



NOTE

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A note on the derivation of quotient rules and their use in QR kinematics

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Abstract QR kinematics have recently gained interest in various fields of mechanics due to its ease of application from an experimenter's standpoint. This method, however, faces restriction owing to its dependence on the coordinate system in which the matrix of the deformation gradient is written and the QR decomposition is performed. Since different experimental setups are more amenable to different coordinate systems, it is important to derive and adopt transformation rules pertinent to QR kinematics that help us navigate from one coordinate system to another with ease. In this short technical note, the quotient rules for transforming vectors and second-order tensors between different coordinate systems obtained from a QR decomposition of the deformation gradient have been derived. The use of these quotient rules in comparing results obtained from two different rheometry methods has also been demonstrated.

1 Introduction

In recent years, QR kinematics have gained interest in various fields of mechanics such as theory of elasticity [7–9, 13, 15], viscoelasticity and damage [3], plasticity [14, 16, 19], rheometry [17], mechanics of plate tectonics [2], and biomechanics [1, 4, 12, 21, 22]. The primary attraction of this framework is its ease of application from an experimenter's point of view. Although the traditional theory of continuum mechanics based on a polar decomposition of the deformation gradient has been extensively used and mathematically rigorous, this theory is difficult to implement in an experimental framework. In particular, the constitutive models in this theory are mostly developed using the invariants of an appropriate metric or strain tensor. Criscione et al. [5] have shown that the covariance between the invariants makes the parametrization of the constitutive models extremely difficult. To overcome this issue, an upper-triangular decomposition of the matrix of the deformation gradient was proposed [9, 11, 20] that has minimum covariance between its components. In this framework, the deformation gradient is expressed in its matrix form in a chosen coordinate system and thereafter a Gram–Schmidt process is applied on this matrix that decomposes the deformation gradient into an orthogonal matrix \mathcal{R} and, an upper-triangular matrix \mathcal{U} , called the Laplace stretch. Unlike the polar decomposition, the orthogonal matrix \mathcal{R} plays an important role in coordinate transformation, whereas the six components of the upper-triangular Laplace stretch *completely* describe the deformation of a body in all possible degrees of freedom. These six components along with their thermodynamic counterparts can be used in defining scalar conjugate stress/strain base pairs which have been used in developing constitutive models for elastic isotropic and anisotropic solids [6–8] and elastic–plastic materials [16].

As mentioned earlier, the QR framework is particularly useful from an experimental standpoint particularly in the field of plasticity and rheometry. In the former, Paul and Freed [14] proposed a new method to experimentally determine the plastic part of Laplace stretch that overcomes the theoretical issue faced by the traditional

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multiplicative decomposition of deformation gradient, i.e., $\mathbf{F} = \mathbf{F}^e \mathbf{F}^p$. The use of **QR** framework seems to be promising in the field of rheometry since the method proposed by Paul et al. [17] can possibly circumvent the problem of simultaneous use of two kinds of rheometers, a cone and plate and a parallel plate rheometer, in determining the rheological properties of material by using *only one* of them.¹ Despite many advantages, this theory is not without its challenges. It is worth noting that the primary kinematic variable of this framework, the Laplace stretch, is derived from a Gram–Schmidt factorization of the matrix of the deformation gradient, expressed in terms of a specified set of base vectors. Therefore, one major caveat of this theory is that in this framework, one cannot work with the kinematic and kinetic variables in their tensorial forms and a coordinate system must be specified. In other words, the **QR** kinematics framework loses the mathematical rigor of the traditional theory (using a polar decomposition) at the expense of the ease of interpretation and its practical application in the experimental setup.

Due to its importance at the very foundation of the **QR** framework, the choice of the associated coordinate system in which the matrix of the deformation gradient is written, poses some important questions. For example, if the deformation gradient is written in a Cartesian coordinate system, then one is left with six choices for a set of base vectors in which the Laplace stretch can be obtained. Needless to say, these six choices will produce six different Laplace stretches and hence this ambiguity will render any constitutive model based on Laplace stretch invalid. To resolve this issue, Paul et al. [18] proposed a coordinate re-indexing strategy² to assign the base vectors required for the physical frame of reference (in which Laplace stretch is written) in a particular sequence. Specifically, the first base vector was chosen in such a way that the side of a representative cube that lies along this vector in the undeformed configuration of the body undergoes minimum amount of transverse shear. The second base vector is chosen such that the plane formed by the first and second base vectors experience minimum amount of in-plane shear. Such a strategy need not be adopted for other coordinate systems for which the coordinate axes bear different physical meanings such as a cylindrical polar coordinate system. For a spherical coordinate system, one needs to use a simpler strategy to re-index the deformation gradient since the number of possible coordinate systems reduces to four.

Although the coordinate re-indexing strategy allows us to use the **QR** framework in different fields of application, this framework is still not without its challenges. It is to note that the base vectors for the physical frame of reference in which Laplace stretch is written are derived by using a successive orthogonal projection on the re-indexed matrix of the deformation gradient. This process makes the coordinate transformations of vectors and tensors from one physical frame of reference to another rather difficult. For example, in their paper, Paul et al. [17] proposed that the characterization of rheological properties may be done using only one rheometer and the use of both cone and plate and a parallel plate rheometer can thus be avoided. In order to show that only one rheometer is sufficient to characterize the materials, one needs to show that the ‘post-processed’ results obtained from both the rheometers are comparable. Since the two rheometers are more amenable to two different coordinate systems, it is likely that the measurable quantities such as force on a plate or torque will be derived in two different physical frames of reference. To compare the results, one must transform them into the same coordinate system. However, the derivation of the base vectors using a successive orthogonal projection makes the coordinate transformation quite convoluted. This short paper addresses this particular issue where we derive the quotient rules required to transform different quantities obtained in different physical frames of reference.

In this paper, transformation rules for vectors and tensorial quantities have been derived from one physical frame of reference to another. It has been shown that a direct transformation of vectors and tensors through base vectors would lead to erroneous results since these base vectors are derived by using Laplace’s successive orthogonal projection. The rest of the paper is organized as follows. In Sect. 2, the relevant derivations and theory of **QR** kinematics is revisited. The main derivation of the quotient rules constitutes Sect. 3. In Sect. 4, the use of the quotient rules is shown with the help of the problems in rheometry. Finally, the results are summarized and drawn to conclusion. In this paper, vectors and second-order tensors have been represented by boldfaced lower and upper case letters, respectively. Their components are represented using the same letters without the boldface. ‘[]’ has been used to write the components of a second-order tensor in its matrix form.

¹ The experimental verification of the proposed methods is yet to be conducted.

² One can draw an analogy between this re-indexing strategy and material frame indifference. The coordinate re-indexing strategy restricts the coordinate system in which the deformation gradient is to be written, and therefore, the choice of different coordinate systems is taken away. Needless to say that this method is quite restrictive as compared to the traditional method.

2 Preliminaries

Let us consider a simply connected body \mathcal{B} embedded in a three-dimensional Euclidean point space. The body undergoes a motion $\mathcal{X}(\mathbf{X}, t)$ that maps points from the undeformed configuration of the body $\kappa_r(\mathcal{B})$ into its current (deformed) configuration $\kappa_t(\mathcal{B})$. Let \mathbf{X} and \mathbf{x} denote the position vectors of a point in the undeformed and current configuration of the body, respectively. The deformation gradient of the motion can be defined as

$$\mathbf{F} = \frac{\partial \mathcal{X}(\mathbf{X}, t)}{\partial \mathbf{X}}. \quad (1)$$

The deformation gradient maps a tangent vector from the undeformed configuration of the body and places it into the tangent space of its current configuration, κ_t . Let us choose a mutually orthogonal coordinate system $\{\vec{\mathbf{e}}_J\}$ in which the matrix of the deformation gradient can be written as

$$[F] = \begin{bmatrix} F_{11} & F_{12} & F_{13} \\ F_{21} & F_{22} & F_{23} \\ F_{31} & F_{32} & F_{33} \end{bmatrix} = [f_1 \ f_2 \ f_3] \text{ where } f_I = F_{JI} \vec{\mathbf{e}}_J. \quad (2)$$

Here, we work within a Lagrangian frame of reference with an implicit assumption that the same set of base vectors $\{\vec{\mathbf{e}}_J\}$ is in use for the undeformed and deformed configuration of the body. A Gram–Schmidt process on the matrix of the deformation gradient yields a set of base vectors $\{\vec{\mathcal{E}}_i\}$ given as

$$\vec{\mathcal{E}}_1 = \frac{f_1}{\|f_1\|}, \quad (3a)$$

$$\vec{\mathcal{E}}_2 = \frac{f_2 - (f_2 \cdot \vec{\mathcal{E}}_1) \vec{\mathcal{E}}_1}{\|f_2 - (f_2 \cdot \vec{\mathcal{E}}_1) \vec{\mathcal{E}}_1\|}, \quad (3b)$$

$$\vec{\mathcal{E}}_3 = \frac{f_3 - (f_3 \cdot \vec{\mathcal{E}}_1) \vec{\mathcal{E}}_1 - (f_3 \cdot \vec{\mathcal{E}}_2) \vec{\mathcal{E}}_2}{\|f_3 - (f_3 \cdot \vec{\mathcal{E}}_1) \vec{\mathcal{E}}_1 - (f_3 \cdot \vec{\mathcal{E}}_2) \vec{\mathcal{E}}_2\|}. \quad (3c)$$

The decomposition of the matrix of the deformation gradient, thus, can be written as

$$\mathbf{F} = \mathcal{R} \mathcal{U} \quad \text{where} \quad (4a)$$

$$[\mathcal{R}] = [\vec{\mathcal{E}}_1 \mid \vec{\mathcal{E}}_2 \mid \vec{\mathcal{E}}_3] \quad \text{and} \quad [\mathcal{U}] = \begin{bmatrix} a & a\gamma & a\beta \\ 0 & b & b\alpha \\ 0 & 0 & c \end{bmatrix}. \quad (4b)$$

The orthogonal matrix \mathcal{R} plays an important role in coordinate transformation; specifically, it maps vectors from the undeformed configuration of the body to our physical frame of reference in which $\{\mathcal{E}_J\}$ acts as a set of base vectors. In this coordinate system, the matrix of the deformation gradient takes an upper-triangular form. This upper-triangular matrix \mathcal{U} represents deformation of a representative cube in all *six* degrees of freedom and is called a Laplace stretch.

The diagonal elements of the Laplace stretch, a , b and c , represent the extension of a representative cube along the directions $\vec{\mathcal{E}}_J$, whereas the off-diagonal elements α , β and γ represent the magnitude of shear. Note that the **QR** decomposition is valid for any mutually orthogonal coordinate system. For a specific coordinate system such as a Cartesian or a spherical polar coordinate system, the matrix of the deformation gradient needs to be re-indexed first as per the strategy laid out by Paul et al. [18] in order to preserve the unambiguity of the Laplace stretch, \mathcal{U} . The Laplace stretch is then obtained by using Eq. (4) on the re-indexed matrix of the deformation gradient.

3 Derivation of quotient rules

In this section, we derive quotient rules that take vectors and second-order tensors from one physical frame of reference to another. In an experimental setup, one is free to choose any coordinate system that is most suitable to the apparatus. For example, in rheometry experiments, a cylindrical polar coordinate system is adopted for a parallel plate rheometer and a spherical polar coordinate system is adopted for a cone and plate rheometer.

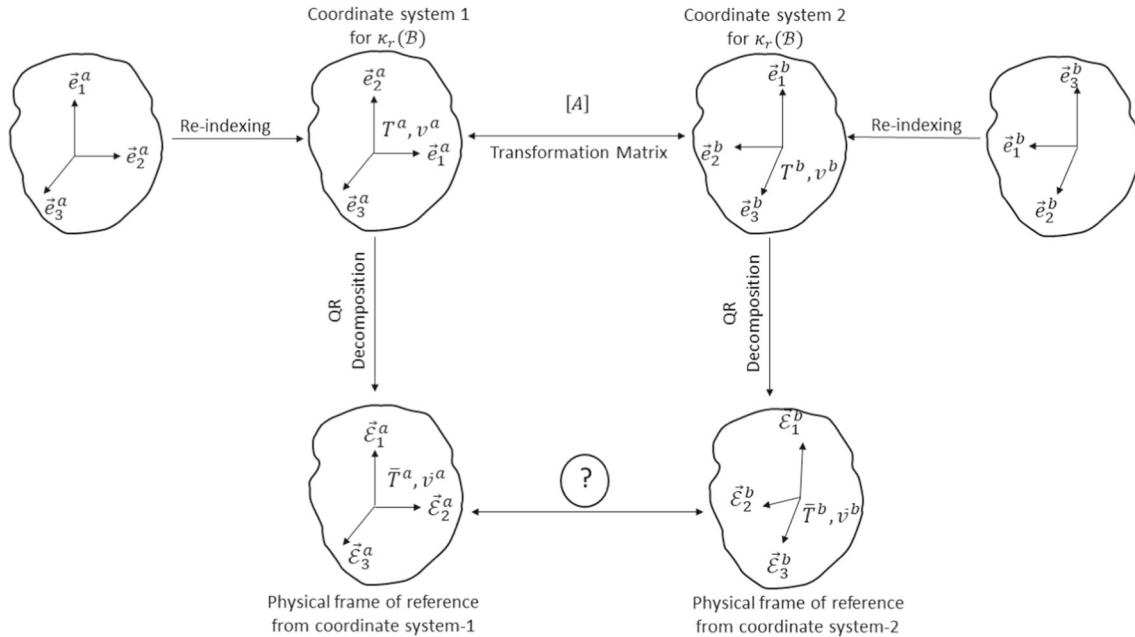


Fig. 1 Different coordinate systems and the problem statement

In this case, the choice of coordinate system is governed by the geometry of the respective experimental setups. From Eq. (3), it can be clearly understood that the base vectors of the physical frame of reference solely depend on the matrix of the deformation gradient, written in the chosen coordinate system. Therefore, comparing results obtained from two different experimental setups will require transformation of vectors and tensors from one physical frame of reference to another. The properties of the base vectors of our physical frame of reference make this transformation rather complicated for a general, fully populated deformation gradient matrix. Here, we will derive the transformation rules for vectors and second-order tensors written in different physical frames of reference derived from two different coordinate systems (cf. Fig. 1). For the sake of generality, no restriction has been provided on the coordinate systems in which the deformation gradient is written except that *the matrix of the deformation gradient has been re-indexed* according to the strategies provided by Paul et al. [18]. Transformation rules for a convected coordinate system have already been derived by Freed and Zamani [10] and therefore will be omitted here.

Let us consider two coordinate systems with base vectors $\{\vec{e}_I^a\}$ and $\{\vec{e}_I^b\}$ in which the matrix of the deformation gradient is written. We assume that the matrices of the deformation gradient are already re-indexed such that for both these coordinate systems, the base vectors carry unique physical meanings and therefore are not interchangeable. For convenience in notation, let us denote the matrix of deformation gradient expressed in these sets of base vectors as $[F^a]$ and $[F^b]$, respectively. If $\{f_I^a\}$, $\alpha = a, b$ and, $I = 1, 2, 3$ denote the column vectors forming the respective matrices of the deformation gradient, then the matrices of the respective deformation gradients can be written as

$$[F^a] = [f_1^a \mid f_2^a \mid f_3^a] \quad \text{and} \quad [F^b] = [f_1^b \mid f_2^b \mid f_3^b]. \quad (5)$$

Let $[A]$ denote the transformation matrix between the coordinate systems $\{\vec{e}_I^a\}$ and $\{\vec{e}_I^b\}$. Therefore, the relationship between the two matrices of deformation gradient is provided as

$$[F^a] = [A]^T [F^b] [A]. \quad (6)$$

Note that the transformation rule (6) is valid because of the assumption that the undeformed and deformed configuration of the body has the same set of base vectors. The base vectors of a physical frame of reference corresponding to a particular matrix of the deformation gradient can be derived using Eq. (3). To derive the quotient rules, or in other words, to transform vectors and tensors from one physical frame of reference to another, one needs to find an inverse expression for Eq. (3). Thus, the column vectors of the matrix of the respective deformation gradient should now be expressed as a linear combination of the base vectors of the

corresponding physical frame of reference. A routine calculation using Eq. (3) enables one to write the base vectors $\vec{\mathcal{E}}_I$ in terms of the column vectors of the matrix of the deformation gradient as

$$\left[\vec{\mathcal{E}}_1^\alpha \mid \vec{\mathcal{E}}_2^\alpha \mid \vec{\mathcal{E}}_3^\alpha \right] = \left[\mathbf{f}_1^\alpha \mid \mathbf{f}_2^\alpha \mid \mathbf{f}_3^\alpha \right] \underbrace{\begin{bmatrix} C_1^\alpha & C_2^\alpha & C_4^\alpha \\ 0 & C_3^\alpha & C_5^\alpha \\ 0 & 0 & C_6^\alpha \end{bmatrix}}_{[C^\alpha]}. \quad (7)$$

Note that the matrix $[C^\alpha]$ is an upper-triangular matrix with

$$C_1^\alpha = 1 / \|\mathbf{f}_1^\alpha\|, \quad (8a)$$

$$C_2^\alpha = -(\mathbf{f}_1^\alpha \cdot \mathbf{f}_2^\alpha) / \|\mathbf{h}_1^\alpha\|, \quad (8b)$$

$$C_3^\alpha = \|\mathbf{f}_1^\alpha\|^2 / \|\mathbf{h}_1^\alpha\|, \quad (8c)$$

$$C_4^\alpha = \left[\|\mathbf{f}_1^\alpha\|^2 (\mathbf{f}_1^\alpha \cdot \mathbf{f}_2^\alpha)(\mathbf{f}_2^\alpha \cdot \mathbf{f}_3^\alpha) - \|\mathbf{h}_1^\alpha\|^2 (\mathbf{f}_1^\alpha \cdot \mathbf{f}_3^\alpha) - (\mathbf{f}_1^\alpha \cdot \mathbf{f}_2^\alpha)^2 (\mathbf{f}_1^\alpha \cdot \mathbf{f}_3^\alpha) \right] / \|\mathbf{h}_2^\alpha\|, \quad (8d)$$

$$C_5^\alpha = \left[(\mathbf{f}_1^\alpha \cdot \mathbf{f}_2^\alpha)(\mathbf{f}_1^\alpha \cdot \mathbf{f}_3^\alpha) \|\mathbf{f}_1^\alpha\|^2 - \|\mathbf{f}_1^\alpha\|^4 (\mathbf{f}_2^\alpha \cdot \mathbf{f}_3^\alpha) \right] / \|\mathbf{h}_2^\alpha\|, \quad (8e)$$

$$C_6^\alpha = \left[\|\mathbf{h}_1^\alpha\|^2 \|\mathbf{f}_1^\alpha\|^2 \right] / \|\mathbf{h}_2^\alpha\| \quad (8f)$$

where

$$\mathbf{h}_1^\alpha = \|\mathbf{f}_1^\alpha\|^2 \mathbf{f}_2^\alpha - (\mathbf{f}_1^\alpha \cdot \mathbf{f}_2^\alpha) \mathbf{f}_1^\alpha \quad \text{and} \quad \mathbf{h}_2^\alpha = \|\mathbf{f}_1^\alpha\|^2 \|\mathbf{h}_1^\alpha\|^2 \mathbf{f}_3^\alpha - \|\mathbf{h}_1^\alpha\|^2 (\mathbf{f}_1^\alpha \cdot \mathbf{f}_3^\alpha) \mathbf{f}_1^\alpha - \|\mathbf{f}_1^\alpha\|^2 (\mathbf{f}_3^\alpha \cdot \mathbf{h}_1^\alpha) \mathbf{h}_1^\alpha.$$

It is worth noting that although the vectors $\{\mathbf{f}_I^\alpha\}$ do not act as base vectors, this set of vectors is still able to span the associated vector space. To derive the quotient rules that transform vectors and tensors between different coordinate systems, the easiest and expected path would be to use the base vectors instead of using $\{\mathbf{f}_I^\alpha\}$. For a general case, however, the relationship between $\{\vec{\mathcal{E}}_I^a\}$ and $\{\vec{\mathcal{E}}_I^b\}$ is difficult to find and the computation is very cumbersome.

From Eq. (7), it can be easily understood that the column vectors of $[F^\alpha]$ can be written as a linear combination of the set of base vectors $\vec{\mathcal{E}}_I^\alpha$. This relationship is implicit in nature since the associated scalar components will have terms involving the inner products of different \mathbf{f}_I^α 's. This implicit relationship, however, will not cause any severe issue since the matrices of the deformation gradient in both the coordinate systems are always known. The inverse relation of Eq. (3) can be written as

$$\left[\mathbf{f}_1^\alpha \mid \mathbf{f}_2^\alpha \mid \mathbf{f}_3^\alpha \right] = \left[\vec{\mathcal{E}}_1^\alpha \mid \vec{\mathcal{E}}_2^\alpha \mid \vec{\mathcal{E}}_3^\alpha \right] \underbrace{\begin{bmatrix} 1 & B_1^\alpha & B_2^\alpha \\ 0 & 1 & B_3^\alpha \\ 0 & 0 & 1 \end{bmatrix}}_{[B^\alpha]}. \quad (9)$$

where

$$B_1^\alpha = \|\mathbf{f}_1^\alpha\|, \quad (10a)$$

$$B_2^\alpha = (\mathbf{f}_1^\alpha \cdot \mathbf{f}_2^\alpha) / \|\mathbf{f}_1^\alpha\|, \quad (10b)$$

$$B_3^\alpha = \|\mathbf{h}_1^\alpha\| / \|\mathbf{f}_1^\alpha\|^2, \quad (10c)$$

$$B_4^\alpha = (\mathbf{f}_1^\alpha \cdot \mathbf{f}_3^\alpha) / \|\mathbf{f}_1^\alpha\|, \quad (10d)$$

$$B_5^\alpha = (\mathbf{f}_3^\alpha \cdot \mathbf{h}_1^\alpha) / \|\mathbf{h}_1^\alpha\|, \quad (10e)$$

$$B_6^\alpha = \|\mathbf{h}_2^\alpha\| / \left(\|\mathbf{f}_1^\alpha\|^2 \|\mathbf{h}_1^\alpha\|^2 \right). \quad (10f)$$

Note that the matrix $[B^\alpha]$ is also an upper-triangular matrix. Needless to say that this matrix acts as a transformation matrix between the coordinate system in which the deformation gradient is written and the physical frame of reference. In the derivation of Eq. (9), it has been assumed that the deformation gradient is written in a coordinate system with mutually perpendicular base vectors.

Any vector \mathbf{v} and second-order tensor \mathbf{T} can be expressed with respect to the base vectors of the physical frame of reference $\vec{\mathcal{E}}_I^\alpha$. Since f_I^α also span the same vector space, it is also possible to express the vector \mathbf{v} and tensor \mathbf{T} in terms of f_I^α . Therefore, the vector \mathbf{v} can be written as

$$\mathbf{v} = \bar{v}_I^\alpha \vec{\mathcal{E}}_I^\alpha = v_I^\alpha f_I. \quad (11)$$

Similarly, for any second-order tensor \mathbf{T} , we can write

$$\mathbf{T} = \bar{T}_{IJ} \vec{\mathcal{E}}_I^\alpha \otimes \vec{\mathcal{E}}_J^\alpha = T_{IJ}^\alpha f_I \otimes f_J. \quad (12)$$

Once the coordinate transformation is complete, one should write the vectors in terms of the original base vectors of the physical frame of reference. For two coordinate systems $\{\vec{\mathbf{e}}_I^a\}$ and $\{\vec{\mathbf{e}}_I^b\}$, the column vectors of $[F^a]$ and $[F^b]$ are related to each other through the transformation matrix $[A]$ by

$$[F^a] = [A]^T [F^b] [A]. \quad (13)$$

Our objective is to find a relationship between the components of the vector and second-order tensor expressed in two different physical frames of reference, i.e., between \bar{v}_I^a and \bar{v}_I^b and \bar{T}_{IJ}^a and \bar{T}_{IJ}^b .

One can observe that although the vectors \mathbf{f}_I^a are *not* the base vectors of the Lagrangian coordinate system $\{\vec{\mathbf{e}}_I^a\}$, these vectors are capable of spanning the tangent space of the undeformed configuration of the body. We will use this property to write the components of the vector and second-order tensor \mathbf{v} and \mathbf{T} in the Lagrangian coordinate system in terms of \bar{v}_I^a and \bar{T}_{IJ}^a , respectively. Using Eq. (7), the components of \mathbf{v} and \mathbf{T} in terms of \mathbf{f}_I^a can be written as

$$v_I^a = C_{IJ}^a \bar{v}_J^a \implies \{v^a\} = [C^a] \{\bar{v}^a\} \quad (14a)$$

and,

$$T_{IJ}^a = C_{IK}^a \bar{T}_{KL}^a C_{JL}^a \implies [T^a] = [C^a] [\bar{T}^a] [C^a]^T. \quad (14b)$$

Needless to say that the matrix $[C^a]$ acts as a transformation matrix between the spanning vectors $\{\mathbf{f}_I^a\}$ and $\{\vec{\mathcal{E}}_I^a\}$. Now, the components of vector \mathbf{v} and second-order tensor \mathbf{T} can be easily written in terms of \mathbf{f}_I^b by using Eq. (6) as

$$v_R^b = v_I^a A_{QI} F_{PQ}^b A_{PJ} F_{RJ}^{b-1} \implies \{v^b\} = [F^b]^{-1} [A]^T [F^b] [A] \{v^a\} \quad (15a)$$

and,

$$\begin{aligned} T_{RS}^b &= F_{RK}^{b-1} A_{QK} F_{QP}^b A_{PI} T_{IJ}^a A_{JM} F_{NM}^b A_{LM} F_{SL}^{b-1} \\ &\implies [T^b] = [F^b]^{-1} [A]^T [F^b] [A] [T^a] [A]^T [F^b] [A] [F^b]^{-1}. \end{aligned} \quad (15b)$$

To find a quotient rule between the two physical frames of reference, we need to obtain the transformation rules between the Lagrangian and its corresponding physical frame of reference. Using Eq. (9), the components of the vector \mathbf{v} and tensor \mathbf{T} as

$$\bar{v}_C^b = v_R^b B_{RC}^b \implies \{\bar{v}^b\} = [B^b] \{v^b\} \quad (16a)$$

and,

$$\bar{T}_{CD}^b = B_{RC}^b T_{RS}^b B_{SD}^b \implies [\bar{T}^b] = [B^b]^T [T^b] [B^b]. \quad (16b)$$

Combining Equations (14), (15) and (16), we finally have

$$\bar{v}_C^b = C_{IJ}^a \bar{v}_J^a A_{QI} F_{PQ}^b A_{PJ} F_{RJ}^{b-1} B_{RC}^b \implies \{\bar{v}^b\} = [B^b] [F^b]^{-1} [F^a] [C^a] \{\bar{v}^a\} \quad (17a)$$

and,

$$\begin{aligned} \bar{T}_{CD}^b &= B_{CR}^b F_{RK}^{b-1} F_{KI}^a C_{IY}^a \bar{T}_{YZ}^a C_{JZ}^a F_{LJ}^a F_{SL}^{b-1} B_{DS}^b \\ &\implies [\bar{T}^b] = [B^b] [F^b]^{-1} [F^a] [C^a] [\bar{T}^a] [C^a]^T [F^a]^T [F^b]^{-T} [B^b]^T. \end{aligned} \quad (17b)$$

4 Applications: rheometry

In this section, we demonstrate the use of the quotient rules with applications to rheometry. Typically, in order to determine the rheological properties of a material, two rheometers are simultaneously used. Specifically, a cone and plate rheometer is used in conjunction with a parallel plate rheometer. Recently, Paul et al. [17] showed that the use of **QR** decomposition opens up a possibility for determining the rheological properties using only one rheometer and thus saving experimental efforts and additional computational costs. This method, however, requires verification through comparison of the results obtained from the two rheometers. In general, the coordinate system used in an experimental setup is chosen as per the geometry of the apparatus. For example, typically a spherical polar coordinate system is chosen for a cone and plate rheometer, whereas a cylindrical polar coordinate system is chosen for a parallel plate rheometer. Moreover, the **QR** decomposition leads to computing the necessary experimental parameters in a physical frame of reference that depends on the matrices of the deformation gradients expressed in these particular coordinate systems. Therefore, a direct comparison between the two results is not possible as they belong to two different coordinate systems. Hence, the results must be obtained in the same coordinate systems using the quotient rules derived in Eq. (17). To demonstrate the utility of these quotient rules, here we take two cases: (i) comparison between the Kirchhoff stresses for a parallel plate and a cone and plate rheometer and (ii) comparison of the same between a parallel plate rheometer and a flow between two coaxial cylinders. The superscripts ‘pp’, ‘cp’ and ‘cc’ denote variables corresponding to a cone and plate, parallel plate and coaxial cylinder rheometers.

4.1 Comparison between a parallel plate and a cone and plate rheometer

Let us assume that the solution, i.e., the Kirchhoff stress in physical frame of reference $\overline{\mathcal{T}}^{pp}$, corresponding to the parallel plate rheometer is known. Moreover, the (re-indexed) matrices of the deformation gradient $[F^{pp}]$ and $[F^{cp}]$ corresponding to a parallel plate and a cone and plate rheometer, respectively, are also known. The Kirchhoff stress, $\overline{\mathcal{T}}^{pp}$, needs to be transformed to a physical frame of reference corresponding to the cone and plate rheometer so that it can be compared with the same obtained experimentally in a cone and plate rheometer for verification purpose. The matrices of the deformation gradient are given as

$$[F^{pp}] = \begin{bmatrix} 1 & 0 & 0 \\ 0 & 1 & \beta_1 \\ 0 & 0 & 1 \end{bmatrix} \text{ and } [F^{cp}] = \begin{bmatrix} 1 & 0 & 0 \\ 0 & 1 & \beta_2 \\ 0 & 0 & 1 \end{bmatrix} \text{ where } \beta_1 = \frac{\partial \omega}{\partial Z}(t - t') \text{ and } \beta_2 = -\frac{\partial \omega}{\partial \Theta}(t - t'). \quad (18)$$

Here, ω is the angular velocity provided on the plates of the two rheometers. All other symbols bear the usual meanings. Since the two rheometry problems are set in two different coordinate systems, one would expect that the results (i.e., Kirchhoff stresses) obtained from these rheometers also will be in different coordinate systems and hence they are not readily comparable. However, a routine calculation using Eq. (17) reveals that the Kirchhoff stress $\overline{\mathcal{T}}^{pp}$ obtained in the physical frame of reference corresponding to a parallel plate rheometer is identical to the one corresponding to a cone and plate rheometer, i.e., $\overline{\mathcal{T}}^{pp} = \overline{\mathcal{T}}^{cp}$ (see Appendix 5 for detailed derivation). This is due to the fact that the re-indexed matrices of the deformation gradient in both the cases are upper-triangular and thus the base vectors of the two physical frames of reference are the same. Since the Kirchhoff stresses are expressed in terms of the same base vectors, they have the same components in both the physical frames of reference. Thus, the results obtained from these two rheometers can be readily compared without any coordinate transformation.

This simple exercise helps us gain a significant insight regarding the quotient rules for **QR** kinematics. This example implies that even though the deformation gradient matrices are written in two different coordinate systems, the kinematic and kinetic quantities in the physical frame of reference (i.e., after **QR** decomposition has been performed) may have the same components. This is due to the fact that the base vectors of our physical frame of reference *solely* depend on the form of the deformation gradient matrix. If the (re-indexed) matrices of the deformation gradient, expressed in two different coordinate systems, are both upper-triangular, then the resulting base vectors of the physical frame of reference are identical and therefore no quotient rules are required. Hence, the need for quotient rules only arises when either of the matrices of the deformation gradient is *not* upper-triangular.

4.2 Comparison between a parallel plate rheometer and flow between coaxial cylinders

In the previous case, we have demonstrated the use of quotient rules between two apparatus which were more amenable for a cylindrical polar and a spherical polar coordinate systems, respectively. Since the base vectors of the physical frame of reference depend on the matrix of the deformation gradient, the problem in comparing results is not limited to results obtained in different coordinate systems when **QR** decomposition is involved. In this demonstration, we take the example of a parallel plate rheometer and a flow between two coaxial cylinders, both of which are amenable to a cylindrical polar coordinate systems. The matrices of the deformation gradients in these two problems are given as

$$[F^{pp}] = \begin{bmatrix} 1 & 0 & 0 \\ 0 & 1 & \beta_1 \\ 0 & 0 & 1 \end{bmatrix} \quad \text{and} \quad [F^{cc}] = \begin{bmatrix} 1 & 0 & 0 \\ \beta_3 & 1 & 0 \\ 0 & 0 & 1 \end{bmatrix} \quad \text{where} \quad \beta_3 = R(\partial\omega/\partial R)(t - t'). \quad (19)$$

Since the base vectors of the physical frame of reference corresponding the two cases are different, we shall use the quotient rule (17) to obtain Kirchhoff stress in the physical frame of reference derived from a parallel plate rheometer to the same in case of the coaxial cylinders. A routine calculation (see Appendix 5) shows that

$$[\bar{T}^b] = \begin{bmatrix} 1/\sqrt{1+\beta_3^2} & \beta_3/\sqrt{1+\beta_3^2} & 0 \\ -\beta_3/\sqrt{1+\beta_3^2} & 1/\sqrt{1+\beta_3^2} & 0 \\ 0 & 0 & 1 \end{bmatrix} [\bar{T}^a] \begin{bmatrix} 1/\sqrt{1+\beta_3^2} & -\beta_3/\sqrt{1+\beta_3^2} & 0 \\ \beta_3/\sqrt{1+\beta_3^2} & 1/\sqrt{1+\beta_3^2} & 0 \\ 0 & 0 & 1 \end{bmatrix}. \quad (20)$$

5 Summary

In this short note, we derive the quotient rules to transform vectors and second-order tensors between two physical frames of reference obtained from a **QR** decomposition of the deformation gradient. It has been shown that a direct transformation of the vectors and tensors through the base vectors of the physical frames of reference is difficult to obtain and involves cumbersome calculation for general, fully populated matrices of the deformation gradient. Therefore, an alternative method has been proposed. The utility of this quotient rule has been demonstrated through comparison of results in case of two different rheometers. One key finding of the paper is that since the base vectors of the physical frames of reference are derived from the matrices of the deformation gradients, the form of these matrices plays a more significant role in the derivation of the quotient rules than the selected coordinate systems in which the matrices of the deformation gradient are written. Specifically, if the matrices of the deformation gradient written in two different coordinate systems are upper-triangular, then the base vectors of our physical frame of reference are identical. Hence, no quotient rule needs to be applied on the vectors and tensor components expressed in the physical frames of reference. On the other hand, even if the matrices of the deformation gradient are written in the same coordinate system, the difference in the forms of these matrices may lead to different physical frames of reference after **QR** decomposition and quotient rules need to be applied.

A Derivation of quotient rules for different types of rheometers

In this section, we provide a detailed derivation of the rheometry problems and related quotient rules given in Sect. 4. The fluid flows in rheometry problems are traditionally analyzed using a convected coordinate system since this method allows one to obtain analytical solutions for complex flow problems using the solution of a simpler, similar problems via a selection of an appropriate coordinate system. For example, the solution for a cone and plate rheometer can be obtained with the help of a solution to the problem of flow between a stationary and a moving parallel plate. This method, however, involves cumbersome calculations, and often it is difficult to obtain a globally convected coordinate system for many such problems. To overcome this difficulty, a new analytical method involving **QR** decomposition has been proposed [17] that retains the advantages of using a convected coordinate system without the computational difficulties.

Rheometry is typically a strain-controlled test where the test specimen is subjected to a given angular velocity. Three kinetic quantities, namely the total force on the plate, the couple required to keep the plate stationary and the pressure at a point on the plate, are measured for this given fluid flow in order to determine its rheological properties. In the following, we briefly describe the **QR** kinematics and the use of quotient rules pertaining to cone and plate, parallel plate and coaxial cylinder rheometers.

To describe the motion of the test specimen in different rheometers, different coordinate systems are adopted according to their respective geometries. Specifically, a spherical polar coordinate system is adopted for a cone and plate rheometer, whereas a cylindrical polar coordinate system is used for a parallel plate and a coaxial cylinders rheometer. In the respective coordinate systems, the velocity distribution can be written as

$$v_r^{cp} = 0, \quad v_\theta^{cp} = 0, \quad v_\phi^{cp} = r \sin \Theta \omega(\Theta), \quad (21a)$$

$$v_r^{pp} = 0, \quad v_\theta^{pp} = r\omega(Z), \quad v_z^{pp} = 0, \quad (21b)$$

$$v_r^{cc} = 0, \quad v_\theta^{cc} = r\omega(R), \quad v_z^{cc} = 0. \quad (21c)$$

A simple integration of the velocity distributions in Eqs. (21a)–(21c) leads to the deformation map as

$$r^{cp} = R^{cp}; \quad \theta^{cp} = \Theta^{cp}; \quad \phi^{cp} = \Phi^{cp} - \omega(\Theta^{cp})(t - t'), \quad (22a)$$

$$r^{pp} = R^{pp}; \quad \theta^{pp} = \Theta^{cp}(Z) + \omega(t - t'); \quad z^{pp} = Z^{pp}, \quad (22b)$$

$$r^{pp} = R^{pp}; \quad \theta^{pp} = \Theta^{cp}(R) + \omega(t - t'); \quad z^{pp} = Z^{pp}. \quad (22c)$$

From these deformation maps, the (re-indexed) matrices of the deformation gradients can be easily obtained as

$$[F^{cp}] = \begin{bmatrix} 1 & 0 & 0 \\ 0 & 1 & \beta_2 \\ 0 & 0 & 1 \end{bmatrix}, \quad [F^{pp}] = \begin{bmatrix} 1 & 0 & 0 \\ 0 & 1 & \beta_1 \\ 0 & 0 & 1 \end{bmatrix}, \quad [F^{cc}] = \begin{bmatrix} 1 & 0 & 0 \\ \beta_3 & 1 & 0 \\ 0 & 0 & 1 \end{bmatrix} \quad (23)$$

where $\beta_2 = -\frac{\partial\omega}{\partial\Theta}(t - t')$, $\beta_1 = \frac{\partial\omega}{\partial Z}(t - t')$ and $\beta_3 = R \frac{\partial\omega}{\partial R}(t - t')$. Based on these deformation gradients

and subsequent Laplace stretches, the normal stress differences and the shear stresses are obtained by using the constitutive relations given in [17]. These stress components are thermodynamic conjugates to the strains defined based on the Laplace stretches and are known as Kirchhoff stress in its tensorial form. Needless to say that the experimentally measurable kinetic variables as mentioned earlier can be obtained from these stress components. The Kirchhoff stresses for different rheometers, however, are expressed in different sets of base vectors (i.e., base vectors of our physical frame of reference). Therefore, quotient rules are required to transform the Kirchhoff stresses for the purpose of comparison.

Parallel plate rheometer → cone and plate rheometer

To transform from the physical frame of reference for a parallel plate rheometer to that for a cone and plate rheometer, we first need to evaluate the transformation matrices $[C^{pp}]$ and $[B^{cp}]$. These matrices are derived from the matrices of deformation gradient $[F^{pp}]$ and $[F^{cp}]$, respectively, using Eqs. (8) and (3) as

$$[C^{pp}] = \begin{bmatrix} 1 & 0 & 0 \\ 0 & 1 & -\beta_1 \\ 0 & 0 & 1 \end{bmatrix} \quad \text{and} \quad [B^{cp}] = \begin{bmatrix} 1 & 0 & 0 \\ 0 & 1 & \beta_2 \\ 0 & 0 & 1 \end{bmatrix} \quad (24)$$

It can be easily verified that the matrices $[C^{pp}]$ and $[B^{cp}]$ are equal to $[F^{pp}]^{-1}$ and $[F^{cp}]$, respectively. Therefore, substitution of these matrices in Eq. (17) renders the Kirchhoff stresses for both the rheometers identical.

Parallel plate rheometer → coaxial cylinders

A similar calculation is carried out for the transformation between parallel plate rheometer and coaxial cylinders. In this case, using Eqs. (8) and (3) on the matrices of the deformation gradient, $[F^{PP}]$ and $[F^{CC}]$, we arrive at

$$[C^{PP}] = \begin{bmatrix} 1 & 0 & 0 \\ 0 & 1 & -\beta_1 \\ 0 & 0 & 1 \end{bmatrix} \quad \text{and} \quad [B^{CC}] = \begin{bmatrix} \sqrt{1 + \beta_3^2} & \beta_3/\sqrt{1 + \beta_3^2} & 0 \\ 0 & 1/\sqrt{1 + \beta_3^2} & 0 \\ 0 & 0 & 1 \end{bmatrix}. \quad (25)$$

Substitution of Eq. (25) into Eq. (17) leads to the transformation rule for Kirchhoff stress from the physical frame of reference corresponding to a parallel plate rheometer to that for the coaxial cylinders as given in Eq. (20).

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