Explicit representation for the SO(3) rotation tensor of deformable bodies

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Abstract

Computation of rotation tensor is essential in the analysis of deformable bodies. This paper propose an explicit expression for rotation tensor $R$ of deformation gradient $F$, and successfully establishes an intrinsic relation between the exponential mapping $Q = \exp A$ and the deformation $F$. As an application, Truesdell’s simple shear deformation is revisited. For easy use of our formulation, we provide a Maple code for a general 2D problem.

Keywords: finite deformation, deformation gradient, rotation tensor, polar decomposition, eigenvalues

1. Introduction

In continuum physics, the representations and computations of SO(3) rotation tensor are vital in all aspects of theoretical study and practical applications. For deformable bodies, the deformation gradient is defined by $F = \chi \otimes \nabla$, where $\nabla$ is the del operator with respect to $X$ and $\chi(X, t)$ is a mapping from a point $X$ in the reference configuration to a point $x$ in the current configuration through time $t$, namely $\chi : X \rightarrow x$. The deformation gradient $F$ can be split into stretch and rotation components by the polar multiplication decomposition $[1, 2]: F = R \cdot U = V \cdot R$, where “$\cdot$” denotes the dot product and $U$, $V$, and $R$ are the right stretch, left stretch, and rotation tensors, respectively. The rotation
tensor satisfies the orthogonality condition $R \cdot R^T = R^T \cdot R = I$ and $\det(R) = 1$.

From the polar decomposition and orthogonality condition, the right and left Cauchy–Green stretch tensors can be defined as $C = F^T \cdot F = U \cdot U = U^2$ and $B = F \cdot F^T = V \cdot V = V^2$, respectively. The algorithm for computing the rotation tensor is

$$ R = F \cdot U^{-1} = F \cdot (C)^{-\frac{1}{2}} = V^{-1} \cdot F = (B)^{-\frac{1}{2}} \cdot F. \quad (1) $$

As [3] pointed out, such a direct analysis requires to perform square root and inverse operations on symmetric tensors, and this may bring computational difficulties for both $(C)^{1/2}$ and $(C)^{-1/2}$. Although there were some attempts to find an explicit representation of the rotation tensor [3, 4, 5, 6, 7], however, all proposed algorithms are rather complicated for application. It is highly demanded to have a simple and practical representation of rotation tensor $R$ that is explicitly expressed in the deformation gradient tensor $F$.

Another issue is that, in mathematics, an arbitrary SO(3) rotation tensor $Q$ is given by

$$ Q = I + \frac{\sin \omega}{\omega} A + \frac{1 - \cos \omega}{\omega^2} A^2. \quad (2) $$

where $A$ is an arbitrary order-2 skew-symmetric tensor, namely $A^T = -A$, which has an axial vector $\omega = \varepsilon : A = -2(A_{32} G^1 + A_{13} G^2 + A_{21} G^3) = \omega_1 G^1 + \omega_2 G^2 + \omega_3 G^3$. Hence, $\omega_1 = -2A_{32}$, $\omega_2 = -2A_{13}$, $\omega_3 = -2A_{21}$, and $\omega = \sqrt{\omega \cdot \omega}$. Because $\varepsilon : \varepsilon = 2I$, we have that $\varepsilon \cdot \omega = \varepsilon \cdot (\varepsilon : A) = \varepsilon \cdot \varepsilon \cdot A = 2I \cdot A = 2A$; therefore, $A = \frac{1}{2} \varepsilon \cdot \omega$.

Note that the rotation tensor expression in Eq. (2) is not derived from the deformation gradient $F = R \cdot U$, and so the rotation tensor $Q$ is not equal to the rotation tensor $R$, namely $Q \neq R$, which means that $Q$ is nothing to do with $R$.

Although the rotation tensor in Eq. (2) is widely used in the formulation of continuum physics, no expression has yet been obtained for $A$ in terms of the right Cauchy–Green tensor $C$ and deformation gradient $F$. The relationship between $A$ and tensors such as the deformation gradient tensor $F$ and the right
Cauchy–Green tensor $C$ remains one of the fundamental unsolved problems in continuum physics.

In this Letter, we will focus on the above-mentioned open problems, and propose alternative ways to find explicit formulas for the rotation tensor $R$, and find an intrinsic relation between the exponential mapping $Q = \exp A$ and the deformation gradient tensor $F$.

2. Rotation tensor expressed in the deformation gradient

Given a deformation gradient $F$, we can easily get the right Cauchy–Green stretch tensor $C = F^T \cdot F$ and its eigenvalues $\lambda_k$ from the characteristic equation $\det(C - \lambda I) = 0$.

To find the explicit expression of rotation tensor $R$, it is clear that we must find the expression of $(C)^{1/2}$ and/or its inverse $(C)^{-1/2}$ that can be expressed in the deformation gradient tensor $F$ explicitly.

According to the Cayley–Hamilton theorem and the Cauchy tensor representation theory [1, 2, 8, 9, 10], the explicit expression of $(C)^{1/2}$ can be set in the following form:

$$C^{1/2} = \alpha_0 I + \alpha_1 C + \alpha_2 C^2,$$

in which the coefficients $\alpha_0$, $\alpha_1$, and $\alpha_2$ can be determined by simply replacing the $C$ with the eigenvalues $\lambda_1$, $\lambda_2$ and $\lambda_3$ in Eq. 3 in this way, we can get three equations as follows:

$$
\begin{pmatrix}
\sqrt{\lambda_1} \\
\sqrt{\lambda_2} \\
\sqrt{\lambda_3}
\end{pmatrix} =
\begin{pmatrix}
1 & \lambda_1 & (\lambda_1)^2 \\
1 & \lambda_2 & (\lambda_2)^2 \\
1 & \lambda_3 & (\lambda_3)^2
\end{pmatrix}
\begin{pmatrix}
\alpha_0 \\
\alpha_1 \\
\alpha_2
\end{pmatrix},
$$

hence, we can find the coefficients $\alpha_0$, $\alpha_1$ and $\alpha_2$ as follows

$$
\begin{pmatrix}
\alpha_0 \\
\alpha_1 \\
\alpha_2
\end{pmatrix} =
\begin{pmatrix}
1 & \lambda_1 & (\lambda_1)^2 \\
1 & \lambda_2 & (\lambda_2)^2 \\
1 & \lambda_3 & (\lambda_3)^2
\end{pmatrix}^{-1}
\begin{pmatrix}
\sqrt{\lambda_1} \\
\sqrt{\lambda_2} \\
\sqrt{\lambda_3}
\end{pmatrix},
$$

The coefficients $\alpha_1$, $\alpha_2$, and $\alpha_3$ are given in the appendix.
If two of the eigenvalues is repeated $\lambda_i = \lambda_j$, $i \neq j$, then Eq. 4 will yield two identical equations, and therefore will not be a set of 3 independent equations.

If $\lambda_1 = \lambda_2 = \lambda$, we can reformulate the first equation in Eq. 4 as follows:

$$\frac{d}{d\lambda} [\lambda^{1/2} - (\alpha_0 + \alpha_1 \lambda + \alpha_2 \lambda^2)] |_{\lambda = \lambda} = 0,$$

namely

$$\frac{1}{2} \lambda^{-1/2} - (\alpha_1 + 2\alpha_2 \lambda) = 0.$$

Hence, Eq. 4 becomes

$$\begin{pmatrix} \frac{1}{\sqrt{\lambda}} \\ \sqrt{\lambda} \\ \sqrt{\lambda_3} \end{pmatrix} = \begin{pmatrix} 0 & 1 & 2\lambda \\ 1 & \lambda & (\lambda)^2 \\ 1 & \lambda_3 & (\lambda_3)^2 \end{pmatrix} \begin{pmatrix} \alpha_0 \\ \alpha_1 \\ \alpha_2 \end{pmatrix}, \quad (6)$$

Therefore, we can get the coefficients $\alpha_0$, $\alpha_1$ and $\alpha_2$ as follows

$$\begin{pmatrix} \alpha_0 \\ \alpha_1 \\ \alpha_2 \end{pmatrix} = \begin{pmatrix} 0 & 1 & 2\lambda \\ 1 & \lambda & (\lambda)^2 \\ 1 & \lambda_3 & (\lambda_3)^2 \end{pmatrix}^{-1} \begin{pmatrix} \frac{1}{\sqrt{\lambda}} \\ \sqrt{\lambda} \\ \sqrt{\lambda_3} \end{pmatrix}. \quad (7)$$

In the same way, we can formulate $C^{-\frac{1}{2}}$ as

$$(C)^{-1/2} = \beta_0 I + \beta_1 C + \beta_2 C^2, \quad (8)$$

in which $\beta_0$, $\beta_1$, and $\beta_2$ are again determined by the eigenvalues $\lambda_k$, $(k = 1, 2, 3)$ of $C$:

$$\begin{pmatrix} \beta_0 \\ \beta_1 \\ \beta_2 \end{pmatrix} = \begin{pmatrix} 1 & \lambda_1 & (\lambda_1)^2 \\ 1 & \lambda_2 & (\lambda_2)^2 \\ 1 & \lambda_3 & (\lambda_3)^2 \end{pmatrix}^{-1} \begin{pmatrix} \frac{1}{\sqrt{\lambda_1}} \\ \frac{1}{\sqrt{\lambda_2}} \\ \frac{1}{\sqrt{\lambda_3}} \end{pmatrix}. \quad (9)$$

their expressions can also be found in the appendix.

If $\lambda_1 = \lambda_2 = \lambda$, from Eq. 8, we have

$$\frac{d}{d\lambda} [\lambda^{-1/2} - (\beta_0 + \beta_1 \lambda + \beta_2 \lambda^2)] |_{\lambda = \lambda} = 0,$$

namely

$$-\frac{1}{2} \lambda^{-3/2} - (\beta_1 + 2\beta_2 \lambda) = 0.$$

Hence, Eq. 8 becomes

$$\begin{pmatrix} \beta_0 \\ \beta_1 \\ \beta_2 \end{pmatrix} = \begin{pmatrix} 0 & 1 & 2\lambda \\ 1 & \lambda & (\lambda)^2 \\ 1 & \lambda_3 & (\lambda_3)^2 \end{pmatrix}^{-1} \begin{pmatrix} -\frac{1}{2} \lambda^{-3/2} \\ \frac{1}{\sqrt{\lambda}} \\ \frac{1}{\sqrt{\lambda_3}} \end{pmatrix}. \quad (10)$$

If all eigenvalues are identical, namely $\lambda_1 = \lambda_2 = \lambda_3$, in this case, the deformation has no rotation but pure stretching.
Using $C = F^T \cdot F$, we obtain explicit expressions for $U$ and $U^{-1}$:

$$U = \alpha_0 I + \alpha_1 (F^T \cdot F) + \alpha_2 (F^T \cdot F)^2,$$

(11)

and

$$U^{-1} = \beta_0 I + \beta_1 (F^T \cdot F) + \beta_2 (F^T \cdot F)^2.$$  

(12)

With these formulas, we can write the rotation tensor $R$ as follows:

$$R = F \cdot U^{-1} = F \cdot (\beta_0 I + \beta_1 C + \beta_2 C^2)$$

$$= F \cdot [\beta_0 I + \beta_1 (F^T \cdot F) + \beta_2 (F^T \cdot F)^2].$$

(13)

The explicit expressions in Eqs. (11)–(13) have not previously been seen in the literature.

From Eq.13, and notice the definition $U^2 = C = F^T \cdot F$ and $V^2 = B = F \cdot F^T$, hence the rotation tensor in Eq.13 can be rewritten as follows

$$R = F \cdot U^{-1}$$

$$= \beta_0 F \cdot I + \beta_1 F \cdot F^T \cdot F + \beta_2 F \cdot (F^T \cdot F) \cdot (F^T \cdot F)$$

$$= \beta_0 F + \beta_1 V \cdot F + \beta_2 V \cdot F \cdot C$$

$$= \beta_0 F + \beta_1 B \cdot F + \beta_2 B^2 \cdot F$$

$$= (\beta_0 I + \beta_1 B + \beta_2 B^2) \cdot F.$$  

(14)

Since $R = V^{-1} \cdot F$, comparing with the above relation, hence we have

$$V^{-1} = \beta_0 I + \beta_1 B + \beta_2 B^2$$

$$= \beta_0 I + \beta_1 F \cdot F^T + \beta_2 (F \cdot F^T)^2.$$  

(15)

### 3. 2D deformation

For the 2D deformation, the eigenvalues of $C$ are

$$\lambda_{1,2} = \frac{C_{11} + C_{22}}{2} \pm \frac{1}{2} \sqrt{(C_{11} - C_{22})^2 + 4C_{12}^2}.$$  

(16)

We can easily write the tensors $U$, $U^{-1}$, and $R$ as follows:

$$U = \frac{(\lambda_2 \sqrt{\lambda_1} - \lambda_1 \sqrt{\lambda_2}) I + (\sqrt{\lambda_2} - \sqrt{\lambda_1}) C}{\lambda_2 - \lambda_1},$$

(17)
and its inverse
\[
U^{-1} = \frac{(\lambda_2^{3/2} - \lambda_1^{3/2}) I + (\lambda_1^{1/2} - \lambda_2^{1/2}) C}{(\lambda_2 - \lambda_1) \sqrt{\lambda_1 \lambda_2}},
\]
(18)

and rotation tensor
\[
R = \frac{F \cdot \left[ (\lambda_2^{3/2} - \lambda_1^{3/2}) I + (\lambda_1^{1/2} - \lambda_2^{1/2}) C \right] (\lambda_2 - \lambda_1) \sqrt{\lambda_1 \lambda_2}}{(\lambda_2 - \lambda_1) \sqrt{\lambda_1 \lambda_2}}.
\]
(19)

This 2D deformation rotation tensor expression has not previously been seen in the literature.

For the easy use of our formulation, we have written a Maple code for a general 2D problem as follows:

with(LinearAlgebra):

R := proc (F)
local C, Eigen, lambda1, lambda2, alpha0, alpha1, beta0, beta1, U, Uinverse;

C := Multiply(Transpose(F), F);
Eigen := Eigenvalues(C);
lambda1 := Eigen(1);
lambda2 := Eigen(2);
alpha0 := simplify((lambda2*sqrt(lambda1)-lambda1*sqrt(lambda2))/(lambda2-lambda1));
alpha1 := simplify((sqrt(lambda2)-sqrt(lambda1))/(lambda2-lambda1));
beta0 := simplify((lambda2/sqrt(lambda1)-lambda1/sqrt(lambda2))/(lambda2-lambda1));
beta1 := simplify((1/sqrt(lambda2)-1/sqrt(lambda1))/(lambda2-lambda1));
U := simplify(alpha0*Matrix([[1, 0], [0, 1]])+alpha1*C);
Uinverse := simplify(beta0*Matrix([[1, 0], [0, 1]])+beta1*C);
simplify(Multiply(F, Uinverse))
end proc

The code is general and can be easily upgraded to the 3D problem.
4. Relations between SO(3) rotation tensor and deformation gradient

We now find the skew-symmetric tensor $A$ expressed in terms of the deformation gradient tensor $F$. Mathematically speaking, the rotation tensor in Eq. (2) is an exponential mapping of a second-order skew-symmetric tensor $A$, that is, $Q = e^A$. As $A^T = -A$ and $tr A = 0$ for the skew-symmetric tensor $A$, we have that $\det A = e^{tr A} = e^0 = 1$, and so $Q^T \cdot Q = e^{A^T} \cdot e^A = e^{-A+A} = e^0 = I = e^{A-A} = e^A \cdot e^{A^T} = Q \cdot Q^T = I$.

One approach is to set $Q = e^A = R = F \cdot U^{-1}$, such that $A = \ln(F \cdot U^{-1})$. However, this is not an explicit expression owing to the logarithm operation. Another method is to use the rotation tensor in Eq. (13) and let $Q = R$, that is, $I + \frac{\sin \omega}{\omega} A + \frac{1 - \cos \omega}{\omega^2} A^2 = F : (\beta_0 I + \beta_1 C + \beta_2 C^2)$, (20)

Transposing both sides of this equation gives

$I - \frac{\sin \omega}{\omega} A + \frac{1 - \cos \omega}{\omega^2} A^2 = (\beta_0 I + \beta_1 C + \beta_2 C^2) \cdot F^T$, (21)

Equation (20) minus Eq. (21) gives an explicit expression of the skew-symmetric tensor $A$. For the 3D case, we have

$A = \frac{\omega \beta_0}{2 \sin \omega} (F - F^T) + \frac{\omega \beta_1}{2 \sin \omega} (F \cdot C - C \cdot F^T)$
$+ \frac{\omega \beta_2}{2 \sin \omega} (F \cdot C^2 - C^2 \cdot F^T)$. (22)

and for the 2D deformation case, we have

$A = \frac{\omega}{2 \sin \omega} \left[ \frac{(\lambda_2^{3/2} - \lambda_1^{3/2})(F - F^T)}{(\lambda_2 - \lambda_1)\sqrt{\lambda_1 \lambda_2}} + \frac{(\lambda_1^{1/2} - \lambda_2^{1/2})(F \cdot C - C \cdot F^T)}{(\lambda_2 - \lambda_1)\sqrt{\lambda_1 \lambda_2}} \right]$. (23)

Equations (22) is the intrinsic linkages between the rotation tensor $Q$ and the deformation gradient tensor $F$, as well as the Cauchy–Green tensor $C$. These relations reveal that the skew-symmetric tensor $A$ is not only related to the antisymmetric tensor $F - F^T$, but also to other two antisymmetric tensors as well: $F \cdot C - C \cdot F^T$ and $F \cdot C^2 - C^2 \cdot F^T$. If the deformation gradient $F$ is symmetric, i.e., $F = F^T$, then $A = 0$ and $Q = I$. 

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5. Approximation of rotation tensor

In co-moving coordinates, the deformation gradient is defined by \( F = g_k \otimes G^k \); thus, \( F^T = C = g_{ij}G^i \otimes G^j \), and \( C^2 = g_{ij}g_{k\ell}G^jG^i \otimes G^\ell \). Substituting these formulas into Eq. (13) leads to another form of the rotation tensor.

If we introduce the displacement vector \( u \) from the reference to the current configuration, the deformation mapping becomes \( \chi(X) = X + u \) and the deformation gradient tensor is \( F = I + u \otimes \nabla \). Hence, its transpose \( F^T = I + \nabla \otimes u \), \( C = F^T \cdot F = I + u \otimes \nabla + \nabla \otimes u + (\nabla \otimes u) \cdot (u \otimes \nabla) \), and \( C^2 = I + 2(u \otimes \nabla + \nabla \otimes u) + (u \otimes \nabla) \cdot (u \otimes \nabla) \). Substituting these expressions into Eq. (13), we have the rotation tensor \( R \) expressed in terms of the displacement vector \( u \), namely \( R = (I + u \otimes \nabla) \cdot (\beta_0 I + \beta_1 C + \beta_2 C^2) \).

With this displacement form of the rotation tensor, we propose two consistent approximations of the rotation tensor based on the order of \( u \otimes \nabla \), for instance, the first order rotation tensor
\[
R_{1st} \approx (\beta_0 + \beta_1 + \beta_2)I + (\beta_0 + 2\beta_1 + 4\beta_2)u \otimes \nabla \\
+ (\beta_1 + 2\beta_2)\nabla \otimes u + O([u \otimes \nabla]^2), \tag{24}
\]
and the second order rotation tensor
\[
R_{2nd} \approx (\beta_0 + \beta_1 + \beta_2)I + (\beta_0 + 2\beta_1 + 4\beta_2)u \otimes \nabla \\
+ (\beta_1 + 2\beta_2)\nabla \otimes u + (\beta_1 + 10\beta_2)(u \otimes \nabla) \cdot (\nabla \otimes u) \\
+ \beta_2([u \otimes \nabla]^2 + (\nabla \otimes u)^2) + O([u \otimes \nabla]^3). \tag{25}
\]
Those two approximations of the rotation tensor have not been reported in the literature. The rotation tensor approximation here can be used to the formulations of thin-shells modelling, it is anticipated that the order estimation of rotation of shell middle surface can be rigorously investigated.

In summary, all of the explicit expressions for \( U \), its inverse \( U^{-1} \) and rotation tensor \( R \) derived in this letter have been formulated without using the
eigenvectors of $C$, it is an essential feature of our formulation that is different from traditional ones.

6. Generalization to order-n tensor

Although our focus is 3D deformation, the algorithm of computing the rotation tensor and relevant tensor is universal for any order tensor and even can be used to differential operators such as in quantum mechanics. It is worth to give a general formulation.

For instance, if $F$ is order-n tensor, we still have a polar decomposition $F = R \cdot U$, and tensor $C = F^T \cdot F$. We can compute the eigenvalues $\lambda_k (k = 1, \ldots, n)$ of $C$ by the characteristic equation $\det(C - \lambda I) = 0$. Once we have the eigenvalues $\lambda_k$, we can compute $C^{-1/2}$.

Set $C^{-1/2} = \sum_{j=0}^{n-1} c_j C^j$, according to the Cayley-Hamilton theory, the eigenvalues satisfy the polynomial corresponding equation, namely $\lambda_k^{-1/2} = \sum_{j=0}^{n-1} c_j \lambda_k^j$.

This operation will produce n-equations as follows

\[
\begin{pmatrix}
1 & \lambda_1 & \ldots & \lambda_1^{n-1} \\
1 & \lambda_2 & \ldots & \lambda_2^{n-1} \\
1 & \ldots & \ldots & \ldots \\
1 & \lambda_1 & \ldots & \lambda_n^{n-1}
\end{pmatrix}
\begin{pmatrix}
c_0 \\
c_1 \\
\ldots \\
c_{n-1}
\end{pmatrix}
= 
\begin{pmatrix}
1/\sqrt{\lambda_1} \\
1/\sqrt{\lambda_2} \\
\ldots \\
1/\sqrt{\lambda_n}
\end{pmatrix}
\]

(26)

We can solve the equation and find the coefficient vector

\[
\begin{pmatrix}
c_0 \\
c_1 \\
\ldots \\
c_{n-1}
\end{pmatrix}
= 
\begin{pmatrix}
1 & \lambda_1 & \ldots & \lambda_1^{n-1} \\
1 & \lambda_2 & \ldots & \lambda_2^{n-1} \\
1 & \ldots & \ldots & \ldots \\
1 & \lambda_1 & \ldots & \lambda_n^{n-1}
\end{pmatrix}^{-1}
\begin{pmatrix}
1/\sqrt{\lambda_1} \\
1/\sqrt{\lambda_2} \\
\ldots \\
1/\sqrt{\lambda_n}
\end{pmatrix}
\]

(27)
From the obtained \( c_k, k = 0, ..., n - 1 \), we have \( C^{-1/2} = \sum_{j=0}^{n-1} c_j C^j \), and rotation tensor
\[
R = F \cdot C^{-1/2} = F \cdot \sum_{j=0}^{n-1} c_j C^j
\]
\[
= F \cdot (c_0 I + c_1 C + c_2 C^2 + ... + c_{n-1} C^{n-1}).
\] (28)

If there were repeated eigenvalues, similar approaches in the previous section can be adopted.

7. Applications

To verify our new formulations, we present the following two examples.

(1) A 2D deformation:
Consider the deformation given by the mapping (see Example 3.7.1 in [11])
\[
\chi(X) = \frac{1}{4}[4X_1 - (9 - 3X_1 - 5X_2 - X_1X_2)t]G^1 + \frac{1}{4}[4X_2 + (16 + 8X_1)t]G^2.
\] (29)
For \( X = (0, 0), t = 1 \), determine the symmetric stretch tensor \( U \) and rotation tensor \( R \).

From the deformation mapping in Eq. (29), we have the deformation gradient
\[
F = \frac{1}{4}(G^1 \otimes G^1 - 5G^1 \otimes G^2 + 8G^2 \otimes G^1 + 4G^2 \otimes G^2)
\] or in matrix \([F] = \begin{pmatrix} \frac{1}{4} & -\frac{5}{4} \\ 2 & 1 \end{pmatrix}\).

Applying the Maple code to the this problem, and just input \( R((1/4) * Matrix([[1, -5], [8, 4]])) \) in Maple command line, we can get following results.

The right Cauchy–Green tensor \( C = \frac{1}{16}(65G^1 \otimes G^1 + 27G^1 \otimes G^2 + 27G^2 \otimes G^1 + 41G^2 \otimes G^2) \), or in matrix
\[
[C] = [F]^T [F] = \frac{1}{16} \begin{pmatrix} 65 & 27 \\ 27 & 41 \end{pmatrix}
\].

From the eigenvalue equation \(|C - \lambda I| = 0\), we obtain two eigenvalues of \( C \) as follows: \( \lambda_1 = \frac{53}{16} + \frac{3}{16} \sqrt{97} \) and \( \lambda_2 = \frac{53}{16} - \frac{3}{16} \sqrt{97} \).

Hence, the coefficients are \( \alpha_0 = \frac{11}{1067} \sqrt{194} \), \( \alpha_1 = \frac{27}{1067} \sqrt{194} \) and \( \beta_0 = \frac{75}{1067} \sqrt{194}, \beta_1 = -\frac{8}{1067} \sqrt{194} \). Therefore, we have \( U = \frac{\sqrt{194}}{1067} \begin{pmatrix} 81 & 27 \\ 27 & 57 \end{pmatrix} \), its inverse
\[ [U]^{-1} = \frac{1}{\sqrt{194}} \begin{pmatrix} 85 & -27 \\ -27 & 109 \end{pmatrix}, \text{ and the rotation tensor } [R] = \frac{1}{\sqrt{194}} \begin{pmatrix} 5 & -13 \\ 13 & 5 \end{pmatrix}, \]

and its transpose \([R]^T = \frac{1}{\sqrt{194}} \begin{pmatrix} 5 & 13 \\ -13 & 5 \end{pmatrix} \).

The correctness of the above results can be easily validated, since \(R \cdot R^T = R^T \cdot R = I\) and \(\det [R] = 1\).

(2) A 3D deformation: Given a deformation gradient matrix \([F] = \begin{pmatrix} 1 & 2 & 3 \\ 3 & 1 & 3 \\ 3 & 2 & 1 \end{pmatrix}\), by a Maple code of our formulation, we can find the corresponding rotation \([R] = \frac{1}{\sqrt{59}} \begin{pmatrix} -\frac{\sqrt{59}}{2} + \frac{3}{2} & \frac{3}{2} + \frac{\sqrt{59}}{2} \\ 5 & -3 \\ \frac{3}{2} + \frac{\sqrt{59}}{2} & 5 - \frac{\sqrt{59}}{2} + \frac{3}{2} \end{pmatrix}\). The interesting feature of this rotation is that it is symmetric. We can show that it is a rotation, because it satisfies the rotation definition \(\det [R] = 1\), and \([R]^T [R] = [R] [R]^T = [I]\).

(3) Simple shear deformation:

This shear deformation is defined to be a set of line elements whose lengths and orientations are unchanged, as shown in \(\text{Fig. 1}\). The deformation mapping in this case is \(\chi(X) = (X_1 + \gamma X_2) G^1 + X_2 G^2 + X_3 G^3\). We find that the deformation gradient tensor is \(F = I + \gamma G^1 \otimes G^2 = G^1 \otimes G^1 + \gamma G^1 \otimes G^2 + G^2 \otimes G^2 + G^3 \otimes G^3\) and its transpose is \(F^T = I + \gamma G^2 \otimes G^1 = G^1 \otimes G^1 + \gamma G^2 \otimes G^1 + G^2 \otimes G^2 + G^3 \otimes G^3\). The Cauchy–Green tensor is written as \(C = F^T \cdot F = I + \gamma G^1 \otimes G^2 + \gamma G^2 \otimes G^1 + \gamma^2 G^2 \otimes G^2\), and its square is \(C^2 = (1 + \gamma^2) G^1 \otimes G^1 + (2 \gamma + \gamma^3) G^1 \otimes G^2 + (2 \gamma + \gamma^3) G^2 \otimes G^1 + (\gamma^4 + 3 \gamma^2 + 1) G^2 \otimes G^2 + G^3 \otimes G^3\). The eigenvalues of
\( \mathbf{C} \) are \( \lambda_1 = 1, \lambda_2 = \frac{1}{2} \gamma^2 + 1 + \frac{1}{2} \sqrt{\gamma^4 + 4 \gamma^2}, \) and \( \lambda_3 = \frac{1}{2} \gamma^2 + 1 - \frac{1}{2} \sqrt{\gamma^4 + 4 \gamma^2} \).

Applying our new formulation or using the Maple code, the right stretch tensor is obtained as
\[
U^{-1} = s_0 \mathbf{I} + s_1 \mathbf{C} + s_2 \mathbf{C}^2 = (U^{-1})_{11} \mathbf{G}^1 \otimes \mathbf{G}^1 + (U^{-1})_{12} \mathbf{G}^1 \otimes \mathbf{G}^2 + (U^{-1})_{21} \mathbf{G}^2 \otimes \mathbf{G}^1 + (U^{-1})_{22} \mathbf{G}^2 \otimes \mathbf{G}^2 + \mathbf{G}^3 \otimes \mathbf{G}^3
\]
and the rotation tensor is
\[
\mathbf{R} = R_{11} \mathbf{G}^1 \otimes \mathbf{G}^1 + R_{12} \mathbf{G}^1 \otimes \mathbf{G}^2 + R_{21} \mathbf{G}^2 \otimes \mathbf{G}^1 + R_{22} \mathbf{G}^2 \otimes \mathbf{G}^2 + \mathbf{G}^3 \otimes \mathbf{G}^3,
\]
where the coefficients \( s_0, s_1, s_2, \) and other elements are given in the appendix.

The right stretch tensor \( \mathbf{U} \), its inverse \( \mathbf{C}^{-1} \), and the rotation tensor \( \mathbf{R} \) obtained here for the shear deformation have no geometrical constraints. From Fig. 2, it is clear to see that the coefficients \( s_0 \) and \( s_1 \) vary dramatically, with \( s_0 \) being positive and \( s_1 \) being negative; \( s_2 \) is positive and smooth, and has a maximum value of approximately 0.37498.

![Figure 2: Coefficient comparisons: \( s_0, s_1, \) and \( s_2 \).](image)

For small shear deformations, Truesdell’s both eigenvalues and rotation tensor can be obtained from our formulation after omitting orders higher than \( O(\gamma^2) \) terms. The reduced eigenvalues of \( \mathbf{C} \) are \( \lambda_1 = 1, \lambda_2 = 1 + \frac{1}{2} \gamma, \) and
\[ \lambda_2 = 1 - \frac{1}{2}\gamma; \text{ and rotation tensor is} \]
\[
R_{\text{Truesdell}} = \begin{pmatrix}
\frac{1}{\sqrt{1+\gamma^2/4}} & \frac{\gamma}{\sqrt{4+\gamma^2}} & 0 \\
-\frac{\gamma}{\sqrt{4+\gamma^2}} & \frac{1}{\sqrt{1+\gamma^2/4}} & 0 \\
0 & 0 & 1
\end{pmatrix}.
\] (30)

The components of this rotation tensor are plotted in Fig. 3 below. The drawing show that both components \( R_{11} \) and \( R_{22} \) are vary slowly vs the \( \gamma \), but the \( R_{12} \) and \( R_{21} \) vary with \( \gamma \).

![Figure 3: Rotation tensor component vs. shear deformation \( \gamma \).](image)

Through numerical comparisons, we found that Truesdell’s results are extreme accurate at around of errors margin of \( O(10^{-13}) \). Therefore, the second-order or nonlinear effects of the simple shear deformation can be omitted.

8. Conclusions

In conclusion, our algorithm successfully produces explicit formulas for \( C^{1/2} \), \( C^{-1/2} \) and the rotation tensor \( R \) as well. The key feature of the new algorithm is that there is no need to find the eigenvector of \( C \), and even more remarkable is that, for the first time, we have established the intrinsic relation between the rotation tensor (i.e., an exponential mapping) \( Q = \exp \mathbf{A} \) and the deformation gradient tensor \( \mathbf{F} \). For higher order tensor, we have given some formulations.
for any order tensor. Finally, as an application, we have evaluated Truesdell’s approximate results for simple shear deformation using our exact solution, and have confirmed that Truesdell’s results are extremely accurate.

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Appendix

\[ \alpha_0 = \frac{\lambda_2 \lambda_3 \sqrt{\lambda_1}}{\lambda_1^2 - \lambda_1 \lambda_2 - \lambda_1 \lambda_3 - \lambda_2 \lambda_3} \]
\[ - \frac{\lambda_1 \lambda_2 \sqrt{\lambda_3}}{\lambda_1 \lambda_2 - \lambda_1 \lambda_3 - \lambda_2 \lambda_3 + \lambda_3^2} + \frac{\lambda_1 \lambda_2 \sqrt{\lambda_3}}{\lambda_1 \lambda_2 - \lambda_1 \lambda_3 - \lambda_2 \lambda_3 + \lambda_3^2} \]

\[ \alpha_1 = -\frac{(\lambda_1 + 1) \sqrt{\lambda_2}}{\lambda_1^2 - \lambda_1 \lambda_2 - \lambda_1 \lambda_3 + \lambda_2 \lambda_3} + \frac{(\lambda_1 + 1) \sqrt{\lambda_2}}{\lambda_1 \lambda_2 - \lambda_1 \lambda_3 - \lambda_2 \lambda_3 + \lambda_3^2} - \frac{(\lambda_1 + 1) \sqrt{\lambda_3}}{\lambda_1 \lambda_2 - \lambda_1 \lambda_3 - \lambda_2 \lambda_3 + \lambda_3^2} \]

\[ \alpha_2 = \frac{\sqrt{\lambda_1}}{\lambda_1^2 - \lambda_1 \lambda_2 - \lambda_1 \lambda_3 + \lambda_2 \lambda_3} \]
\[ - \frac{\sqrt{\lambda_2}}{\lambda_1 \lambda_2 - \lambda_1 \lambda_3 - \lambda_2 \lambda_3 + \lambda_3^2} + \frac{\sqrt{\lambda_3}}{\lambda_1 \lambda_2 - \lambda_1 \lambda_3 - \lambda_2 \lambda_3 + \lambda_3^2} \]

\[ \beta_0 = \frac{\lambda_2 \lambda_3}{\sqrt{\lambda_1 \lambda_2 - \lambda_1 \lambda_3 - \lambda_2 \lambda_3}} \]
\[ - \frac{\lambda_1 \lambda_2}{\sqrt{\lambda_2 \lambda_1 \lambda_2 - \lambda_1 \lambda_3 - \lambda_2 \lambda_3}} + \frac{\lambda_1 \lambda_2}{\sqrt{\lambda_3 \lambda_1 \lambda_2 - \lambda_1 \lambda_3 - \lambda_2 \lambda_3 + \lambda_3^2}} \]

\[ \beta_1 = \frac{\lambda_2 + \lambda_3}{\sqrt{\lambda_1 \lambda_2 - \lambda_1 \lambda_3 - \lambda_2 \lambda_3}} \]
\[ + \frac{\lambda_1 + \lambda_2}{\sqrt{\lambda_2 \lambda_1 \lambda_2 - \lambda_1 \lambda_3 - \lambda_2 \lambda_3}} + \frac{\lambda_1 + \lambda_2}{\sqrt{\lambda_3 \lambda_1 \lambda_2 - \lambda_1 \lambda_3 - \lambda_2 \lambda_3 + \lambda_3^2}} \]

\[ \beta_2 = \frac{1}{\sqrt{\lambda_1 \lambda_2 - \lambda_1 \lambda_3 - \lambda_2 \lambda_3}} \]
\[ - \frac{1}{\sqrt{\lambda_2 \lambda_1 \lambda_2 - \lambda_1 \lambda_3 - \lambda_2 \lambda_3}} + \frac{1}{\sqrt{\lambda_3 \lambda_1 \lambda_2 - \lambda_1 \lambda_3 - \lambda_2 \lambda_3 + \lambda_3^2}} \]

\[ s_0 = \frac{1}{2} \frac{\gamma^2}{\gamma^2} + \frac{\gamma^2 - \sqrt{\gamma^4 + 4 \gamma^2} + 2}{(\gamma^2 + \sqrt{\gamma^4 + 4 \gamma^2}) \sqrt{\gamma^4 + 4 \gamma^2} \sqrt{1/2 \gamma^2 + 1 + 1/2 \sqrt{\gamma^4 + 4 \gamma^2}}} \]
\[ - \frac{\gamma^2 + \sqrt{\gamma^4 + 4 \gamma^2} + 2}{(\gamma^2 - \sqrt{\gamma^4 + 4 \gamma^2}) \sqrt{\gamma^4 + 4 \gamma^2} \sqrt{1/2 \gamma^2 + 1 - 1/2 \sqrt{\gamma^4 + 4 \gamma^2}}} \]
\[ s_1 = 1 + \frac{2}{\gamma^2} - \frac{\gamma^2 - \sqrt{\gamma^4 + 4\gamma^2 + 4}}{\gamma^2 + \sqrt{\gamma^4 + 4\gamma^2}} \\sqrt{\gamma^4 + 4\gamma^2} + \frac{1}{2} + \frac{1}{2\sqrt{\gamma^4 + 4\gamma^2}} \]  
\[ s_2 = \frac{1}{\gamma^2} + \frac{2}{\gamma^2 + \sqrt{\gamma^4 + 4\gamma^2}} \gamma^4 + 4\gamma^2 \sqrt{\gamma^4 + 4\gamma^2} + \frac{1}{2} + \frac{1}{2\sqrt{\gamma^4 + 4\gamma^2}} \]  
\[ (U^{-1})_{11} = \frac{1}{\sqrt{2\gamma^2 + 4 - 2\gamma\sqrt{\gamma^2 + 4}}} + \frac{1}{\sqrt{2\gamma^2 + 4 + 2\gamma\sqrt{\gamma^2 + 4}}} \]  
\[ (U^{-1})_{12} = (U^{-1})_{21} = \frac{2}{\sqrt{\gamma^2 + 4} \sqrt{2\gamma^2 + 4 + 2\gamma\sqrt{\gamma^2 + 4}}} - \frac{2}{\sqrt{\gamma^2 + 4} \sqrt{2\gamma^2 + 4 - 2\gamma\sqrt{\gamma^2 + 4}}} \]  
\[ (U^{-1})_{22} = -\frac{1}{\sqrt{2\gamma^2 + 4 - 2\gamma\sqrt{\gamma^2 + 4}}} + \frac{1}{\sqrt{2\gamma^2 + 4 + 2\gamma\sqrt{\gamma^2 + 4}}} \]  
\[ R_{11} = \frac{1}{\sqrt{2\gamma^2 + 4 - 2\gamma\sqrt{\gamma^2 + 4}}} + \frac{1}{\sqrt{2\gamma^2 + 4 + 2\gamma\sqrt{\gamma^2 + 4}}} \]  
\[ R_{12} = R_{21} = \frac{2}{\sqrt{\gamma^2 + 4} \sqrt{2\gamma^2 + 4 + 2\gamma\sqrt{\gamma^2 + 4}}} - \frac{2}{\sqrt{\gamma^2 + 4} \sqrt{2\gamma^2 + 4 - 2\gamma\sqrt{\gamma^2 + 4}}} \]  
\[ R_{22} = -\frac{1}{\sqrt{2\gamma^2 + 4 - 2\gamma\sqrt{\gamma^2 + 4}}} + \frac{1}{\sqrt{2\gamma^2 + 4 + 2\gamma\sqrt{\gamma^2 + 4}}} \]  
\[ + \frac{1}{\sqrt{\gamma^2 + 4} \sqrt{2\gamma^2 + 4 - 2\gamma\sqrt{\gamma^2 + 4}}} - \frac{1}{\sqrt{\gamma^2 + 4} \sqrt{2\gamma^2 + 4 + 2\gamma\sqrt{\gamma^2 + 4}}} \]