orthogonal matrices $Q$ that represent rotations constitute points on a particular manifold:

$$SO(3) := \{Q|Q^{-1} = Q^T, \det Q = 1\}.$$  

The matrix $Q$ is also called the direction cosine matrix, which is a configuration space of a rigid-body motion. The object of every orientational investigation is to study the time evolution of $Q$ as a function of initial conditions and of the parameters introduced in a model of physical application. The time evolution of $Q$ is summarized as a second order differential equation on $SO(3)$ (Lang, 1985). Therefore, one has the mapping:

$$t \mapsto Q \in SO(3),$$  

where the particular structure of $SO(3)$ makes the problem of devising suitable integrators interesting (Austin, Krishnaprasad and Wang, 1993; Buss, 2000; Celledoni and Owren, 2003).

Among many classical Lie groups, the three-dimensional rotation $SO(3)$ is one of the most widely used groups. For its numerous physical applications, deriving a proper algorithm to calculate $SO(3)$ has received a considerable attention in the literature, and this subject is in fact of primary interest in the computational mechanics. A comprehensive review of its applications on the spacecraft attitude was given by Shuster (1993) and on the solid mechanics was given by Atluri and Cazzani (1995) up to the 1990s. The mathematical role of finite rotations in both continuum mechanics and multi rigid-body dynamics has presented in the latter paper. More recently, a new framework of minimal parameterizations of the rotation matrix was proposed by Bauchau and Trainelli (2003).

According to the polar decomposition theorem, the deformation gradient $F$ is equal to $RU$ and also $VR$, in which $R$ is the rotation tensor and $U$ and $V$ are the material stretch tensors. Utilizing $R$, many authors have put much emphases on a particular reference frame or configuration on which $R = I_3$, $I_3$ being the third order identity tensor. The reference configuration is indeed the pull-back of the current configuration under $R$. By such a rotation-free configuration/co-rotated frame, Green and Naghdi (1965) have defined the rotated stress tensor as the pull-back of the Cauchy stress tensor under $R$ and many constitutive equations are then established on such a rotation-free configuration. For example, based on this frame, Green and McInnis (1967) generalized the concept of hypoelasticity, and Simo and Marsden (1984) formulated the constitutive equations of
both hyper- and hypo-elasticity. All the aforementioned works have the same goal of removing the complexity induced by the rigid-body rotation in the formulation of large deformation problem. However, contemplating the relation \( W = \dot{R}R^T + R(\dot{U}U^{-1} + U^{-1}\dot{U})R^T/2 \) (the so-called spin tensor), we realize that the spin due to the material stretching \( (\dot{U}U^{-1} - U^{-1}\dot{U})/2 \) still exists even if the rigid-body rotation has been gotten rid of.

Besides, more definitions about the spin tensor different from the above one are seen in the literature. Diens (1979), Dafalias (1983), Lee, Mallett and Wertheimer (1983), Paulun and Pecherski (1985), Sowerby and Chu (1985) and Xiao, Bruhns and Meyers (1997) have replaced the previous \( \dot{W} \) by some other \( \dot{\overline{W}} \) and suggested a modified Jaumann stress rate to eliminate the oscillatory stress in the simple shear problem; see Liu and Hong (1999) for a further discussion. The effects of different objective stress rates on the plasticity equations have been discussed by Liu and Hong (2001) and Liu (2004). However, the purpose of searching for a suitable spin tensor by these authors, in a word, is to find a reference configuration with zero spin throughout the whole motion such that the constitutive equation for a rate-type material under large deformation can be objectively integrated.

By the principle of material frame-indifference, many constitutive laws require for a reference purpose the rotation-free configuration where the rotation tensor equals identity. Nevertheless, a reference configuration with zero spin throughout the whole motion history might be more relevant for a rate-type material under large deformation to be properly described by an objective constitutive equation. To characterize this spin-free reference configuration/co-rotational frame, an orthogonal transformation tensor \( Q \) is connecting the spin-free and the fixed configurations due to the non-zero spin tensor denoted by \( W \), such that the tensorial differential equation

\[
\dot{Q} = WQ
\]

is necessary. It does not lose any generality to assume that the initial condition of \( Q \) is identity, i.e., \( Q(0) = I_3 \). Throughout this paper, a superimposed dot denotes the differential with respect to the current time \( t \). Computational techniques were proposed by Hughes and Winget (1980), Rubinstein and Atluri (1983) and Flanagan and Taylor (1987) for integrating Eq. (1), which require a constant rate of rotation for each finite time step.

On the other hand, special attention has also been paid on the finite rotation effect in the structural mechanics of flexible bodies, including beam, plate, shell, etc. Atluri (1984) has considered finite rotations as direct independent variables in the variational formulations of finitely deformed continua and shells. Han, Rajendran and Atluri (2005) have formulated an effective MLPG approach for solving the nonlinear structural problems of beam with large deformation and rotation. They have shown that the MLPG is more effective than the FEM.

A recent progress to dealing with the finite rotations in beams, plates and shells was also summarized in a special issue of CMES. Lin and Hsiao (2003) have solved the buckling problems of 3-D beams by using the co-rotational formulation. Gotou, Kuwataka, Nishihara and Iwakuma (2003) have introduced the rotational angles associated with the Cartesian coordinates as additional degrees of freedom, where the Euler’s angles are used to describe finite rotations. The accuracy of the co-rotational formulation for 3-D Timoshenko’s beam is discussed from a theoretical viewpoint by Iura, Suetake and Atluri (2003). Beda (2003) introduced three rotation angles and solved the elastica problem of spatial Euler-Bernoulli beam. Suetake, Iura and Atluri (2003) have derived a symmetric tangent stiffness operator for thick shells undergoing finite rotation. Basar and Kintzel (2003) have developed a finite element model for finite rotation and large strain thin-walled shells. From those papers one can understand that the finite rotations are important in the mechanical analysis of flexible body. Equally, for the rigid multibody dynamics the finite rotations are also important as shown by Rochinha and Sampaio (2000) and Huston and Liu (2005).

To describe finite rotation, it should be noted that the history of \( Q \) can be represented by the histories of three Euler’s angles \( \delta, \zeta \) and \( \eta \) as follows (Goldstein, 1980):

\[
Q = \begin{pmatrix}
\cos \psi \cos \phi - \cos \theta \sin \phi \sin \psi \\
- \sin \psi \cos \phi - \cos \theta \sin \phi \cos \psi \\
\sin \theta \sin \phi
\end{pmatrix}
\begin{pmatrix}
\cos \psi \sin \phi + \cos \theta \cos \phi \sin \psi \\
- \sin \psi \sin \phi + \cos \theta \cos \phi \cos \psi \\
- \sin \theta \cos \phi
\end{pmatrix},
\]

and the corresponding differential equations are

\[
\omega_1 = \dot{\theta} \cos \phi + \dot{\psi} \sin \theta \sin \phi,
\]
\[ \omega_2 = \dot{\Theta} \sin \phi - \Psi \sin \theta \cos \phi, \]  

\[ \omega_3 = \dot{\phi} + \Psi \cos \theta. \]  

Supposing that the angular velocities \( \omega_1, \omega_2 \) and \( \omega_3 \) are given, the above nonlinear equations with assumed zero initial values need be integrated by a time-stepping technique.

By searching an effective representation of the rotation matrix has led to the development of numerous techniques in the last several decades, and reviewing the properties, advantages and shortcomings of these parameterization techniques can be found in the papers by Ibrahimbegovic (1997), Borri, Trainelli and Bottasso (2000), and Bauchau and Trainelli (2003). For the three-dimensional rotation the minimal number of parameters is three as the Euler parameters, the Rodrigues and modified Rodrigues parameters are. However, these representations contain singularities, and their governing equations are nonlinear in nature. The procedures for finding the solutions of rotation matrix involving such nonlinear systems are usually not so easy.

The remaining sections of this paper are arranged as follows. For a motivation of the present study we mention of the quaternionic representations in Section 2. In Section 3 we point out that the quaternionic representations are undertaken in a larger six-dimensional Lie algebra space \( so(4) \). In Section 4 we propose a novel decomposition of the rotation matrix \( Q = FQ_1 \), where \( F \) can be obtained exactly and \( Q_1 \) is amenable to a simpler treatment than \( Q \). In Section 5 we consider a projective realization of \( Q_1 \), the Lie algebra of which is just \( so(3) \) with dimensions much smaller than \( so(4) \). In order to give a more effective numerical computation of \( Q_1 \), we develop a fully new representation in terms of nilpotent differential equations system in Section 6. In Section 7 we consider the computations of \( Q \) and compare the performances of different numerical methods discussed in this paper through numerical examples in Section 8. Finally, we conclude some results in Section 9.

## 2 Quaternionic representations

For a comparison purpose let us mention other representations of the rotation matrix in this section. It is known that the spatial orientation \( Q \in SO(3) \) of rigid body can be expressed in terms of unit quaternion (Rochinha and Sampaio, 2000; San Miguel, 2003):

\[
\dot{Q} = \left( \begin{array}{ccc}
q_0^2 + q_1^2 - q_2^2 - q_3^2 & 2(q_1q_2 + q_0q_3) & 2(q_1q_3 - q_0q_2) \\
2(q_1q_2 - q_0q_3) & q_0^2 - q_1^2 + q_2^2 - q_3^2 & 2(q_2q_3 + q_0q_1) \\
2(q_1q_3 + q_0q_2) & 2(q_2q_3 - q_0q_1) & q_0^2 - q_1^2 - q_2^2 + q_3^2
\end{array} \right).
\]

These parameters are obtained by using the stereographic projection of

\[
S^3 := \{ q = (q, q_0) \in \mathbb{R}^4 | \|q\|^2 + q_0^2 = 1 \}
\]

onto \( \mathbb{R}^3 \) by a two-fold covering; see, e.g., Goldstein (1980). In above we use \( \|q\| \) to denote the Euclidean norm of \( q \in \mathbb{R}^3 \). Corresponding to Eq. (1) the governing equation of \( \dot{Q} \) is

\[
\dot{Q} = \bar{Q} \bar{W},
\]

where \( \bar{W}_{ij} = \varepsilon_{ijk} \omega_k \) is the transpose of \( W_{ij} = \varepsilon_{ijk} \omega_k \). The above \( \varepsilon_{ijk} \) is a three-dimensional permutation symbol. Consequently, one has \( \bar{Q} = Q^T \).

In terms of the unit quaternion the governing Eq. (8) can be written as

\[
\frac{d}{dt} \left( \begin{array}{c}
q \\
q_0
\end{array} \right) = \frac{1}{2} \left( \begin{array}{cc}
-\bar{W} & \omega \\
-\omega^T & 0
\end{array} \right) \left( \begin{array}{c}
q \\
q_0
\end{array} \right),
\]

where \( \omega = (\omega_1, \omega_2, \omega_3)^T \) is the vector of angular velocity. In terms of \( (q, q_0) \), Liu (2002) has considered the following homogeneous coordinates:

\[
s := \frac{q}{q_0}
\]

known as the Rodrigues parameters, and from Eq. (9) one can obtain the following differential equation:

\[
\dot{s} = \frac{1}{2} \omega - \frac{1}{2} \bar{W} s + \frac{1}{2} (\omega \cdot s) s.
\]

From Eqs. (10) and (7) one has

\[
q_0 = \frac{1}{\sqrt{1 + \|s\|^2}}.
\]
The rotation matrix in terms of $s$ is read as (Schaub, Tsio-
tras and Junkins, 1995)

$$
\mathbf{Q} = \frac{1}{1 + \|\mathbf{s}\|^2} \begin{pmatrix}
1 + s_2^2 - s_3^2 - s_1^2 & 2(s_1 s_2 + s_3) \\
2(s_1 s_2 - s_3) & 1 - s_1^2 + s_2^2 - s_3^2 \\
2(s_1 s_3 + s_2) & 2(s_2 s_3 - s_1)
\end{pmatrix}.
$$

(13)

On the other hand, Marandi and Modi (1987) have intro-
duced the modified Rodrigues parameters

$$
\mathbf{S} := \frac{\mathbf{q}}{1 + q_0}.
$$

(14)

The parameters $\mathbf{S} = (S_1, S_2, S_3)^T$ are well defined for ev-
every rotation through the angle $\phi \in [0, 2\pi)$, in contrast to the ordinary Rodrigues parameters which are defined
only for the rotation through the angle $\phi \in [0, \pi)$.

From Eqs. (14) and (7) it follows that

$$
q_0 = \frac{1 - \|\mathbf{S}\|^2}{1 + \|\mathbf{S}\|^2}.
$$

(15)

Now, taking the time differential of Eq. (14), then using
Eqs. (9) and (15) and through some arrangements we ob-
tain

$$
\dot{\mathbf{S}} = \frac{1}{4}(1 - \|\mathbf{S}\|^2)\mathbf{\omega} - \frac{1}{2}\mathbf{W}\mathbf{S} + \frac{1}{2}(\mathbf{\omega} \cdot \mathbf{S})\mathbf{S}.
$$

(16)

The rotation matrix in terms of $\mathbf{S}$ is read as (Schaub and
Junkins, 1996; Schaub, Tsiotras and Junkins, 1995)

$$
\dot{\mathbf{Q}} = \frac{1}{(1 + \|\mathbf{S}\|^2)^2} \begin{pmatrix}
4(S_2^2 - S_3^2 - S_1^2) + S^2 & 8S_1S_2 - 4S_3S \\
8S_1S_2 - 4S_3S & 8S_1S_3 + 4S_2S \\
8S_1S_2 + 4S_3S & 8S_1S_3 - 4S_2S \\
4(-S_1^2 + S_2^2 - S_3^2) + S^2 & 8S_2S_3 + 4S_1S \\
8S_2S_3 - 4S_1S & 4(-S_1^2 - S_2^2 + S_3^2) + S^2
\end{pmatrix},
$$

where

$$
\mathbf{S} := 1 - \|\mathbf{S}\|^2.
$$

(17)

It has a higher degree of nonlinearity than the corre-
sponding matrix in terms of the Rodrigues parameters. Even though, the modified Rodrigues parameters are
used frequently in the attitude control theory for their
singularity-free interval is larger than that of the Ro-
drigues parameters; see, e.g., Akella (2001), Akella, Hal-
bert and Kotamraju (2003), and El-Gohary (2005).

Both the singularities of $\mathbf{s}$ and $\mathbf{S}$ occur at infinity, i.e.,
$\|\mathbf{s}\| = \infty$ and $\|\mathbf{S}\| = \infty$, which correspond respectively to $q_0 = 0$ and $q_0 = -1$. Conversely, when $q_0 = 0$ the $\mathbf{s}$
defined by Eq. (10) is infinite, since $\mathbf{q} \neq 0$ in view of the constraint in Eq. (7). That is, the singularity of $\mathbf{s}$ is of
the form finite/0. But, when $q_0 = -1$ the $\mathbf{S}$ defined by
Eq. (14) is of the form $\mathbf{0}/0$, since it is also $\mathbf{q} = \mathbf{0}$ when
$q_0 = -1$ in view of the constraint in Eq. (7). This is the
reason that the singularity-free interval of $\mathbf{S}$ is larger
than that of $\mathbf{s}$.

3 A Lie algebra study

In order to give a Lie algebra aspect of Eqs. (11) and (16),
we write them with the following componential forms:

$$
\dot{s}_i = -\frac{1}{2}\hat{W}_{ij}s_j + \frac{1}{2}[\delta_{ij} + s_is_j]\omega_j,
$$

(18)

$$
\dot{s}_j = -\frac{1}{2}\hat{W}_{ij}s_j + \frac{1}{2}[\delta_{ij} + s_is_j]\omega_j - \frac{1}{4}[1 + \|\mathbf{S}\|^2]d_{ij}\omega_j,
$$

(19)

where $\delta_{ij}$ is the Kronecker delta symbol. These equations
can be viewed as the affine nonlinear systems with $\omega_j$
and $\hat{W}_{ij}$ as inputs and $s_j$ or $S_j$ as outputs, which means
that the above equations are linear in both $\omega_j$ and $\hat{W}_{ij}$
but nonlinear in $s_j$ or $S_j$ (Isidori, 1989).

For the nonlinear dynamical system:

$$
\frac{dx^\mu(t)}{dt} = \eta^\mu(x^1, \ldots, x^n, t), \quad 1 \leq \mu \leq n,
$$

(20)

if the general solution $x(t) = (x^1(t), \ldots, x^n(t))^T$
can be expressed as a function of $m$ particular solutions
$x^1(t), \ldots, x^m(t)$ and $n$ integration constants $c_1, \ldots, c_n$
such that

$$
x(t) = F(x^1, \ldots, x^n, c_1, \ldots, c_n),
$$

(21)

then Eq. (20) is said to admit a superposition principle;
see, e.g. Hong and Liu (1997) and Cariñena, Grabowski

Lie has proved that Eq. (20) admits a superposition prin-
ciple iff it can be written as

$$
\frac{dx}{dt} = \sum_{i=1}^{s} Z_i(t)\xi_i(x),
$$

(22)
and its vector fields

\[ Y_i = \xi^\mu_i(x) \frac{\partial}{\partial x^\mu}, \quad i = 1, \ldots, s, \quad (23) \]

constitute a finite-dimensional Lie algebra, the dimension \( r \) of which satisfies \( s \leq r \leq mn \).

The three vector fields of Eq. (18) corresponding to the three inputs of \( \omega_j/2, \ j = 1, 2, 3 \) are

\[ g_j = \delta_{ij}e_i + s_j s_j e_i, \quad 1 \leq j \leq 3, \quad (24) \]

where \( e_i, i = 1, 2, 3 \) are unit bases. The vector forms of \( g_j, j = 1, 2, 3 \) are

\[ g_1 = \begin{pmatrix} 1 + s_1^2 \\ s_1 s_2 \\ s_1 s_3 \end{pmatrix}, \quad g_2 = \begin{pmatrix} s_1 s_2 \\ 1 + s_2^2 \\ s_2 s_3 \end{pmatrix}, \quad g_3 = \begin{pmatrix} s_1 s_3 \\ s_2 s_3 \\ 1 + s_3^2 \end{pmatrix}. \quad (25) \]

Similarly, the three vector fields generated from \( \tilde{W}_{23}/2 = \omega_1/2, -\tilde{W}_{13}/2 = \omega_2/2 \) and \( \tilde{W}_{12}/2 = \omega_3/2 \) are

\[ w_k = \varepsilon_{kij}s_j e_i, \quad 1 \leq k \leq 3, \quad (26) \]

or in terms of the vector forms:

\[ w_1 = \begin{pmatrix} 0 \\ s_3 \\ -s_2 \end{pmatrix}, \quad w_2 = \begin{pmatrix} -s_3 \\ 0 \\ s_1 \end{pmatrix}, \quad w_3 = \begin{pmatrix} -s_1 \\ 0 \\ s_2 \end{pmatrix}. \quad (27) \]

The Lie bracket of \( g_\alpha \) and \( g_\beta \) is

\[ [g_\alpha, g_\beta] = \frac{\partial g_\beta}{\partial s} g_\alpha - \frac{\partial g_\alpha}{\partial s} g_\beta. \quad (28) \]

From Eqs. (24) and (26) it follows that

\[ \frac{\partial g^i_\alpha}{\partial s^j} = s_j \delta_{\alpha j} + s_\alpha \delta_{ij}, \quad (29) \]

\[ \frac{\partial w^i_k}{\partial s^j} = \varepsilon_{kij}, \quad (30) \]

where \( g^i_\alpha \) is the \( i \)th component of \( g_\alpha \), and \( w^i_k \) is the \( i \)th component of \( w_k \).

By using the above equations we can prove that

\[ [g_\alpha, g_\beta] = s_\beta g_\alpha - s_\alpha g_\beta. \quad (31) \]

Inserting Eq. (24) for \( g \), the above right-hand side can be further reduced to

\[ s_\beta g_\alpha - s_\alpha g_\beta = -s_j (\delta_{j \alpha} \delta_{\beta k} - \delta_{j \beta} \delta_{\alpha k}) e_i. \quad (32) \]

Reminding that

\[ \varepsilon_{kij} \varepsilon_{k_{\beta \alpha}} = \delta_{j \alpha} \delta_{\beta k} - \delta_{j \beta} \delta_{\alpha k}, \quad (33) \]

and from Eqs. (31) and (32) we have

\[ [g_\alpha, g_\beta] = -\varepsilon_{k_{\beta \alpha}} \varepsilon_{k_{ij}} s_j e_i. \quad (34) \]

From Eqs. (34) and (26) it follows that

\[ [w_k, g_\alpha] = \varepsilon_{kaj} g_\beta. \quad (35) \]

Furthermore, by Eqs. (29), (30), (24) and (26) through some calculations we find that

\[ [w_k, w_j] = \varepsilon_{jim} w^m_k e_i - \varepsilon_{kim} w^m_j e_i = \varepsilon_{kij} w_l. \quad (37) \]

Therefore, the three vector fields in Eq. (25) and the three vector fields in Eq. (27) constitute a finite-dimensional Lie algebra, which is indeed the algebra \( so(4) \) of the 4-dimensional proper rotation group \( SO(4) \) with dimensions six.

Dividing both the denominator and the nominator on the right-hand side of Eq. (14) by \( q_0 \), and inserting Eq. (10) for \( q/(q_0) \) and Eq. (12) for \( q_0 \) we obtain

\[ S := \frac{s}{1 + \sqrt{1 + ||s||^2}}. \quad (38) \]

Conversely, dividing both the denominator and the nominator on the right-hand side of Eq. (10) by \( 1 + q_0 \), and inserting Eq. (14) for \( q/(1 + q_0) \) and Eq. (15) for \( q_0 \) we obtain

\[ S := \frac{2S}{1 - ||S||^2}. \quad (39) \]

These two equations give relations between the modified and unmodified Rodrigues parameters. Substituting the above equation into Eq. (11) we can obtain Eq. (16). By the same token, substituting Eq. (38) into Eq. (16) we can obtain Eq. (11). Similarly, the vector fields of Eq. (19) constitute a six-dimensional Lie algebra.
Euler’s equations (3)-(5) as well as the kinematic equations (11) and (16) in terms of Rodrigues and modified Rodrigues kinematics are nonlinear. Procedures for finding solutions of these problems involving nonlinear systems are usually complicated. In contrast, our approach below is to find a differential equations system through the projective transformation, the result of which is a parametric representation of the rotation group in terms of two scalar variables with the singularity-free interval being largely extended.

4 A decomposition of $Q$

To commence with the derivations of our results we denote the spin matrix by

$$W = \begin{pmatrix} 0 & -\omega_3 & \omega_2 \\ \omega_3 & 0 & -\omega_1 \\ -\omega_2 & \omega_1 & 0 \end{pmatrix},$$

(40)

and the corresponding angular velocity vector by

$$\omega = (\omega_1, \omega_2, \omega_3)^T$$

(41)

with a magnitude

$$\|\omega\| := (\omega_1^2 + \omega_2^2 + \omega_3^2)^{\frac{1}{2}}.$$  

(42)

Also the instantaneous spin axis in the three-dimensional space is denoted by

$$(\eta_1, \eta_2, \eta_3)^T := \frac{1}{\|\omega\|} (\omega_1, \omega_2, \omega_3)^T.$$  

(43)

When the spin axis is fixed, it can be defined as a two-dimensional spin since the rotation only occurs on the plane perpendicular to this fixed axis. While the spin axis changes with time, it is defined as a three-dimensional spin.

In what follows, we present a novel calculus to explore an analytical decomposition of $Q$. Since $Q$ is orthogonal, it belongs to the special orthogonal group with dimensions three, i.e., $Q \in SO(3)$. Therefore, although Eq. (1) can be divided into nine simultaneous ODEs, only three of them are independent. In the differential geometry, $Q$, an element of $SO(3)$, represents a certain three-dimensional algebraic surface in a real space of nine dimensions. It is unwise to find the analytical solution of Eq. (1) by solving these simultaneous ODEs.

To the later derivations, let us define a matrix operator $F$ which applies to $W$ and results in the following Rodrigues form:

$$F(W) := I_3 + \frac{\sin \phi}{\|\omega\|} W + \left(1 - \cos \phi \right) W^2,$$

(44)

where

$$\phi := \int_0^t \|\omega(\tau)\|d\tau.$$  

(45)

Recalling Eq. (40), we define the following two-dimensional spin matrix

$$W_1 = \begin{pmatrix} 0 & 0 & 0 \\ 0 & 0 & -\omega_1 \\ 0 & \omega_1 & 0 \end{pmatrix},$$

(46)

from which we have

$$F(W_1) = \begin{pmatrix} 1 & 0 & 0 \\ 0 & \cos \overline{\omega}_1 & -\sin \overline{\omega}_1 \\ 0 & \sin \overline{\omega}_1 & \cos \overline{\omega}_1 \end{pmatrix},$$

(47)

where

$$\overline{\omega}_1(t) := \int_0^t \omega_1(\tau)d\tau.$$  

(48)

It is cunning to presume that $Q$ can be decomposed to

$$Q = F(W_1)Q_1,$$

(49)

with $Q_1$ an unknown matrix belonging to $SO(3)$. Substituting it into Eq. (1) leads to

$$\dot{Q}_1 = AQ_1, \quad Q_1(0) = I_3,$$

(50)

where

$$A := F(W_1)^T[WF(W_1) - F(W_1)] = \begin{pmatrix} 0 & -\dot{u}_1 & -\dot{u}_2 \\ \dot{u}_1 & 0 & 0 \\ \dot{u}_2 & 0 & 0 \end{pmatrix}$$

(51)

is skew-symmetric with

$$\dot{u}_1 := \omega_3 \cos \overline{\omega}_1 - \omega_2 \sin \overline{\omega}_1,$$

(52)

$$\dot{u}_2 := -\omega_2 \cos \overline{\omega}_1 - \omega_3 \sin \overline{\omega}_1.$$  

(53)
Tsiontiras and Longuski (1995) have developed a superficially similar decomposition to Eq. (49), and called it the two perpendicular rotations.

The decomposition made in Eq. (49) leads to a simpler spin matrix for Q₁ in Eq. (51) with only two independent inputs ῦ₁ and ῦ₂. For a given angular velocity (ω₁(τ), ω₂(τ), ω₃(τ)), it is easy to find the matrix F by Eq. (47). However, in order to obtain Q we still require an effort to find Q₁. In this paper, some mathematical procedures will be developed to solve this problem for arbitrary inputs ῦ₁ and ῦ₂.

5 A projective transformation

The system of equations generated by A in Eq. (51) can be written as

$$\dot{X} = AX,$$  \hspace{1cm} (54)

where

$$X := \left( \begin{array}{c} X_0 \\ X_1 \\ X_2 \end{array} \right) = \left( \begin{array}{c} X_0 \\ X_1 \\ X_2 \end{array} \right).$$  \hspace{1cm} (55)

The initial values of X₀, X₁ and X₂ are assumed to be X₀(0), X₁(0) and X₂(0), respectively. So the determination of Q₁(t) is now equivalent to searching a general solution of Eq. (54), i.e.,

$$X(t) = Q₁(t)X(0).$$  \hspace{1cm} (56)

How to obtain Q₁(t) from X(t) will be presented in Section 7.

Let

$$x₁ := \frac{X₁}{X₀}, \quad x₂ := \frac{X₂}{X₀}$$  \hspace{1cm} (57)

be the homogeneous coordinates for \( \mathbb{R}^3 \). Then, the use of Eq. (54) implies

$$\frac{\dot{X₀}}{X₀} = -x \cdot \dot{u},$$

$$\frac{d}{dt}(X₀x) = X₀\dot{u},$$

where

$$x := \left( \begin{array}{c} x₁ \\ x₂ \end{array} \right), \quad \dot{u} := \left( \begin{array}{c} \dot{u₁} \\ \dot{u₂} \end{array} \right)$$

are, respectively, the output and input of Eqs. (58) and (59). By integrating Eq. (59) from 0 to t we obtain

$$x(t) = X₀(0)x(0) + \int₀ᵗ \frac{X₀(τ)}{X₀(t)}\dot{u}(τ)dτ,$$  \hspace{1cm} (61)

and substituting it for x(t) into Eq. (58) we obtain

$$\dot{X₀}(t) = -X₀(0)x(0) \cdot \dot{u}(τ) - \int₀ᵗ \dot{u}(τ) \cdot \dot{u}(τ)X₀(τ)dτ.$$  \hspace{1cm} (62)

The inner product of Eq. (59) with x and the use of Eq. (58) render

$$x \cdot \dot{x} = -\frac{\dot{X₀}}{X₀}(\|x\|^2 + 1).$$  \hspace{1cm} (63)

Integrating Eq. (63) leads to

$$\|x(t)\|^2 = \frac{\|X₀(0)\|^2}{X₀(t)} - 1,$$  \hspace{1cm} (64)

where \( \|x(0)\|^2 = (X₁²(0) + X₂²(0))/X₀²(0) \) was considered. By using Eq. (57), Eq. (64) is equivalent to \( \|X(t)\| = \|X(0)\| \), i.e., the length of the vector X is preserved under the action of the group of SO(3). Obviously, X(0) cannot equal zero; otherwise, X(t) will be zero.

By eliminating X₀, Eqs. (58) and (59) can be combined into a single nonlinear differential equations system for x:

$$x - (\dot{u} \cdot x)x = \dot{u}.$$  \hspace{1cm} (65)

The transformation made in this section sends each three-dimensional vector \((X₀,X₁,X₂) transport it into a two-dimensional vector \((x₁,x₂)\) in the topological space \( \mathbb{R}P^3 \), which is correlated intimately with the two independent inputs of \( \dot{u} \), and leads to the following feasible formulae:

$$X₀(t) = \frac{\|X(0)\|}{\sqrt{1 + \|x(t)\|^2}},$$  \hspace{1cm} (66)

$$X₁(t) = X₀(t)x₁(t) = \frac{x₁(t)\|X(0)\|}{\sqrt{1 + \|x(t)\|^2}},$$  \hspace{1cm} (67)

$$X₂(t) = X₀(t)x₂(t) = \frac{x₂(t)\|X(0)\|}{\sqrt{1 + \|x(t)\|^2}}.$$  \hspace{1cm} (68)
The first equation is obtained from Eq. (64), while the other two are the direct results of definition and Eq. (66).

As that done for Eq. (11), the Lie algebra for Eq. (65) can be proved to be \( so(3) \). Even the variables \((x_1, x_2)\) used in this formulation are minimal with numbers two only, it still has a singularity at \( X_0 = 0 \), i.e., \( \|x\| = \infty \).

Eqs. (66)-(68) indeed provide a minimal representation of the rotation matrix, which preserve the length \( \|X(t)\| = \|X(0)\| \), and the resulting transformation is an element of the group \( SO(3) \).

6 The nilpotent form of rotation matrix

6.1 The Peano-Baker formula

\( Q_1(t) \) is a fundamental solution matrix of system (54). Let

\[
\Phi(t, t_0) := Q_1(t)Q_1^{-1}(t_0) \tag{69}
\]

be the state transition matrix (Rugh, 1993). In general, it may not be possible to derive a closed-form expression of \( \Phi(t, t_0) \) associated with arbitrary matrix \( A(t) \). For the time-varying case, we usually use a power series expansion, called the Peano-Baker formula (Rugh, 1993), to express \( \Phi(t, t_0) \) by

\[
\Phi(t, t_0) = I_3 + \int_{t_0}^{t} A(\tau_1) d\tau_1 + \int_{t_0}^{t} \int_{t_0}^{\tau_1} A(\tau_1)A(\tau_2) d\tau_2 d\tau_1 + \cdots
\]

\[
+ \int_{t_0}^{t} \int_{t_0}^{\tau_1} \cdots \int_{t_0}^{\tau_{n-1}} A(\tau_1)A(\tau_2)\cdots A(\tau_n) d\tau_n \cdots d\tau_2 d\tau_1 + \cdots \tag{70}
\]

As observed by Hausdorff (1906), Eq. (50) can be translated to a differential equation of the underlying algebra \( \sigma(t) \in so(3) \) with

\[
\sigma(t) = \sum_{k=0}^{\infty} \frac{B_k}{k!} \text{ad}_x^k A(t), \quad \sigma(0) = 0_3, \tag{71}
\]

where \( B_k \) are the Bernoulli numbers, and the adjoint operator \( \text{ad}_x y \) with \( x, y \in so(3) \) is defined by an iterated commutation (Isidori, 1989),

\[
\text{ad}_x y = y, \quad \text{ad}_x^k y = [x, \text{ad}_x^{k-1} y], \quad k \in \mathbb{N}. \tag{72}
\]

Here, \([x, y] = xy - yx\) denotes the Lie commutator.

Magnus (1954) showed that

\[
\sigma(t) = \int_{0}^{t} \int_{0}^{\tau_1} A(\tau_1) d\tau_1 + \frac{1}{2} \int_{0}^{t} \int_{0}^{\tau_1} [A(\tau_1), A(\tau_2)] d\tau_2 d\tau_1
\]

\[
+ \frac{1}{4} \int_{0}^{t} \int_{0}^{\tau_1} \int_{0}^{\tau_2} [[A(\tau_3), A(\tau_2)], A(\tau_1)] d\tau_3 d\tau_2 d\tau_1
\]

\[
+ \frac{1}{12} \int_{0}^{t} \int_{0}^{\tau_1} \int_{0}^{\tau_2} \int_{0}^{\tau_3} [[A(\tau_4), [A(\tau_3), A(\tau_2)]], A(\tau_1)] d\tau_4 d\tau_3 d\tau_2 d\tau_1
\]

\[
+ \cdots, \tag{73}
\]

and proved that \( Q_1(t) = \exp \sigma(t) \) is a solution of Eq. (50).

6.2 The main results

No matter which formula, Eq. (70) or Eq. (73), is used to calculate the state transition matrix, we need to calculate many multivariate integrals of the matrix functions and the infinite sums. Especially, the latter further requires to calculate a large number of commutators and a single exponential of a matrix function with complicated argument. Here we propose a new method to transform the time-varying linear system (54) to an index two nilpotent time-varying linear system:

\[
\dot{Y}(t) = N(t)Y(t), \quad N^2(t) = 0.
\]

Due to this good nilpotent property of \( N(t) \), it is believed that the new system is more effective to develop numerical method than the original system (54).

For this purpose let us rewrite Eqs. (61) and (62) to be

\[
X_s(t) = X_s(0) + \int_{0}^{t} X_0(\tau) \dot{u}(\tau) d\tau, \tag{74}
\]

\[
\dot{X}_0(t) = -X_s(0) \cdot \dot{u}(t) - \int_{0}^{\tau} \dot{u}(\tau) X_0(\tau) d\tau, \tag{75}
\]

where \( X_0(t)X(t) \) was replaced by \( X_s(t) \).

The main results are given below.

Theorem 1. Corresponding to the linear system (54) with \( A \) satisfying

\[
A^T + A = 0, \tag{76}
\]

there exists a linear system

\[
\dot{Y}(t) = N(t)Y(t), \tag{77}
\]
where \( N \) is a zero trace nilpotent matrix function, satisfying
\[
\text{tr} N = 0, \quad N^2 = 0.
\]

**Proof.** Integrating Eq. (75) we obtain
\[
X_0(t) = X_0(0) - v^T(t)X_s(0) - \int_0^t [v^T(t) - v^T(\xi)]\dot{u}(\xi)X_0(\xi)d\xi,
\]
where \( v(t) = u(t) - u(0) \).

Left multiplying Eq. (79) by \( (v^T \dot{u}^T)^T \) we obtain a three-dimensional vectorial integral equation:
\[
\begin{pmatrix} v^T \dot{u} & u^T \end{pmatrix} X_0 =
\begin{pmatrix} v^T \dot{u} & u^T \end{pmatrix} \int_0^t \begin{pmatrix} 1 & -v^T(t) \end{pmatrix} \begin{pmatrix} v^T(\xi)\dot{u}(\xi) \\ u^T(\xi) \end{pmatrix} X_0(\xi)d\xi
+ \begin{pmatrix} v^T \dot{u}[X_0(0) - v^T X_s(0)] \\ uX_0(0) - \dot{u}v^T X_s(0) \end{pmatrix}.
\]

Upon introducing
\[
N := \begin{pmatrix} v^T \dot{u} & u^T \end{pmatrix} \begin{pmatrix} 1 & -v^T \end{pmatrix},
\]

\[
\begin{pmatrix} Y_0(t) \\ Y_s(t) \end{pmatrix} := \int_0^t \begin{pmatrix} v^T(\xi)\dot{u}(\xi) \\ u^T(\xi) \end{pmatrix} X_0(\xi)d\xi + \begin{pmatrix} X_0(0) \\ X_s(0) \end{pmatrix},
\]

by means of Eq. (80) we obtain a linear equations system as that given by Eq. (77), where \( N \) can be proved to satisfy Eq. (78). \[\Box\]

From Eqs. (74), (82), (81) and (77) the relations between \( X \) and \( Y \) are obtained:
\[
\begin{pmatrix} X_0 \\ X_s \end{pmatrix} = \begin{pmatrix} 1 & -v^T \\ 0_{2 \times 1} & I_2 \end{pmatrix} \begin{pmatrix} Y_0 \\ Y_s \end{pmatrix},
\]

\[
\begin{pmatrix} Y_0 \\ Y_s \end{pmatrix} = \begin{pmatrix} 1 & v^T \\ 0_{2 \times 1} & I_2 \end{pmatrix} \begin{pmatrix} X_0 \\ X_s \end{pmatrix}.
\]

The above two equations render us easily to prove the following result.

**Theorem 2.** The \( N \) defined by Eq. (81) satisfies
\[
N^T \eta + \eta N = \begin{pmatrix} 0 & \dot{u}^T \\ u & -\dot{u}v^T + \dot{u}v^T \end{pmatrix},
\]

where
\[
\eta := \begin{pmatrix} 1 & -v^T \\ -v & I_2 + vv^T \end{pmatrix}
\]
is a positive definite matrix function. Moreover,
\[
N^T \eta + \eta N + \dot{\eta} = 0.
\]

**Proof.** Substituting Eq. (81) for \( N \) and Eq. (86) for \( \eta \) into the left-hand side of Eq. (85) and through some calculations we obtain the right-hand side of Eq. (85). For any nonzero \( Y = (Y_0, Y_s) \in \mathbb{R}^3 \) we have
\[
\begin{pmatrix} Y_0 \\ Y_s \end{pmatrix} = \begin{pmatrix} 1 & -v^T \\ -v & I_2 + vv^T \end{pmatrix} \begin{pmatrix} Y_0 \\ Y_s \end{pmatrix} = (v^T Y_s - Y_0)^2 + \|Y_s\|^2.
\]

Since the right-hand side is positive, by definition \( \eta \) is positive definite. Taking the time derivative of Eq. (86) and noting \( \dot{v} = \dot{u} \), then substituting the resultant into Eq. (87) which together Eq. (85) leads to Eq. (87). \[\Box\]

**Theorem 3.** The fundamental matrix \( Q_1 \) for Eq. (50) with \( A \) satisfying Eq. (76) has the following representation:
\[
Q_1 = \begin{pmatrix} 1 & -v^T \\ 0_{2 \times 1} & I_2 \end{pmatrix} K,
\]

where \( K \in SL(3, \mathbb{R}) \) is the fundamental matrix for Eq. (77), satisfying
\[
K = NK, \quad K(0) = I_3.
\]

\[
K^T \eta K = I_3.
\]

System (77) possesses the following first integral:
\[
Y^T \eta Y = Y^T(0) \eta(0) Y(0).
\]

**Proof.** With \( K \) satisfied Eq. (89), the solution of Eq. (77) can be expressed by
\[
Y(t) = K(t) Y(0).
\]
Substituting it into Eq. (83) and using \( \mathbf{Y}(0) = \mathbf{X}(0) \) we obtain
\[
\mathbf{X}(t) = \begin{pmatrix}
1 & -v^T \\
0_{2 \times 1} & \mathbf{I}_2
\end{pmatrix} \mathbf{K} \mathbf{X}(0),
\] (93)
which comparing with the solution of Eq. (54), \( \mathbf{X}(t) = \mathbf{Q}_1(t) \mathbf{X}(0) \) with \( \mathbf{Q}_1(t) \) satisfying Eq. (50), we obtain Eq. (88). Since \( \text{tr} \mathbf{N} = 0 \) as shown in Eq. (78), the property of \( \det \mathbf{K} = 1 \) follows from the Abel formula and \( \det \mathbf{K}(0) = 1 \). It indicates that \( \mathbf{K} \in SL(3, \mathbb{R}) \).

Substituting Eq. (88) for \( \mathbf{Q}_1 \) into the identity
\[
\mathbf{Q}_1^T \mathbf{Q}_1 = \mathbf{I}_3,
\] (94)
and noting that
\[
\begin{pmatrix}
1 & 0_{1 \times 2} \\
-v & \mathbf{I}_2
\end{pmatrix} \mathbf{I}_3 \begin{pmatrix}
1 & -v^T \\
0_{2 \times 1} & \mathbf{I}_2
\end{pmatrix} = \eta,
\] (95)
where \( \eta \) is given in Eq. (86), we can prove Eq. (90).

It is well known that \( \mathbf{X}^T \mathbf{X} \) is an invariant form of system (54) as discussed before. Substituting Eq. (83) for \( \mathbf{X} \) into \( \mathbf{X}^T \mathbf{X} \), we obtain an invariant form \( \mathbf{Y}^T \mathbf{Y} \) of system (77). Substituting Eq. (92) for \( \mathbf{Y} \) into the above quadratic form and using Eq. (90) and \( \eta(0) = \mathbf{I}_3 \) we can prove that \( \mathbf{Y}^T \eta \mathbf{Y} = \mathbf{Y}^T(0) \eta(0) \mathbf{Y}(0) \) is a first integral of system (77).

From the above we know that \( \eta \) is a noncanonical metric in the underlying space for \( \mathbf{Y} \) and \( \mathbf{I}_3 \) is a canonical metric in the underlying space for \( \mathbf{X} \). The two metrics are related through a similar transformation as shown in Eq. (95), both of which are positive definite. The matrix \( \mathbf{K} \) preserves the orthogonality under the metric \( \eta \) as shown by Eq. (90). Therefore, the mathematical role of \( \mathbf{K} \) is a noncanonical orthogonal matrix in the \( \eta \)-metric space. In Table 1 we compare the Lie groups, Lie algebras and other properties for these two systems \( \mathbf{X} \) and \( \mathbf{Y} \) about the rotations in the Euclidean space, as well as with Eqs. (9), (11), (16) and (65). The dimensions are referred to the numbers of the independent variables used in these equations, not to the dimensions of the Lie algebras.

6.3 Numerical methods

In this section, we first derive numerical methods for system (77) by utilizing the nilpotent matrix property. By means of the Peano-Baker formula the state transition matrix \( \mathbf{\Phi}(t, t_0) \) for system (77), which maps the state vector \( \mathbf{Y}(t_0) \) at time \( t_0 \) to the state vector \( \mathbf{Y}(t) \) at time \( t \), can be expressed as:
\[
\mathbf{\Phi}(t, t_0) = \mathbf{I}_3 + \int_{t_0}^{t} \mathbf{N}(\tau_1) d\tau_1 + \int_{t_0}^{t} \int_{\tau_0}^{\tau_1} \mathbf{N}(\tau_1) \mathbf{N}(\tau_2) d\tau_2 d\tau_1 + \cdots
\] (96)
For developing a numerical scheme we search a state transition matrix from state \( \mathbf{Y}_t \) at time \( t \) to state \( \mathbf{Y}_{t+1} \) at time \( t_{t+1} \) with \( \Delta t = t_{t+1} - t_t \) small enough. Upon letting \( t_0 \) be \( t_t \) and \( t \) to be \( t_{t+1} \) in the above integrals, then approximating of which by the trapezoidal rule and taking advantage of \( \mathbf{N}^2(t) = \mathbf{0} \) for all \( t \in \mathbb{R}^+ \), we obtain
\[
\mathbf{\Phi}(t_{t+1}, t_t) = \mathbf{I}_3 + \frac{\Delta t}{2} [\mathbf{N}(t_t) + \mathbf{N}(t_{t+1})] + \frac{(\Delta t)^2}{4} \mathbf{N}(t_{t+1})\mathbf{N}(t_t),
\] (97)
which being substituted into
\[
\mathbf{Y}_{t+1} = \mathbf{\Phi}(t_{t+1}, t_t) \mathbf{Y}_t,
\] (98)
results in a numerical scheme for system (77):
\[
\mathbf{Y}_{t+1} = \left( \mathbf{I}_3 + \frac{\Delta t}{2} [\mathbf{N}(t_t) + \mathbf{N}(t_{t+1})] + \frac{(\Delta t)^2}{4} \mathbf{N}(t_{t+1})\mathbf{N}(t_t) \right) \mathbf{Y}_t.
\] (99)
Then, by means of Eq. (83) we can calculate \( \mathbf{X} \) forward step-by-step.

It should be emphasized that the matrix resulting from the Peano-Baker formula is not equal to \( \exp \int_{t_0}^{t} \mathbf{N}(\tau)d\tau \), and is not guaranteed to be an element of \( SL(3, \mathbb{R}) \) even \( \mathbf{N} \) is an element of the Lie algebra \( sl(3, \mathbb{R}) \), i.e., \( \text{tr} \mathbf{N} = 0 \). In order to obtain this type numerical scheme which preserving \( SL(3, \mathbb{R}) \), let us return to system (77). The resulting \( \mathbf{N} \) makes us easily to derive the so-called group preserving scheme as follows:
\[
\mathbf{Y}_{t+1} = \exp[\Delta \mathbf{N}(\bar{t})] \mathbf{Y}_t = [\mathbf{I}_3 + \Delta \mathbf{N}(\bar{t})] \mathbf{Y}_t,
\] (100)
where \( \mathbf{N}(\bar{t}) = \mathbf{N}(t_t + \Delta t/2) \). The higher order terms disappear due to \( \mathbf{N}^k = \mathbf{0}, \ k \geq 2 \). Obviously, \( \mathbf{I}_3 + \Delta \mathbf{N}(\bar{t}) \in SL(3, \mathbb{R}) \).
7 The computation of $Q$

First, we calculate $Q_1$ by the method of Eq. (65). Select three independent set of the initial values of $X(0)$ with $X_0(0) \neq 0$, for example,

$$
\begin{pmatrix}
X_0^1(0) & X_0^2(0) & X_0^3(0) \\
X_1^1(0) & X_1^2(0) & X_1^3(0) \\
X_2^1(0) & X_2^2(0) & X_2^3(0)
\end{pmatrix}
= \begin{pmatrix}
1/\sqrt{3} & 1/\sqrt{2} & 1/\sqrt{6} \\
1/\sqrt{3} & -1/\sqrt{2} & 1/\sqrt{6} \\
1/\sqrt{6} & 0 & -2/\sqrt{6}
\end{pmatrix}.
$$

The corresponding solutions are denoted by

$$
\begin{pmatrix}
X_0^1(t) & X_0^2(t) & X_0^3(t) \\
X_1^1(t) & X_1^2(t) & X_1^3(t) \\
X_2^1(t) & X_2^2(t) & X_2^3(t)
\end{pmatrix},
$$

and from Eq. (56) we obtain

$$
Q_1(t) = \begin{pmatrix}
X_0^1(t) & X_0^2(t) & X_0^3(t) \\
X_1^1(t) & X_1^2(t) & X_1^3(t) \\
X_2^1(t) & X_2^2(t) & X_2^3(t)
\end{pmatrix} \\
\times \\
\begin{pmatrix}
1/\sqrt{3} & 1/\sqrt{3} & 1/\sqrt{3} \\
1/\sqrt{2} & -1/\sqrt{2} & 0 \\
1/\sqrt{6} & 1/\sqrt{6} & -2/\sqrt{6}
\end{pmatrix}.
$$

Then, inserting the above equation for $Q_1(t)$ and Eq. (47) for $F$ into Eq. (49) we obtain

$$
Q(t) = \begin{pmatrix}
1 & 0 & 0 \\
0 & \cos \omega_1 & -\sin \omega_1 \\
0 & \sin \omega_1 & \cos \omega_1
\end{pmatrix} \\
\times \\
\begin{pmatrix}
X_0^1(t) & X_0^2(t) & X_0^3(t) \\
X_1^1(t) & X_1^2(t) & X_1^3(t) \\
X_2^1(t) & X_2^2(t) & X_2^3(t)
\end{pmatrix} \\
\times \\
\begin{pmatrix}
1/\sqrt{3} & 1/\sqrt{3} & 1/\sqrt{3} \\
1/\sqrt{2} & -1/\sqrt{2} & 0 \\
1/\sqrt{6} & 1/\sqrt{6} & -2/\sqrt{6}
\end{pmatrix}.
$$

For other methods of Eqs. (99) and (100) we can suppose the simplest initial conditions with $(X_0^1(0), X_1^1(0), X_2^1(0)) = (1, 0, 0)$, $(X_0^2(0), X_1^2(0), X_2^2(0)) = (0, 1, 0)$ and $(X_0^3(0), X_1^3(0), X_2^3(0)) = (0, 0, 1)$. Therefore, the matrix function presented in Eq. (102) is just the matrix of $Q_1$ and $Q = FQ_1$ is obtained. If we use Eqs. (11) and (13) to calculate $Q = \hat{Q}^T$ we can select the initial condition of $s$ to be $(s_1(0), s_2(0), s_3(0)) = (0, 0, 0)$. Similarly, for Eqs. (16) and (17) we use $(s_1(0), s_2(0), s_3(0)) = (0, 0, 0)$. The integrations of these three nonlinear equations (11), (16) and (65) can be performed very well by the fourth-order Runge-Kutta method RK4.

8 Numerical tests

In order to give a criterion to assess our numerical methods we first derive a closed-form solution of $Q_1$ in the Appendix under the angular velocities $\omega_1 = \Omega - \omega$, $\omega_2 = -\sin \Omega t$ and $\omega_3 = \cos \Omega t$, where $\Omega$ and $\omega$ are angular frequencies parameters.

Then, for the purpose of comparison we also consider a naive approach to Eq. (54) by discretizing the state transition matrix given in Eq. (70) with a similar procedure as that for Eq. (97). Through some calculations we find that

$$
\Phi(t_{t+1}, t_t) = I_3 + \frac{\Delta t}{2} [A(t_t) + A(t_{t+1})] \\
+ \frac{\Delta t^2}{4} [A^2(t_{t+1}) + A(t_{t+1})A(t_t)] \\
+ \cdots + \left(\frac{\Delta t}{2}\right)^n [A^n(t_{t+1}) + A^{n-1}(t_{t+1})A(t_t)] \\
+ \cdots
$$

However, because $A$ is not a nilpotent matrix the higher order terms appear.

After given the closed-form solutions we compare our numerical results with them. In Fig. 1 we have employed different numerical methods as compared in Table 1 to calculate the rotation matrix $Q$, where $\omega = 2$, $\Omega = 3$ and a fixed time step of $\Delta t = 0.001$ sec were used. Because Eq. (65) has a singular point at $X_0 = 0$ we can only proceed the calculations to a final time $t_f = 0.5$ sec. The errors of the components of $Q$, called the componental errors, are obtained by taking the absolute of the differences between the numerical solutions with the closed-form solutions. The error of orthogonality is defined as $\|QQ^T - I_3\|$ with $Q$ calculated by the numerical methods. The componental errors are only plotted for the numerical methods based on Eqs. (65), (11) and (99), because the ones with Eq. (16) are closer to that of Eq. (11) and the ones with Eq. (100) are close to that of Eq. (99). However, the errors of orthogonality were plotted totally...
Figure 1: Comparing the componential errors and the errors of orthogonality for five types numerical methods within the range of small rotation.

Table 1: Comparisons of six formulations for rotations in the Euclidean space \( \mathbb{R}^3 \) (Dims. means Dimensions)

<table>
<thead>
<tr>
<th>Variables</th>
<th>Eqs.</th>
<th>Metrics</th>
<th>Lie Algebras</th>
<th>Lie Groups</th>
<th>Invariants</th>
<th>Dims.</th>
<th>Linearity</th>
<th>Singularity</th>
</tr>
</thead>
<tbody>
<tr>
<td>((q,q_0))</td>
<td>(9)</td>
<td>(I_4)</td>
<td>(so(4))</td>
<td>(SO(4))</td>
<td>(</td>
<td>q</td>
<td>^2 + q_0^2)</td>
<td>4</td>
</tr>
<tr>
<td>(s)</td>
<td>(11)</td>
<td>(I_3)</td>
<td>(so(4))</td>
<td>(SO(4))</td>
<td>(\times)</td>
<td>3</td>
<td>nonlinear</td>
<td>Yes</td>
</tr>
<tr>
<td>(S)</td>
<td>(16)</td>
<td>(I_3)</td>
<td>(so(4))</td>
<td>(SO(4))</td>
<td>(\times)</td>
<td>3</td>
<td>nonlinear</td>
<td>Yes</td>
</tr>
<tr>
<td>(x)</td>
<td>(65)</td>
<td>(\mathbb{R}P^3)</td>
<td>(so(3))</td>
<td>(SO(3))</td>
<td>(\times)</td>
<td>2</td>
<td>nonlinear</td>
<td>Yes</td>
</tr>
<tr>
<td>(X)</td>
<td>(54)</td>
<td>(I_3)</td>
<td>(so(3))</td>
<td>(SO(3))</td>
<td>(X^T I_3 X)</td>
<td>3</td>
<td>linear</td>
<td>No</td>
</tr>
<tr>
<td>(Y)</td>
<td>(77)</td>
<td>(\eta)</td>
<td>nilpotent</td>
<td>(SL(3, \mathbb{R}))</td>
<td>(Y^T \eta Y)</td>
<td>3</td>
<td>linear</td>
<td>No</td>
</tr>
</tbody>
</table>
The Computations of Large Rotation Through an Index Two Nilpotent Equation

Figure 2: Comparing the errors of orthogonality for four types numerical methods in the range of large rotation.

as shown in Fig. 1(j). It can be seen that the componential errors by Eqs. (65) and (11) are of the same order of $10^{-10}$ and that with Eq. (99) are in the order of $10^{-7}$. As expected, the errors of orthogonality by Eqs. (11) and (16) are almost zero, that of Eq. (65) is in the order of $10^{-9}$ and that of Eqs. (99) and (100) are in the order of $10^{-7}$.

The better accuracy of the numerical methods based on the three Eqs. (11), (16) and (65) are due to the high accuracy of RK4. We have employed RK4 to the quaternionic Eq. (9) and found that its errors no matter in the components or in the orthogonality increase rapidly to the order of $10^{-2}$. Obviously, RK4 cannot retain the invariant of Eq. (7), and thus leads to a larger error.

Now, let us turn to the case of large rotation in Figs. 2 and 3, where $\omega = 10$ and $\Omega = 5$ were used. Under these parameters, Eq. (11) can be computed by the RK4 until 0.5 sec, and Eq. (16) until 1 sec with a time step of $\Delta t = 0.01$ sec; however, Eq. (65) is still survived. As shown in Fig. 2 the error of orthogonality induced by the numerical method based on Eq. (65) is the smallest one, and then sequentially by Eq. (105) with $n = 2$, and Eqs. (100) and (99). The above calculations are performed under a fixed time step of $\Delta t = 0.001$ sec until the final time of $t_f = 5$ sec. Next, we investigate a long-term rotation behavior by increasing the final time to $t_f = 50$ sec in Fig. 3, where $\Delta t = 0.01$ sec were used for all calculations. By the same token, Eq. (65) preserves the orthogonality best, and then Eqs. (105) and (100). It can be seen that the scheme (100) is stable, but the scheme (105) slowly increases its errors on the orthogonality as shown in Fig. 3(c), and more obviously its componential errors are increased rapidly as shown in Fig. 3(a) for the $Q_{11}$ component and Fig. 3(b) for the $Q_{22}$ component. For the other components they are also of this situation even we do not plot them in this figure.

To assess the performance of a numerical scheme on the computation of rotation, there are four factors should be considered: stability, accuracy, the preservation of orthogonality and the free of singularity. The scheme based on Eq. (65) has a good advantage in its dimension is minimum; however, an inherent singularity at $X_0 = 0$ is not easily removed, and its singularity seems to depend on the parameters of angular frequencies as that in Fig. 1 with $\omega = 2$ and $\Omega = 3$ it fails to be applicable until time 0.5 sec, but that with $\omega = 10$ and $\Omega = 5$ in Fig. 3 we can apply it on the computation until 50 sec. A naive approach as that given in Eq. (105) has several advantages including a reasonable accuracy and the free of singularity; however, its long-term behaviors show the spill-over
Figure 3: Comparing the componential errors and the errors of orthogonality for three types numerical methods in the long-term range under very large rotation.

In order to keep the invariant in Eq. (91) unchanged, we modify the numerical method when applied the RK4 on Eq. (77) by considering a unit vector $n$:

\[ n := \frac{Y}{\|Y\|}. \]  

(106)

As suggested by Liu (2006), we can insert it into Eq. (91) to solve $\|Y_\ell\|$ by the following formula:

\[ \|Y_\ell\| = \sqrt{\frac{\|Y(0)\|^2}{n_\ell^T \eta_\ell n_\ell}}, \]  

(107)

because of $\eta(0) = I_3$. Upon $\|Y_\ell\|$ is obtained, from Eq. (106) we obtain a new $Y_\ell$ by

\[ Y_\ell = \|Y_\ell\| n_\ell, \]  

(108)

which is guaranteed to satisfy the invariant in Eq. (91). This numerical method is indeed a projection of the numerical solutions onto the invariant manifold.

Under the same parameters as that used in Fig. 3, we plot the numerical results calculated by the RK4 method with the above modification in Fig. 4. It can be seen that this method gives highly accurate numerical com-
components of $Q$ and also preserves the orthogonality very well. Through these investigations, the scheme based on Eqs. (106)-(108) is a rather stable one in all aspects of the accuracy and the preservation of orthogonality. More importantly, it is free of singularity, and is very simple to implement as a numerical program.

The same modification strategy can also be applied on Eqs. (99) and (100) to improve their performance; however, these numerical results are similar to that in Fig. 4.

9 Concluding remarks

In this paper we have developed two new mathematical procedures to calculate $Q$. The first one is obtained by transforming the governing equations in a space of $\mathbb{R}^3$, whose singularity-free interval is largely extended. Then, we developed a second method to express $Q$ in terms of a noncanonical orthogonal matrix, the governing equation of which is a linear ODEs system with the state matrix being nilpotent with index two.

We have examined different methods on the computation of $Q$ from a theoretical aspect. There are three linear
equations (9), (54) and (77), which are singularity-free and have invariants. There are also three nonlinear equations (11), (16) and (65), each of which has a singular point at infinity. The first three equations (9), (11) and (16) use a slightly larger algebra of \(so(4)\) to realize their representations of \(SO(3)\). Both equations (65) and (54) use the Lie algebra \(so(3)\) to realize their representations of \(SO(3)\). Especially, Eq. (77) employed a nilpotent Lie algebra to realize its representation of \(SO(3)\).

Through numerical examples testing we concluded that the new methods can pass all the requirements of larger singularity-free interval, long-term stability, accuracy and easy implementation. They are therefore amenable to the calculations of large rotation.

References


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Noting that the differential of Eq. (75) again gives
\[ u_X \]
Further differentiating yields
where
\[ m_0 := \sqrt{1 + \omega^2}, \quad f_1 = \frac{X_0(0)}{m_0^2} + \frac{\omega X_2(0)}{m_0^2}, \]
\[ f_2 = -\frac{X_1(0)}{m_0}, \quad f_0 = \frac{\omega^2 X_0(0)}{m_0^3} - \frac{\omega X_2(0)}{m_0^3}. \tag{A.6} \]
Taking the differential of Eq. (58) and using Eq. (59), thus substituting Eqs. (A.1) and (A.2) into those results and noting that Eq. (57), we obtain
\[ \cos \omega t X_1 + \sin \omega t X_2 = -\dot{X}_0, \tag{A.7} \]
\[ \omega \sin \omega t X_1 - \omega \cos \omega t X_2 = \ddot{X}_0 + X_0. \tag{A.8} \]
Solutions of the above two equations for \( X_1 \) and \( X_2 \) render
\[ X_1 = \frac{1}{\omega} \left[ \sin \omega t (\dot{X}_0 + X_0) - \omega \cos \omega t \dot{X}_0 \right], \tag{A.9} \]
\[ X_2 = -\frac{1}{\omega} \left[ \cos \omega t (\dot{X}_0 + X_0) + \omega \sin \omega t \dot{X}_0 \right]. \tag{A.10} \]
Finally, substituting Eq. (A.5) and its differentials into the above equations we obtain
\[ X_1(t) = \frac{1}{\omega} \sin \omega t \left( f_0 - f_1 \omega^2 \cos m_0 t - f_2 \omega^2 \sin m_0 t \right) + \cos \omega t \left( f_1 m_0 \sin m_0 t - f_2 m_0 \cos m_0 t \right), \tag{A.11} \]
\[ X_2(t) = \frac{1}{\omega} \cos \omega t \left( f_1 \omega^2 \cos m_0 t + f_2 \omega^2 \sin m_0 t - f_0 \right) + \sin \omega t \left( f_1 m_0 \sin m_0 t - f_2 m_0 \cos m_0 t \right). \tag{A.12} \]
In the form of Eq. (56) the components of \( Q_1 \) can be written as follows:
\[ Q_{1,11} = \frac{\cos m_0 t + \omega^2}{m_0^2}, \tag{A.13} \]
\[ Q_{1,12} = -\frac{\sin m_0 t}{m_0}, \tag{A.14} \]
\[ Q_{1,13} = \frac{\omega \left( \cos m_0 t - 1 \right)}{m_0^2}, \tag{A.15} \]
\[ Q_{1,21} = \frac{\omega \sin \omega t \left( 1 - \cos m_0 t \right)}{m_0^2} + \frac{\cos \omega t \sin m_0 t}{m_0}. \tag{A.16} \]
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\[ Q_{1,22} = \frac{\omega \sin \omega t \sin m_0 t}{m_0} + \cos \omega t \cos m_0 t, \]  \hspace{1cm} (A.17)

\[ Q_{1,23} = \frac{\omega \cos \omega t \sin m_0 t}{m_0} - \frac{\sin \omega t (1 + \omega^2 \cos m_0 t)}{m_0^2}, \]  \hspace{1cm} (A.18)

\[ Q_{1,31} = \frac{\omega \cos \omega t (\cos m_0 t - 1)}{m_0^2} + \frac{\sin \omega t \sin m_0 t}{m_0}, \]  \hspace{1cm} (A.19)

\[ Q_{1,32} = \sin \omega t \cos m_0 t - \frac{\omega \cos \omega t \sin m_0 t}{m_0}, \]  \hspace{1cm} (A.20)

\[ Q_{1,33} = \frac{\cos \omega t (1 + \omega^2 \cos m_0 t)}{m_0^2} + \frac{\omega \sin \omega t \sin m_0 t}{m_0}. \]  \hspace{1cm} (A.21)