 doi:10.20944/preprints202004.0440.v1

# Explicit Representation of SO(3) Rotation Tensor for Deformable Bodies

Bo-Hua SUN[1]

[1] Institute of Mechanics and Technology & School of Civil Engineering
Xi'an University of Architecture and Technology, Xi'an 710055, China
http://imt.xauat.edu.cn
email: sunbohua@xauat.edu.cn

Computing the rotation tensor is vital in the analysis of deformable bodies. This paper describes an explicit expression for the SO(3) rotation tensor $\boldsymbol{R}$ of the deformation gradient $\boldsymbol{F}$, and successfully establishes an intrinsic relation between the exponential mapping $\boldsymbol{Q} = \exp \boldsymbol{A}$ and the deformation $\boldsymbol{F}$. As an application, Truesdell's simple shear deformation is revisited.

Keywords: finite deformation, deformation gradient, rotation tensor

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 $\boldsymbol{F} = \boldsymbol{\chi} \otimes \boldsymbol{\nabla}$, where $\boldsymbol{\nabla}$ is the del operator with respect to $\boldsymbol{X}$ and $\boldsymbol{\chi}(\boldsymbol{X}, t)$ is a mapping from a point $\boldsymbol{X}$ in the reference configuration to a point $\boldsymbol{x}$ in the current configuration through time $t$, namely $\boldsymbol{\chi} : \boldsymbol{X} \to \boldsymbol{x}$. The deformation gradient $\boldsymbol{F}$ can be split into stretch and rotation components by the polar multiplication decomposition [1, 2]: $\boldsymbol{F} = \boldsymbol{R} \cdot \boldsymbol{U} = \boldsymbol{R} \cdot \boldsymbol{V}$, where "$\cdot$" denotes the dot product and $\boldsymbol{U}$, $\boldsymbol{V}$, and $\boldsymbol{R}$ are the right stretch, left stretch, and rotation tensors, respectively. The rotation tensor satisfies the orthogonality condition $\boldsymbol{R} \cdot \boldsymbol{R}^T = \boldsymbol{R}^T \cdot \boldsymbol{R} = \boldsymbol{I}$ and $\det(\boldsymbol{R}) = 1$. From the polar decomposition and orthogonality condition, the right and left Cauchy–Green stretch tensors can be defined as $\boldsymbol{C} = \boldsymbol{F}^T \cdot \boldsymbol{F} = \boldsymbol{U} \cdot \boldsymbol{U} = \boldsymbol{U}^2$ and $\boldsymbol{B} = \boldsymbol{F} \cdot \boldsymbol{F}^T = \boldsymbol{V} \cdot \boldsymbol{V} = \boldsymbol{V}^2$, respectively. The algorithm for computing the rotation tensor is

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

However, one open problem is that no explicit expressions for both $(\boldsymbol{C})^{\frac{1}{2}}$ and $(\boldsymbol{C})^{-\frac{1}{2}}$ have been obtained.

In mathematics, an arbitrary SO(3) rotation tensor $\boldsymbol{Q}$ is given by

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

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

Note that the rotation tensor expression in Eq. (2) is not derived from the deformation gradient $\boldsymbol{F} = \boldsymbol{R} \cdot \boldsymbol{U}$, and so the rotation tensor $\boldsymbol{Q}$ is not equal to the rotation tensor $\boldsymbol{R}$, namely $\boldsymbol{Q} \neq \boldsymbol{R}$. Although the rotation tensor in Eq. (2) is widely used in the formulation of continuum physics, no expression has yet been reported for $\boldsymbol{A}$ in terms of the right Cauchy–Green tensor $\boldsymbol{C}$ and deformation gradient $\boldsymbol{F}$. The relationship between $\boldsymbol{A}$ and tensors such as the deformation gradient tensor $\boldsymbol{F}$ and the right Cauchy–Green tensor $\boldsymbol{C}$ remains one of the fundamental unsolved problems in continuum physics.

In this short article, we will focus on the abovementioned open problems, and propose explicit formulas for both the rotation tensor $\boldsymbol{R}$ and the skew-symmetric tensor $\boldsymbol{A}$. These formulas will be expressed in terms of the right Cauchy–Green tensor $\boldsymbol{C}$ and the deformation gradient $\boldsymbol{F}$.

According to the Cayley–Hamilton theorem [1–4], the explicit expression of $(\boldsymbol{C})^{\frac{1}{2}}$ can be set in the following form:

$$\boldsymbol{U} = \sqrt{\boldsymbol{C}} = \alpha_0\boldsymbol{I} + \alpha_1\boldsymbol{C} + \alpha_2\boldsymbol{C}^2, \quad (3)$$

in which the coefficients $\alpha_0$, $\alpha_1$, and $\alpha_2$ can be determined by the eigenvalues $\lambda_k$, $(k = 1, 2, 3)$ of $\boldsymbol{C}$ as follows:

$$\begin{pmatrix} \sqrt{\lambda_1} \\ \sqrt{\lambda_2} \\ \sqrt{\lambda_3} \end{pmatrix} = \begin{pmatrix} 1 & \lambda_1 & (\lambda_1)^2 \\ 1 & \lambda_2 & (\lambda_2)^2 \\ 1 & \lambda_3 & (\lambda_3)^2 \end{pmatrix} \begin{pmatrix} \alpha_0 \\ \alpha_1 \\ \alpha_2 \end{pmatrix} \quad (4)$$

Thus, we have the solution

$$\begin{pmatrix} \alpha_0 \\ \alpha_1 \\ \alpha_2 \end{pmatrix} = \begin{pmatrix} 1 & \lambda_1 & (\lambda_1)^2 \\ 1 & \lambda_2 & (\lambda_2)^2 \\ 1 & \lambda_3 & (\lambda_3)^2 \end{pmatrix}^{-1} \begin{pmatrix} \sqrt{\lambda_1} \\ \sqrt{\lambda_2} \\ \sqrt{\lambda_3} \end{pmatrix}. \quad (5)$$

The coefficients $\alpha_1, \alpha_2$, and $\alpha_3$ are derived in the appendix.

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

$$(\boldsymbol{C})^{-1/2} = \beta_0\boldsymbol{I} + \beta_1\boldsymbol{C} + \beta_2\boldsymbol{C}^2, \quad (6)$$

in which $\beta_0$, $\beta_1$, and $\beta_2$ are again determined by the eigenvalues $\lambda_k$, $(k = 1, 2, 3)$ of $\boldsymbol{C}$; their derivation can also be found in the appendix.

Using $\boldsymbol{C} = \boldsymbol{F}^T \cdot \boldsymbol{F}$, we obtain explicit expressions for $\boldsymbol{U}$ and $\boldsymbol{U}^{-1}$:

$$\boldsymbol{U} = \alpha_0\boldsymbol{I} + \alpha_1(\boldsymbol{F}^T \cdot \boldsymbol{F}) + \alpha_2(\boldsymbol{F}^T \cdot \boldsymbol{F})^2, \quad (7)$$

*Preprints* (www.preprints.org) | NOT PEER-REVIEWED | Posted: 24 April 2020 doi:10.20944/preprints202004.0440.v1



and

$$\boldsymbol{U}^{-1} = \beta_0 \boldsymbol{I} + \beta_1 (\boldsymbol{F}^T \cdot \boldsymbol{F}) + \beta_2 (\boldsymbol{F}^T \cdot \boldsymbol{F})^2. \tag{8}$$

With these formulas, we can write the rotation tensor $\boldsymbol{R}$ as follows:

$$\begin{aligned}\boldsymbol{R} &= \boldsymbol{F} \cdot \boldsymbol{U}^{-1} = \boldsymbol{F} \cdot (\beta_0 + \beta_1 \boldsymbol{C} + \beta_2 \boldsymbol{C}^2) \\ &= \boldsymbol{F} \cdot [\beta_0 \boldsymbol{I} + \beta_1 (\boldsymbol{F}^T \cdot \boldsymbol{F}) + \beta_2 (\boldsymbol{F}^T \cdot \boldsymbol{F})^2].\end{aligned} \tag{9}$$

The explicit expressions in Eqs. (7)–(9) have not previously been reported in the literature.

For the 2D case, the eigenvalues of $\boldsymbol{C}$ are $\lambda_1 = \frac{1}{2}C_{22} + \frac{1}{2}C_{11} + \frac{1}{2}\sqrt{C_{11}^2 - 2C_{22}C_11 + 4{C_{12}}^2 + C_{22}^2}$ and $\lambda_2 = \frac{1}{2}C_{22} + \frac{1}{2}C_{11} - \frac{1}{2}\sqrt{C_{11}^2 - 2C_{22}C_11 + 4{C_{12}}^2 + C_{22}^2}$.

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

$$\boldsymbol{U} = \frac{(\lambda_2\sqrt{\lambda_1} - \lambda_1\sqrt{\lambda_2})\boldsymbol{I} + (\sqrt{\lambda_2} - \sqrt{\lambda_1})\boldsymbol{C}}{\lambda_2 - \lambda_1}, \tag{10}$$

$$\boldsymbol{U}^{-1} = \frac{(\lambda_2^{3/2} - \lambda_1^{3/2})\boldsymbol{I} + (\lambda_1^{1/2} - \lambda_2^{1/2})\boldsymbol{C}}{(\lambda_2 - \lambda_1)\sqrt{\lambda_1\lambda_2}}, \tag{11}$$

and

$$\begin{aligned}\boldsymbol{R} &= \frac{\boldsymbol{F} \cdot \left[(\lambda_2^{3/2} - \lambda_1^{3/2})\boldsymbol{I} + (\lambda_1^{1/2} - \lambda_2^{1/2})\boldsymbol{C}\right]}{(\lambda_2 - \lambda_1)\sqrt{\lambda_1\lambda_2}} \\ &= \frac{\boldsymbol{F} \cdot \left[(\lambda_2^{3/2} - \lambda_1^{3/2})\boldsymbol{I} + (\lambda_1^{1/2} - \lambda_2^{1/2})(\boldsymbol{F}^T \cdot \boldsymbol{F})\right]}{(\lambda_2 - \lambda_1)\sqrt{\lambda_1\lambda_2}}.\end{aligned} \tag{12}$$

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

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

One approach is to set $\boldsymbol{Q} = e^{\boldsymbol{A}} = \boldsymbol{R} = \boldsymbol{F} \cdot \boldsymbol{U}^{-1}$, such that $\boldsymbol{A} = \ln(\boldsymbol{F} \cdot \boldsymbol{U}^{-1})$. However, this is the final format. Another method is to use the rotation tensor in Eq. (9) and let $\boldsymbol{Q} = \boldsymbol{R}$, that is,

$$\begin{aligned}&\boldsymbol{I} + \frac{\sin\omega}{\omega}\boldsymbol{A} + \frac{1-\cos\omega}{\omega^2}\boldsymbol{A}^2 \\ &= \boldsymbol{F} \cdot (\beta_0 + \beta_1 \boldsymbol{C} + \beta_2 \boldsymbol{C}^2),\end{aligned} \tag{13}$$

Transposing both sides of this equation gives

$$\begin{aligned}&\boldsymbol{I} - \frac{\sin\omega}{\omega}\boldsymbol{A} + \frac{1-\cos\omega}{\omega^2}\boldsymbol{A}^2 \\ &= (\beta_0 + \beta_1 \boldsymbol{C} + \beta_2 \boldsymbol{C}^2) \cdot \boldsymbol{F}^T,\end{aligned} \tag{14}$$

Equation (13) minus Eq. (14) gives an explicit expression of the skew-symmetric tensor $\boldsymbol{A}$. For the 3D case, we have

$$\begin{aligned}\boldsymbol{A} = &\frac{\omega\beta_0}{2\sin\omega}(\boldsymbol{F} - \boldsymbol{F}^T) + \frac{\omega\beta_1}{2\sin\omega}(\boldsymbol{F}\cdot\boldsymbol{C} - \boldsymbol{C}\cdot\boldsymbol{F}^T) \\ &+ \frac{\omega\beta_2}{2\sin\omega}(\boldsymbol{F}\cdot\boldsymbol{C}^2 - \boldsymbol{C}^2\cdot\boldsymbol{F}^T).\end{aligned} \tag{15}$$

and for the 2D case, we have

$$\begin{aligned}\boldsymbol{A} = &\frac{\omega}{2\sin\omega}\frac{(\lambda_2^{3/2} - \lambda_1^{3/2})(\boldsymbol{F} - \boldsymbol{F}^T)}{(\lambda_2 - \lambda_1)\sqrt{\lambda_1\lambda_2}} \\ &+ \frac{\omega}{2\sin\omega}\frac{(\lambda_1^{1/2} - \lambda_2^{1/2})(\boldsymbol{F}\cdot\boldsymbol{C} - \boldsymbol{C}\cdot\boldsymbol{F}^T)}{(\lambda_2 - \lambda_1)\sqrt{\lambda_1\lambda_2}}.\end{aligned} \tag{16}$$

Equations (15) and (16) are the intrinsic linkages between the rotation tensor $\boldsymbol{Q}$ and the deformation gradient tensor $\boldsymbol{F}$, as well as the Cauchy–Green tensor $\boldsymbol{C}$. These relations reveal that the skew-symmetric tensor $\boldsymbol{A}$ is not only related to the antisymmetric tensor $\boldsymbol{F}-\boldsymbol{F}^T$, but also to another two antisymmetric tensors: $\boldsymbol{F}\cdot\boldsymbol{C} - \boldsymbol{C}\cdot\boldsymbol{F}^T$ and $\boldsymbol{F}\cdot\boldsymbol{C}^2 - \boldsymbol{C}^2\cdot\boldsymbol{F}^T$. If the deformation gradient $\boldsymbol{F}$ is symmetric, i.e., $\boldsymbol{F} = \boldsymbol{F}^T$, then $\boldsymbol{A} = \boldsymbol{0}$ and $\boldsymbol{Q} = \boldsymbol{I}$.

In co-moving coordinates, the deformation gradient is defined by $\boldsymbol{F} = \boldsymbol{g}_k \otimes \boldsymbol{G}^k$; thus, $\boldsymbol{F}^T = \boldsymbol{G}^k \otimes \boldsymbol{g}_k$, $\boldsymbol{C} = g_{ij}\boldsymbol{G}^i \otimes \boldsymbol{G}^j$ and $\boldsymbol{C}^2 = g_{ij}g_{k\ell}G^{jk}\boldsymbol{G}^i \otimes \boldsymbol{G}^\ell$. Substituting these formulas into Eq. (9) leads to another form of the rotation tensor.

If we introduce the displacement vector $\boldsymbol{u}$ from the reference to the current configuration, the deformation mapping becomes $\boldsymbol{\chi}(\boldsymbol{X}) = \boldsymbol{X} + \boldsymbol{u}$ and the deformation gradient tensor is $\boldsymbol{F} = \boldsymbol{I} + \boldsymbol{u}\otimes\boldsymbol{\nabla}$. Hence, its transpose $\boldsymbol{F}^T = \boldsymbol{I} + \boldsymbol{\nabla}\otimes\boldsymbol{u}$, $\boldsymbol{C} = \boldsymbol{F}^T\cdot\boldsymbol{F} = \boldsymbol{I} + \boldsymbol{u}\otimes\boldsymbol{\nabla} + \boldsymbol{\nabla}\otimes\boldsymbol{u} + (\boldsymbol{\nabla}\otimes\boldsymbol{u})\cdot(\boldsymbol{u}\otimes\boldsymbol{\nabla})$, and $\boldsymbol{C}^2 = \boldsymbol{I} + 2(\boldsymbol{u}\otimes\boldsymbol{\nabla} + \boldsymbol{\nabla}\otimes\boldsymbol{u}) + (\boldsymbol{u}\otimes\boldsymbol{\nabla})\cdot(\boldsymbol{\nabla}\otimes\boldsymbol{u}) + 3(\boldsymbol{\nabla}\otimes\boldsymbol{u})\cdot(\boldsymbol{u}\otimes\boldsymbol{\nabla}) + (\boldsymbol{u}\otimes\boldsymbol{\nabla})^2 + (\boldsymbol{\nabla}\otimes\boldsymbol{u})^2 + (\boldsymbol{u}\otimes+\boldsymbol{\nabla}\otimes\boldsymbol{u})\cdot(\boldsymbol{\nabla}\otimes\boldsymbol{u})\cdot(\boldsymbol{u}\otimes\boldsymbol{\nabla}) + (\boldsymbol{\nabla}\otimes\boldsymbol{u})\cdot(\boldsymbol{u}\otimes\boldsymbol{\nabla})\cdot(\boldsymbol{u}\otimes\boldsymbol{\nabla}+\boldsymbol{\nabla}\otimes\boldsymbol{u}) + [(\boldsymbol{\nabla}\otimes\boldsymbol{u})\cdot(\boldsymbol{u}\otimes\boldsymbol{\nabla})]^2$. Substituting these expressions into Eq. (9), we have the rotation tensor $\boldsymbol{R}$ expressed in terms of the displacement vector $\boldsymbol{u}$, namely $\boldsymbol{R} = (\boldsymbol{I}+\boldsymbol{u}\otimes\boldsymbol{\nabla})\cdot(\beta_0\boldsymbol{I} + \beta_1\boldsymbol{C} + \beta_2\boldsymbol{C}^2)$.

With this displacement form of the rotation tensor, we propose two consistent approximations of the rotation tensor based on the order of $\boldsymbol{u}\otimes\boldsymbol{\nabla}$, for instance, the first order rotation tensor

$$\begin{aligned}\boldsymbol{R}_{1\mathrm{st}} = &(\beta_0 + \beta_1 + \beta_2)\boldsymbol{I} + (\beta_0 + 2\beta_1 + 4\beta_2)\boldsymbol{u}\otimes\boldsymbol{\nabla} \\ &+ (\beta_1 + 2\beta_2)\boldsymbol{\nabla}\otimes\boldsymbol{u} + \mathcal{O}[(\boldsymbol{u}\otimes\boldsymbol{\nabla})^2],\end{aligned} \tag{17}$$

and the second order rotation tensor

$$\begin{aligned}\boldsymbol{R}_{2\mathrm{nd}} = &(\beta_0 + \beta_1 + \beta_2)\boldsymbol{I} + (\beta_0 + 2\beta_1 + 4\beta_2)\boldsymbol{u}\otimes\boldsymbol{\nabla} \\ &+ (\beta_1 + 2\beta_2)\boldsymbol{\nabla}\otimes\boldsymbol{u} + (\beta_1 + 10\beta_2)(\boldsymbol{u}\otimes\boldsymbol{\nabla}\cdot\boldsymbol{\nabla}\otimes\boldsymbol{u}) \\ &+ \beta_2[(\boldsymbol{u}\otimes\nabla)^2 + (\boldsymbol{\nabla}\otimes\boldsymbol{u})^2] + \mathcal{O}[(\boldsymbol{u}\otimes\boldsymbol{\nabla})^3].\end{aligned} \tag{18}$$

Those two approximations of the rotation tensor have also not been seen in literature.

 doi:10.20944/preprints202004.0440.v1



In summary, all of the explicit expressions for $\boldsymbol{U}$, $\boldsymbol{U}^{-1}$, and $\boldsymbol{R}$ derived in this letter have been formulated without using the eigenvectors of $\boldsymbol{C}$, an essential feature that is different from traditional algorithms.

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

**(1) a 2D deformation**: Consider the deformation given by the mapping

$$\begin{aligned}\boldsymbol{\chi}(\boldsymbol{X}) = &\frac{1}{4}[4X_1 - (9 - 3X_1 - 5X_2 - X_1X_2)t]\boldsymbol{G}^1 \\ &+ \frac{1}{4}[4X_2 + (16 + 8X_1)t]\boldsymbol{G}^2.\end{aligned} \tag{19}$$

For $\boldsymbol{X} = (0, 0)$, $t = 1$, determine the symmetric stretch tensor $\boldsymbol{U}$ and rotation tensor $\boldsymbol{R}$.

From the deformation mapping in Eq. (19), we have the deformation gradient $\boldsymbol{F} = \frac{1}{4}(\boldsymbol{G}^1 \otimes \boldsymbol{G}^1 - 5\boldsymbol{G}^1 \otimes \boldsymbol{G}^2 + 8\boldsymbol{G}^2 \otimes \boldsymbol{G}^1 + 4\boldsymbol{G}^2 \otimes \boldsymbol{G}^2)$ and the right Cauchy–Green tensor $\boldsymbol{C} = \frac{1}{16}(65\boldsymbol{G}^1 \otimes \boldsymbol{G}^1 + 27\boldsymbol{G}^1 \otimes \boldsymbol{G}^2 + 27\boldsymbol{G}^2 \otimes \boldsymbol{G}^1 + 41\boldsymbol{G}^2 \otimes \boldsymbol{G}^2)$. From the eigenvalue equation $|\boldsymbol{C} - \lambda\boldsymbol{I}| = 0$, we obtain two eigenvalues $\lambda_1 = \frac{53}{16} + \frac{3}{16}\sqrt{97}$ and $\lambda_2 = \frac{53}{16} - \frac{3}{16}\sqrt{97}$. Hence, the coefficients are $\alpha_0 = 0.78975$, $\alpha_1 = 0.28718$ and $\beta_0 = 0.97903$, $\beta_1 = -0.10443$. Therefore, we have $\boldsymbol{U} = 0.1956\boldsymbol{G}^1 \otimes \boldsymbol{G}^1 + 0.484\boldsymbol{G}^1 \otimes \boldsymbol{G}^2 + 0.484\boldsymbol{G}^2 \otimes \boldsymbol{G}^1 + 1.525\boldsymbol{G}^2 \otimes \boldsymbol{G}^2$, its inverse $\boldsymbol{U}^{-1} = 0.554\boldsymbol{G}^1 \otimes \boldsymbol{G}^1 - 0.176\boldsymbol{G}^1 \otimes \boldsymbol{G}^2 - 0.176\boldsymbol{G}^2 \otimes \boldsymbol{G}^1 + 0.711\boldsymbol{G}^2 \otimes \boldsymbol{G}^2$, and the rotation tensor $\boldsymbol{R} = \boldsymbol{F} \cdot \boldsymbol{U}^{-1} = 0.35897\boldsymbol{G}^1 \otimes \boldsymbol{G}^1 - 0.93334\boldsymbol{G}^1 \otimes \boldsymbol{G}^2 + 0.93334\boldsymbol{G}^2 \otimes \boldsymbol{G}^1 + 0.35897\boldsymbol{G}^2 \otimes \boldsymbol{G}^2$. The results are correct because $\boldsymbol{R} \cdot \boldsymbol{R}^T = \boldsymbol{R}^T \cdot \boldsymbol{R} = \boldsymbol{I}$ and $\det \boldsymbol{R} = 1$.

**(2) Simple shear deformation**: This shear deformation is defined to be a set of line elements whose lengths and orientations are unchanged, as shown in Fig. 1. The deformation mapping in this case is $\boldsymbol{\chi}(\boldsymbol{X}) = (X_1 + \gamma X_2)\boldsymbol{G}^1 + X_2\boldsymbol{G}^2 + X_3\boldsymbol{G}^3$. We find that the deformation gradient tensor is $\boldsymbol{F} = \boldsymbol{I} + \gamma\boldsymbol{G}^1 \otimes \boldsymbol{G}^2 = \boldsymbol{G}^1 \otimes \boldsymbol{G}^1 + \gamma\boldsymbol{G}^1 \otimes \boldsymbol{G}^2 + \boldsymbol{G}^2 \otimes \boldsymbol{G}^2 + \boldsymbol{G}^3 \otimes \boldsymbol{G}^3$ and its transpose is $\boldsymbol{F}^T = \boldsymbol{I} + \gamma\boldsymbol{G}^2 \otimes \boldsymbol{G}^1 = \boldsymbol{G}^1 \otimes \boldsymbol{G}^1 + \gamma\boldsymbol{G}^2 \otimes \boldsymbol{G}^1 + \boldsymbol{G}^2 \otimes \boldsymbol{G}^2 + \boldsymbol{G}^3 \otimes \boldsymbol{G}^3$. The Cauchy–Green tensor is written as $\boldsymbol{C} = \boldsymbol{F}^T \cdot \boldsymbol{F} = \boldsymbol{I} + \gamma\boldsymbol{G}^1 \otimes \boldsymbol{G}^2 + \gamma\boldsymbol{G}^2 \otimes \boldsymbol{G}^1 + \gamma^2\boldsymbol{G}^2 \otimes \boldsymbol{G}^2$, and its square is $\boldsymbol{C}^2 = (1 + \gamma^2)\boldsymbol{G}^1 \otimes \boldsymbol{G}^1 + (2\gamma + \gamma^3)\boldsymbol{G}^1 \otimes \boldsymbol{G}^2 + (2\gamma + \gamma^3)\boldsymbol{G}^2 \otimes \boldsymbol{G}^1 + (\gamma^4 + 3\gamma^2 + 1)\boldsymbol{G}^2 \otimes \boldsymbol{G}^2 + \boldsymbol{G}^3 \otimes \boldsymbol{G}^3$. The eigenvalues of $\boldsymbol{C}$ 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, the right stretch tensor is obtained as $\boldsymbol{U}^{-1} = s_0\boldsymbol{I} + s_1\boldsymbol{C} + s_2\boldsymbol{C}^2 = (U^{-1})_{11}\boldsymbol{G}^1 \otimes \boldsymbol{G}^1 + (U^{-1})_{12}\boldsymbol{G}^1 \otimes \boldsymbol{G}^2 + (U^{-1})_{21}\boldsymbol{G}^2 \otimes \boldsymbol{G}^1 + (U^{-1})_{22}\boldsymbol{G}^2 \otimes \boldsymbol{G}^2 + \boldsymbol{G}^3 \otimes \boldsymbol{G}^3$ and the rotation tensor is $\boldsymbol{R} = R_{11}\boldsymbol{G}^1 \otimes \boldsymbol{G}^1 + R_{12}\boldsymbol{G}^1 \otimes \boldsymbol{G}^2 + R_{21}\boldsymbol{G}^2 \otimes \boldsymbol{G}^1 + R_{22}\boldsymbol{G}^2 \otimes \boldsymbol{G}^2 + \boldsymbol{G}^3 \otimes \boldsymbol{G}^3$, where the coefficients $s_0, s_1, s_2$, and other elements are given in the appendix.

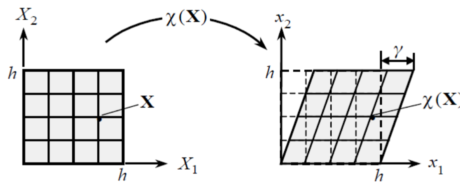


FIG. 1: Simple shear deformation.

The right stretch tensor $\boldsymbol{U}$, its inverse $\boldsymbol{C}^{-1}$, and the rotation tensor $\boldsymbol{R}$ obtained here for the shear deformation have no geometrical constraints. From Fig. 2, 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.

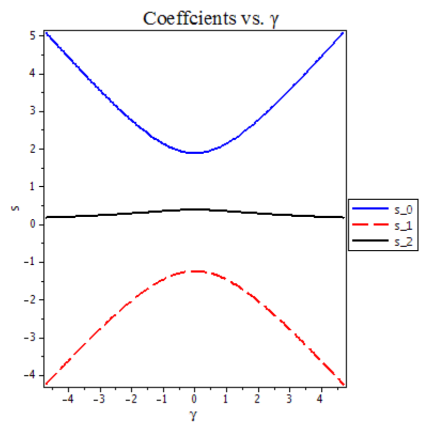


FIG. 2: Coefficient comparisons: $s_0, s_1$, and $s_2$.

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 $\boldsymbol{C}$ are $\lambda_1 = 1$, $\lambda_2 = 1 + \frac{1}{2}\gamma$, and $\lambda_2 = 1 - \frac{1}{2}\gamma$; and rotation tensor is

$$\boldsymbol{R}_{\text{Truesdell}} = \begin{pmatrix} \frac{1}{\sqrt{1+\frac{1}{4}\gamma^2}} & \frac{2\gamma}{\sqrt{1+\frac{1}{4}\gamma^2}} & 0 \\ -\frac{2\gamma}{\sqrt{1+\frac{1}{4}\gamma^2}} & \frac{1}{\sqrt{1+\frac{1}{4}\gamma^2}} & 0 \\ 0 & 0 & 1 \end{pmatrix}. \tag{20}$$

Through numerical comparisons, we found that Truesdell's results are very accurate, with errors of order $10^{-13}$. Therefore, the second-order or nonlinear effects of the simple shear deformation can definitely be omitted.

In conclusion, our algorithm successfully produces explicit formulas for both $\boldsymbol{C}^{-1/2}$ and the rotation tensor $\boldsymbol{R}$. The key feature of the new algorithm is that there is no need to find the eigenvector of $\boldsymbol{C}$, and even more remarkable is that, for the first time, we have established the intrinsic relation between the rotation tensor $Q$ and the deformation gradient tensor $\boldsymbol{F}$. 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.

 doi:10.20944/preprints202004.0440.v1




[1] C. Truesdell and W. Noll, The Non-Linear Field Theories of Mechanics. *Handbuch der Physik*, Editor: S. Flügge, Vol. 3 (Springer-Verlag Berlin,1969).

[2] C. Truesdell and R. Toupin, Principles of Classical Mechanics and Field Theory. *Handbuch der Physik*, Editor: S. Flügge, Vol. 2 (Springer-Verlag Berlin, 1960).

[3] A. Cayley, Philos. Trans. **148**, 17 (1858).

[4] W. R. Hamilton, Lectures on Quaternions (Dublin, 1853).

[5] D. D Fox, A geometrically exact shell theory, PhD Dissertation, Stanford University (1990).


## Appendix

$$\alpha_0 = \frac{\lambda_2\lambda_3\sqrt{\lambda_1}}{{\lambda_1}^2 - \lambda_1\lambda_2 - \lambda_1\lambda_3 + \lambda_2\lambda_3} - \frac{\lambda_1\lambda_3\sqrt{\lambda_2}}{\lambda_1\lambda_2 - \lambda_1\lambda_3 - {\lambda_2}^2 + \lambda_2\lambda_3} + \frac{\lambda_1\lambda_2\sqrt{\lambda_3}}{\lambda_1\lambda_2 - \lambda_1\lambda_3 - \lambda_2\lambda_3 + {\lambda_3}^2}, \tag{21}$$

$$\alpha_1 = -\frac{(\lambda_2+\lambda_3)\sqrt{\lambda_1}}{{\lambda_1}^2 - \lambda_1\lambda_2 - \lambda_1\lambda_3 + \lambda_2\lambda_3} + \frac{(\lambda_1+\lambda_3)\sqrt{\lambda_2}}{\lambda_1\lambda_2 - \lambda_1\lambda_3 - {\lambda_2}^2 + \lambda_2\lambda_3} - \frac{(\lambda_1+\lambda_2)\sqrt{\lambda_3}}{\lambda_1\lambda_2 - \lambda_1\lambda_3 - \lambda_2\lambda_3 + {\lambda_3}^2}, \tag{22}$$

$$\alpha_2 = \frac{\sqrt{\lambda_1}}{{\lambda_1}^2 - \lambda_1\lambda_2 - \lambda_1\lambda_3 + \lambda_2\lambda_3} - \frac{\sqrt{\lambda_2}}{\lambda_1\lambda_2 - \lambda_1\lambda_3 - {\lambda_2}^2 + \lambda_2\lambda_3} + \frac{\sqrt{\lambda_3}}{\lambda_1\lambda_2 - \lambda_1\lambda_3 - \lambda_2\lambda_3 + {\lambda_3}^2}. \tag{23}$$

$$\beta_0 = \frac{\lambda_2\lambda_3}{\sqrt{\lambda_1}({\lambda_1}^2 - \lambda_1\lambda_2 - \lambda_1\lambda_3 + \lambda_2\lambda_3)} - \frac{\lambda_1\lambda_3}{\sqrt{\lambda_2}(\lambda_1\lambda_2 - \lambda_1\lambda_3 - {\lambda_2}^2 + \lambda_2\lambda_3)} + \frac{\lambda_1\lambda_2}{\sqrt{\lambda_3}(\lambda_1\lambda_2 - \lambda_1\lambda_3 - \lambda_2\lambda_3 + {\lambda_3}^2)}, \tag{24}$$

$$\beta_1 = -\frac{\lambda_2+\lambda_3}{\sqrt{\lambda_1}({\lambda_1}^2 - \lambda_1\lambda_2 - \lambda_1\lambda_3 + \lambda_2\lambda_3)} + \frac{\lambda_1+\lambda_3}{\sqrt{\lambda_2}(\lambda_1\lambda_2 - \lambda_1\lambda_3 - {\lambda_2}^2 + \lambda_2\lambda_3)} - \frac{\lambda_1+\lambda_2}{\sqrt{\lambda_3}(\lambda_1\lambda_2 - \lambda_1\lambda_3 - \lambda_2\lambda_3 + {\lambda_3}^2)}, \tag{25}$$

$$\beta_2 = \frac{1}{\sqrt{\lambda_1}({\lambda_1}^2 - \lambda_1\lambda_2 - \lambda_1\lambda_3 + \lambda_2\lambda_3)} - \frac{1}{\sqrt{\lambda_2}(\lambda_1\lambda_2 - \lambda_1\lambda_3 - {\lambda_2}^2 + \lambda_2\lambda_3)} + \frac{1}{\sqrt{\lambda_3}(\lambda_1\lambda_2 - \lambda_1\lambda_3 - \lambda_2\lambda_3 + {\lambda_3}^2)}. \tag{26}$$

$$s_0 = \frac{1}{2} - \frac{1}{\gamma^2} + \frac{\gamma^2 - \sqrt{\gamma^4+4\gamma^2}+2}{(\gamma^2+\sqrt{\gamma^4+4\gamma^2})\sqrt{\gamma^4+4\gamma^2}\sqrt{1/2\,\gamma^2+1+1/2\sqrt{\gamma^4+4\gamma^2}}} - \frac{\gamma^2 + \sqrt{\gamma^4+4\,\gamma^2}+2}{(\gamma^2-\sqrt{\gamma^4+4\,\gamma^2})\sqrt{\gamma^4+4\gamma^2}\sqrt{1/2\gamma^2+1-1/2\sqrt{\gamma^4+4\gamma^2}}} \tag{27}$$

$$s_1 = 1 + \frac{2}{\gamma^2} - \frac{\gamma^2 - \sqrt{\gamma^4+4\gamma^2}+4}{(\gamma^2+\sqrt{\gamma^4+4\gamma^2})\sqrt{\gamma^4+4\gamma^2}\sqrt{1/2\gamma^2+1+1/2\sqrt{\gamma^4+4\gamma^2}}} + \frac{\gamma^2 + \sqrt{\gamma^4+4\gamma^2}+4}{(\gamma^2-\sqrt{\gamma^4+4\gamma^2})\sqrt{\gamma^4+4\gamma^2}\sqrt{1/2\gamma^2+1-1/2\sqrt{\gamma^4+4\gamma^2}}} \tag{28}$$

$$s_2 = -\frac{1}{\gamma^2} + \frac{2}{(\gamma^2+\sqrt{\gamma^4+4\gamma^2})\sqrt{\gamma^4+4\gamma^2}\sqrt{1/2\gamma^2+1+1/2\sqrt{\gamma^4+4\gamma^2}}} - \frac{2}{(\gamma^2-\sqrt{\gamma^4+4\,\gamma^2})\sqrt{\gamma^4+4\gamma^2}\sqrt{1/2\gamma^2+1-1/2\sqrt{\gamma^4+4\gamma^2}}} \tag{29}$$

$$(U^{-1})_{11} = \frac{1}{\sqrt{2\gamma^2+4-2\gamma\sqrt{\gamma^2+4}}} + \frac{1}{\sqrt{2\gamma^2+4+2\gamma\sqrt{\gamma^2+4}}} + \frac{\gamma}{\sqrt{\gamma^2+4}\sqrt{2\gamma^2+4-2\gamma\sqrt{\gamma^2+4}}} - \frac{\gamma}{\sqrt{\gamma^2+4}\sqrt{2\gamma^2+4+2\gamma\sqrt{\gamma^2+4}}} \tag{30}$$

$$(U^{-1})_{12} = (U^{-1})_{21} = \frac{2}{\sqrt{\gamma^2+4}\sqrt{2\gamma^2+4+2\gamma\sqrt{\gamma^2+4}}} - \frac{2}{\sqrt{\gamma^2+4}\sqrt{2\gamma^2+4-2\gamma\sqrt{\gamma^2+4}}} \tag{31}$$

$$(U^{-1})_{22} = -\frac{1}{\sqrt{2\gamma^2+4-2\gamma\sqrt{\gamma^2+4}}} - \frac{1}{\sqrt{2\gamma^2+4+2\gamma\sqrt{\gamma^2+4}}} + \frac{\gamma}{\sqrt{\gamma^2+4}\sqrt{2\gamma^2+4-2\gamma\sqrt{\gamma^2+4}}} - \frac{\gamma}{\sqrt{\gamma^2+4}\sqrt{2\gamma^2+4+2\gamma\sqrt{\gamma^2+4}}} \tag{32}$$

$$R_{11} = \frac{1}{\sqrt{2\gamma^2+4-2\gamma\sqrt{\gamma^2+4}}} + \frac{1}{\sqrt{2\gamma^2+4+2\gamma\sqrt{\gamma^2+4}}} + \frac{\gamma}{\sqrt{\gamma^2+4}\sqrt{2\gamma^2+4+2\gamma\sqrt{\gamma^2+4}}} - \frac{\gamma}{\sqrt{\gamma^2+4}\sqrt{2\gamma^2+4-2\gamma\sqrt{\gamma^2+4}}} \tag{33}$$

$$R_{12} = R_{21} = \frac{2}{\sqrt{\gamma^2+4}\sqrt{2\gamma^2+4+2\gamma\sqrt{\gamma^2+4}}} - \frac{2}{\sqrt{\gamma^2+4}\sqrt{2\gamma^2+4-2\gamma\sqrt{\gamma^2+4}}} \tag{34}$$

$$R_{22} = -\frac{1}{\sqrt{2\gamma^2+4-2\gamma\sqrt{\gamma^2+4}}} - \frac{1}{\sqrt{2\gamma^2+4+2\gamma\sqrt{\gamma^2+4}}} + \frac{\gamma}{\sqrt{\gamma^2+4}\sqrt{2\gamma^2+4-2\gamma\sqrt{\gamma^2+4}}} - \frac{\gamma}{\sqrt{\gamma^2+4}\sqrt{2\gamma^2+4+2\gamma\sqrt{\gamma^2+4}}} \tag{35}$$