Rotations for 3D Cauchy continuum

In this chapter we consider the *classical configuration space* of the nonpolar Cauchy continuum, defined as

$$
\mathcal{C} \doteq \{ \chi \colon \ B \to R^3 \},\tag{3.1}
$$

where χ is the deformation function defined over the reference configuration of the body B. The rotations are calculated from the deformation example of the body D . The rotations are calculated from
gradient, $\mathbf{F} = \nabla \chi$, and are not independent variables.

3.1 Polar decomposition of deformation gradient

In the non-polar Cauchy media, the rotations associated with deformation can be obtained by the polar decomposition of the deformation gradient, which appears in two forms: right and left. The right polar decomposition is given by the formula

$$
\mathbf{F} = \mathbf{R}\mathbf{U},\tag{3.2}
$$

where $\mathbf{U} \doteq (\mathbf{F}^T \mathbf{F})^{\frac{1}{2}}$ is the right stretching tensor (symmetric and positive definite) and $\mathbf{R} = \mathbf{FU}^{-1} \in SO(3)$ is a rotation tensor. The left polar decomposition is

$$
\mathbf{F} = \mathbf{V}\mathbf{R},\tag{3.3}
$$

where $\mathbf{V} \doteq (\mathbf{F}\mathbf{F}^T)^{\frac{1}{2}}$ is the left stretching tensor, also symmetric and positive definite. Then the rotation tensor is calculated as $\mathbf{R} = \mathbf{V}^{-1}\mathbf{F} \in$ $SO(3)$.

Uniqueness of polar decomposition. The proof of uniqueness of the decomposition (3.2) follows the standard lines, and is given, e.g., in [115], p. 77 or [159], p. 93.

Properties of U. The properties of U result from the properties of $\mathbf{C} = \mathbf{F}^T \mathbf{F}$. First, **C** is symmetric as $(\mathbf{F}^T \mathbf{F})^T = \mathbf{F}^T (\mathbf{F}^T)^T = \mathbf{F}^T \mathbf{F}$. Symmetry of U can be shown directly by using the Cayley–Hamilton theorem, see [236], eq. (2.7). Another way is to note that $\mathbb{C}^{\frac{1}{2}}$ is an isotropic function, i.e.

$$
\mathbf{Q}\mathbf{C}^{\frac{1}{2}}\mathbf{Q}^T = (\mathbf{Q}\mathbf{C}\mathbf{Q}^T)^{\frac{1}{2}},\tag{3.4}
$$

for an arbitrary $\mathbf{Q} \in SO(3)$, thus, by Serrin's theorem, it can be represented as $\mathbf{C}^{\frac{1}{2}} = a_0 \mathbf{I} + a_1 \mathbf{C} + a_2 \mathbf{C}^2$. Hence, $\mathbf{U} = \mathbf{C}^{\frac{1}{2}}$ is symmetric as a polynomial of symmetric tensors.

Next, **C** is positive definite, which can be shown by considering a line element, $dx = \mathbf{F} d\mathbf{X}$, where $\det \mathbf{F} \neq 0$ and $d\mathbf{X} \neq 0$. A square of a length of the line element is positive, i.e.

$$
dx \cdot dx = (FdX) \cdot (FdX) = dX \cdot (FTF dX) > 0,
$$
 (3.5)

where the last form is a definition of positive definiteness of $\mathbf{F}^T \mathbf{F} = \mathbf{C}$. By the definition of a square root function in spectral representations, also $U = C^{\frac{1}{2}}$ is positive definite.

Algorithm for calculation of U **for given** C**.** The eigenvalues of C are real and positive and its eigenvectors are pairwise orthogonal. Denote these eigenvalues as λ_i^2 and the eigenvectors as \mathbf{v}_i $(i = 1, 2, 3)$, and arrange them as matrices as follows:

$$
\mathbf{\Lambda} = \text{diag}\left[\lambda_1^2, \lambda_2^2, \lambda_2^2\right], \qquad \mathbf{Q} = [\mathbf{v}_1 | \mathbf{v}_2 | \mathbf{v}_3],
$$

where Λ is a diagonal matrix and $\mathbf Q$ is an orthogonal matrix. Then C is represented as

$$
\mathbf{C} = \mathbf{Q}^T \Lambda \mathbf{Q},\tag{3.6}
$$

where the position of \mathbf{Q} and \mathbf{Q}^T can be interchanged. The standard steps to calculate $\mathbf{U} = \mathbf{C}^{\frac{1}{2}}$ are shown in Table 3.1. Note that \mathbf{U} is not diagonal but is symmetric and positive definite. The algorithm to find a square root of a symmetric positive definite 3×3 matrix is described, e.g., in [75]. Note that for $\mathbf{U} = \mathbf{Q}^T \mathbf{\Lambda} \frac{1}{2} \mathbf{Q}$, we obtain $\mathbf{F} = \mathbf{R} \mathbf{U} = \mathbf{R} \mathbf{Q}^T \mathbf{\Lambda} \frac{1}{2} \mathbf{Q}$, which is a relation for the deformation gradient in which the stretches and the orthogonal tensors are separated.

Properties of R. Orthogonality of **R** is shown as

$$
\mathbf{R}^{T}\mathbf{R} = (\mathbf{U}^{-1})^{T}\mathbf{F}^{T}\mathbf{F}\mathbf{U}^{-1} = \mathbf{U}^{-1}\mathbf{U}^{2}\mathbf{U}^{-1} = \mathbf{I}.
$$
 (3.7)

From this condition we obtain $\det(\mathbf{R}^T \mathbf{R}) = (\det \mathbf{R})^2 = 1$, i.e. a relation for the square of the determinant. To establish the sign of $\det R$, we note that $\det \mathbf{R} = \det(\mathbf{F} \mathbf{U}^{-1}) = (\det \mathbf{F})/(\det \mathbf{U})$. Positive definiteness of **U** implies that the principal stretches $\lambda_i > 0$ and, hence, det **U** = $\lambda_1 \lambda_2 \lambda_3 > 0$. Besides, we must take det $\mathbf{F} > 0$ to exclude annihilation of line elements and negative volumes, see [159], pp. 85 and 87. Hence, $(\det \mathbf{F})/(\det \mathbf{U}) > 0$ and, therefore, $\det \mathbf{R} = +1$.

3.2 Rotation Constraint equation

Instead of calculating **R** as \mathbf{FU}^{-1} , we can find a tensor $\mathbf{Q} \in SO(3)$, by solving the RC equation

$$
\mathfrak{C} \doteq \text{skew}(\mathbf{Q}^T \mathbf{F}) = \mathbf{0}.\tag{3.8}
$$

This it permitted because the equations $\mathbf{Q}^T \mathbf{F} = \mathbf{U}$ and skew $(\mathbf{Q}^T \mathbf{F}) =$ 0, are equivalent, which is shown below.

1. skew $(\mathbf{Q}^T \mathbf{F}) = 0 \Rightarrow \mathbf{Q}^T \mathbf{F} = \mathbf{U}$. From skew $(\mathbf{Q}^T \mathbf{F}) = \mathbf{0}$ we have $\mathbf{Q}^T \mathbf{F} = \mathbf{F}^T \mathbf{Q} = (\mathbf{Q}^T \mathbf{F})^T$, i.e. $\mathbf{Q}^T \mathbf{F}$ is symmetric. Using this symmetry, we have

$$
(\mathbf{Q}^T \mathbf{F})^2 = (\mathbf{Q}^T \mathbf{F})(\mathbf{Q}^T \mathbf{F}) = (\mathbf{Q}^T \mathbf{F})^T (\mathbf{Q}^T \mathbf{F}) = \mathbf{F}^T \mathbf{Q} \mathbf{Q}^T \mathbf{F} = \mathbf{U}^2.
$$
 (3.9)

It remains to show that $\mathbf{Q}^T \mathbf{F} \neq -\mathbf{U}$. Because $\mathbf{U}^2 = \mathbf{C}$ is positive definite, so also is $(Q^T\mathbf{F})^2$. By the definition of a square root function in a spectral representation, also $\mathbf{Q}^T \mathbf{F} = [(\mathbf{Q}^T \mathbf{F})^2]^{\frac{1}{2}}$ is positive definite, similarly as $\mathbf U$ obtained from **C**. This implies that eigenvalues of $\mathbf Q^T \mathbf F$ are positive, similarly as principal stretches λ_i , and that $\mathbf{Q}^T \mathbf{F} = +\mathbf{U}$.

Remark. We can also compare signs of $\mathbf{Q}^T \mathbf{F}$ and U by examining signs of their scalar invariants, but the results are not conclusive because of the first invariant. Both the third invariants are positive, as $det(\mathbf{Q}^T \mathbf{F}) =$ $(\det \mathbf{Q}^T)(\det \mathbf{F}) = \det \mathbf{F} > 0$ and also $\det \mathbf{U} = \lambda_1 \lambda_2 \lambda_3 > 0$, as principal stretches $\lambda_i > 0$. Also, the second invariants are positive, as

$$
\text{tr}(\mathbf{Q}^{\mathrm{T}}\mathbf{F})^2 = \text{tr}(\mathbf{F}^{\mathrm{T}}\mathbf{F}) = \mathbf{F} \cdot \mathbf{F} > 0,
$$
\n(3.10)

using eq. (3.9), and $tr\mathbf{U}^2 = \lambda_1\lambda_2 + \lambda_2\lambda_3 + \lambda_3\lambda_1 > 0$ as $\lambda_i > 0$. For the first invariants, we have $tr \mathbf{U} = \lambda_1 + \lambda_2 + \lambda_3 > 0$ as $\lambda_i > 0$, but there is a problem with $tr(\mathbf{Q}^T\mathbf{F})$. For instance, for the 2D case, when

$$
\mathbf{Q} = \begin{bmatrix} \cos \omega & -\sin \omega \\ \sin \omega & \cos \omega \end{bmatrix}, \qquad \mathbf{F} = \begin{bmatrix} F_{11} & F_{12} \\ F_{21} & F_{22} \end{bmatrix}, \tag{3.11}
$$

we obtain $tr(\mathbf{Q}^T\mathbf{F}) = \mathbf{Q} \cdot \mathbf{F} = \cos \omega (F_{11} + F_{22}) + \sin \omega (F_{21} - F_{12})$. Noting that det $\mathbf{F} = F_{11}F_{22} - F_{12}F_{21} > 0$, and even assuming small rotations, $\omega \approx 0$, for which $tr(\mathbf{Q}^T\mathbf{F}) \approx (F_{11} + F_{22}) + \omega(F_{21} - F_{12})$, it is still difficult to determine the sign of this invariant.

2.
$$
\mathbf{Q}^T \mathbf{F} = \mathbf{U} \Rightarrow \text{skew}(\mathbf{Q}^T \mathbf{F}) = \mathbf{0}.
$$

From the symmetry condition, $\mathbf{U} = \mathbf{U}^T$, we obtain $(\mathbf{Q}^T \mathbf{F}) = (\mathbf{Q}^T \mathbf{F})^T$, which can be rewritten as $skew(Q^TF) = 0$.

This ends the proof that the conditions skew $(\mathbf{Q}^T \mathbf{F}) = \mathbf{0}$ and $\mathbf{Q}^T \mathbf{F} =$ U are fully equivalent. \Box

Finally, we note that the RC equation provides a link between the deformation gradient and the rotations, and can be used to derive mixed formulations including rotations, see Sect. 4.

Relaxed stretching tensors. Using the product $Q^T F$, which was a basis of the RC equation, we can define two relaxed right stretching tensors:

1. the symmetric relaxed right stretching tensor

$$
\tilde{\mathbf{U}} \doteq \text{sym}(\mathbf{Q}^T \mathbf{F}).\tag{3.12}
$$

If skew($\mathbf{Q}^T \mathbf{F}$) = 0, then sym($\mathbf{Q}^T \mathbf{F}$) = U, as in the proof above. 2. the non-symmetric relaxed right stretching tensor

$$
\tilde{\mathbf{U}}_n \doteq \mathbf{Q}^T \mathbf{F}.\tag{3.13}
$$

If skew $(\mathbf{Q}^T \mathbf{F}) = \mathbf{0}$, then $\mathbf{Q}^T \mathbf{F} = \text{sym}(\mathbf{Q}^T \mathbf{F}) = \mathbf{U}$. The tensor $\tilde{\mathbf{U}}_n$ is used in the two-field formulation with unconstrained equations, see Sect. 4.6.

3.3 Interpretation of rotation Q

The rotation Q provided by the RC equation can also be physically interpreted in the range of large rotations, if we parameterize \mathbf{F} in terms of rotations and stretches of a pair of initially ortho-normal vectors.

Fig. 3.1 Deformation of a pair of vectors t_1 and t_2 .

Consider a 2D (planar) body, and denote by t_1 and t_2 two ortho-normal vectors associated with the non-deformed configuration, see Fig. 3.1. Under deformation, each of these vectors is rotated and stretched,

$$
\mathbf{t}_1^* = \mathbf{F} \mathbf{t}_1 = \lambda_1 \mathbf{Q}_1 \mathbf{t}_1, \qquad \mathbf{t}_2^* = \mathbf{F} \mathbf{t}_2 = \lambda_2 \mathbf{Q}_2 \mathbf{t}_2, \tag{3.14}
$$

where $\lambda_1, \lambda_2 > 0$ are scalar stretch parameters and $\mathbf{Q}_1, \mathbf{Q}_2$ are two rotation tensors, each depending on one rotation angle β_{α} , $\alpha = 1, 2$. The length of t_1 and t_2 is preserved if $\lambda_1 = \lambda_2 = 1$ and the angle between them remains unchanged for $\beta_1 = \beta_2$. Note that we can define the deformation gradient as $\mathbf{F} = \lambda_1 \mathbf{Q}_1 (\mathbf{t}_1 \otimes \mathbf{t}_1) + \lambda_2 \mathbf{Q}_2 (\mathbf{t}_2 \otimes \mathbf{t}_2)$ because products of it with t_1 and t_2 yield expressions of eq. (3.14).

For the representations

$$
\mathbf{F} = F_{\alpha\beta} \mathbf{t}_{\alpha} \otimes \mathbf{t}_{\beta},
$$

\n
$$
\mathbf{Q}_{\alpha}(\beta_{\alpha}) = c_{\alpha} (\mathbf{t}_{1} \otimes \mathbf{t}_{1} + \mathbf{t}_{2} \otimes \mathbf{t}_{2}) + s_{\alpha} (\mathbf{t}_{2} \otimes \mathbf{t}_{1} - \mathbf{t}_{1} \otimes \mathbf{t}_{2}), \quad (3.15)
$$

where $s_{\alpha} = \sin \beta_{\alpha}$ and $c_{\alpha} = \cos \beta_{\alpha}$, from eq. (3.14) we obtain

$$
F_{11} = \lambda_1 c_1
$$
, $F_{12} = \lambda_2 (-s_2)$, $F_{21} = \lambda_1 s_1$, $F_{22} = \lambda_2 c_2$, (3.16)

which are algebraic and nonlinear formulas for $F_{\alpha\beta}$ in terms of four new parameters $\{\lambda_1, \lambda_2, \beta_1, \beta_2\}.$

Next, we shall find a relation between the rotation angles β_{α} and the angle ω of the rotation **Q** using the RC equation. For $\mathbf{Q}(\omega) =$ $\cos \omega (\mathbf{t}_1 \otimes \mathbf{t}_1 + \mathbf{t}_2 \otimes \mathbf{t}_2) + \sin \omega (\mathbf{t}_2 \otimes \mathbf{t}_1 - \mathbf{t}_1 \otimes \mathbf{t}_2), \text{ the RC equation becomes}$

$$
(F_{21} - F_{12})\cos\omega - (F_{11} + F_{22})\sin\omega = 0.
$$
 (3.17)

Using the components of the deformation gradients of eq. (3.16), we obtain

$$
[\lambda_1 s_1 - \lambda_2 (-s_2)] \cos \omega - (\lambda_1 c_1 + \lambda_2 c_2) \sin \omega = 0. \tag{3.18}
$$

Assuming $\cos \omega \neq 0$, and $(\lambda_1 c_1 + \lambda_2 c_2) \neq 0$, we obtain

$$
\tan \omega = \frac{\lambda_1 s_1 + \lambda_2 s_2}{\lambda_1 c_1 + \lambda_2 c_2} \approx \frac{s_1 + s_2}{c_1 + c_2},
$$
\n(3.19)

where the last form was obtained for small stretches, $\lambda_{\alpha} \approx 1$. Using trigonometric identities,

$$
\tan \omega \approx \tan \frac{\beta_1 + \beta_2}{2}.
$$
 (3.20)

Hence,

$$
\omega \approx \frac{1}{2}(\beta_1 + \beta_2) + k\pi, \qquad k = 0, \dots, K,
$$
\n(3.21)

i.e. the angle ω yielded by the RC is an average of rotations of vectors t_1 and t_2 . This result, obtained for large rotations, provides a clear physical interpretation of Q.

For rigid body rotation, the length of vectors t_1 and t_2 is constant, and their rotation angles are identical, i.e. $\lambda_1 = \lambda_2 = 1$, and $\beta_1 = \beta_2 = \beta$. Then, eq. (3.14) becomes

$$
\mathbf{Ft}_1 = \mathbf{Q}(\beta) \mathbf{t}_1, \qquad \mathbf{Ft}_2 = \mathbf{Q}(\beta) \mathbf{t}_2 \tag{3.22}
$$

and the deformation gradient $\mathbf{F} = \mathbf{Q}(\beta) (\mathbf{t}_1 \otimes \mathbf{t}_1 + \mathbf{t}_2 \otimes \mathbf{t}_2) = \mathbf{Q}(\beta) \mathbf{I} =$ $\mathbf{Q}(\beta)$. Hence, eq. (3.21) becomes

$$
\omega = \beta + k\pi,\tag{3.23}
$$

i.e. the angle ω yielded by the RC is equal to the angle β of the rigid body rotation.

Summarizing the above two cases, we see that, in general, Q cannot be interpreted as a rigid rotation. This is also true for the rotation R yielded by the polar decomposition of \mathbf{F} , because $\mathbf{R} = \mathbf{Q}$.

3.4 Rate form of RC equation

The rate form of the RC equation has the advantage that it can be equivalently expressed in terms of the angular velocity and the spatial velocity gradient.

Differentiation w.r.t. time of the RC equation (3.8) yields

$$
skew(\dot{\mathbf{Q}}^T \mathbf{F} + \mathbf{Q}^T \dot{\mathbf{F}}) = \mathbf{0}.
$$
 (3.24)

From the definitions of the spatial (left) angular velocity, $\tilde{\boldsymbol{\omega}}^* \doteq \dot{\mathbf{Q}} \mathbf{Q}^T$, and the spatial velocity gradient, $\nabla \mathbf{v} = \dot{\mathbf{F}} \mathbf{F}^{-1}$, we obtain

$$
\dot{\mathbf{Q}} = \tilde{\boldsymbol{\omega}}^* \mathbf{Q}, \qquad \dot{\mathbf{F}} = \nabla \mathbf{v} \mathbf{F}, \tag{3.25}
$$

for which, eq. (3.24) becomes

skew
$$
(\mathbf{Q}^T \mathbf{A} \mathbf{F}) = \mathbf{0}
$$
, where $\mathbf{A} \doteq -\tilde{\boldsymbol{\omega}}^* + \nabla \mathbf{v}$. (3.26)

Next, we apply the rotation-forward operation, $\mathbf{Q}(\cdot) \mathbf{Q}^T$ and rewrite eq. (3.26) as

$$
\mathbf{AV} - \mathbf{VA}^T = \mathbf{0},\tag{3.27}
$$

where $\mathbf{V} \doteq \mathbf{Q} \mathbf{U} \mathbf{Q}^T = \mathbf{F} \mathbf{Q}^T$ is the left stretching tensor, symmetric and positive definite. The split of A into a symmetric part and a skewsymmetric part yields $\mathbf{A} = \mathbf{A}_s + \mathbf{A}_a$, where $\mathbf{A}_s \doteq \text{sym}\nabla \mathbf{v}$ and $A_a \doteq -\tilde{\omega}^* + \text{skew}\nabla v$. Then eq. (3.26) becomes

$$
(\mathbf{A}_s \mathbf{V} - \mathbf{V} \mathbf{A}_s) + (\mathbf{A}_a \mathbf{V} - \mathbf{V} \mathbf{A}_a^T) = \mathbf{0}.
$$
 (3.28)

Note that the first part,

$$
\mathbf{A}_s \mathbf{V} - \mathbf{V} \mathbf{A}_s = 2 \,\text{skew}(\mathbf{A}_s \mathbf{V}) = \mathbf{0},\tag{3.29}
$$

because a skew part of a symmetric tensor is equal to zero. Hence, only the second part of eq. (3.28) remains,

$$
\mathbf{A}_a \mathbf{V} + \mathbf{V} \mathbf{A}_a = \mathbf{0},\tag{3.30}
$$

in which A_a is skew-symmetric, and V is symmetric and positive definite. By Lemma 3.1 in [214], this equation is satisfied only if $\mathbf{A}_a = \mathbf{0}$, which yields

$$
\tilde{\boldsymbol{\omega}}^* - \text{skew}\nabla \mathbf{v} = \mathbf{0}.\tag{3.31}
$$

This relation is equivalent to the rate form of the RC equation of eq. (3.24).

3.5 Rotations calculated from the RC equation

Assume that \mathbf{F} is given, and find the rotations from the RC equation.

The solution of the RC of eq. (3.8) is trivial for a rigid rotation, when $\mathbf{F} = \mathbf{Q}$, as then skew $(\mathbf{Q}^T \mathbf{F}) = \text{skew}(\mathbf{Q}^T \mathbf{Q}) = \text{skew} \mathbf{I} = \mathbf{0}$, i.e. the RC equation is an identity.

For large rotations, the RC of eq. (3.8) yields a system of non-linear equations for $\{\psi_1, \psi_2, \psi_3\}$, where $\psi_i \doteq (\psi)_i$ and ψ is the rotation vector, e.g. the canonical vector of eq. (8.79). Methods of solution of these nonlinear equations for a 2D problem are discussed in Sect. 12.1.

If we assume that rotations are small, then $\mathbf{Q} \approx \mathbf{I} + \psi$, where $\tilde{\psi} = \psi \times I \in so(3)$. Then the RC equation becomes

$$
\mathfrak{C} \doteq \text{skew}(\mathbf{Q}^T \mathbf{F}) = \text{skew}\left[(\mathbf{I} + \tilde{\boldsymbol{\psi}})^T \mathbf{F} \right] = \text{skew}\mathbf{F} + \text{skew}(\tilde{\boldsymbol{\psi}}^T \mathbf{F}) = \mathbf{0}. \tag{3.32}
$$

These are three equations which can be rewritten as

$$
\begin{bmatrix}\n-F_{31} & -F_{32} & (F_{11} + F_{22}) \\
F_{21} & -(F_{11} + F_{33}) & F_{23} \\
(F_{22} + F_{33}) & -F_{12} & -F_{13}\n\end{bmatrix}\n\begin{bmatrix}\n\psi_1 \\
\psi_2 \\
\psi_3\n\end{bmatrix} = -\n\begin{bmatrix}\nF_{12} - F_{21} \\
F_{13} - F_{31} \\
F_{23} - F_{32}\n\end{bmatrix},
$$
\n(3.33)

where $F_{ij} \doteq (\mathbf{F})_{ij}$. Note that for $\mathbf{F} = \mathbf{I}$, the determinant of the matrix is equal to 8 and the r.h.s. vector is equal to zero. Hence, a unique solution exists and is equal to zero.

A unique solution does not exist, e.g., when (i) the off-diagonal components are equal to zero, i.e. $F_{\alpha 3} = F_{3\alpha} = 0$ and $F_{12} = F_{21} = 0$, and (ii) at least one of the following conditions for the diagonal components is satisfied: $F_{11} = -F_{22}$ or $F_{11} = -F_{33}$ or $F_{22} = -F_{33}$.