4

3D formulations with rotations

In this chapter, the formulations including rotations as an independent (primary) variable are derived for a 3D continuum. The derived functionals amount to various forms of the potential energy modified by the Rotation Constraint; their extensions to the Hu–Washizu and Hellinger–Reissner functionals are provided in Sect. 12. Some of these 3D formulations are used in subsequent chapters as a basis for derivation of shell equations.

Extended configuration space. The classical configuration space of the non-polar Cauchy continuum is defined as

$$\mathcal{C} \doteq \{\boldsymbol{\chi}: \ B \rightarrow R^3\}, \tag{4.1}$$

where $\boldsymbol{\chi}$ is the deformation function defined over the reference configuration of the body B. In the present section, we consider the *extended configuration* space, defined in terms of the deformation function $\boldsymbol{\chi}$ and rotations $\mathbf{R} \in \mathrm{SO}(3)$. We do not account for gradients of rotations, similarly as in the pseudo-Cosserat continuum, see [59, 128, 238]. The rotations are generated by the (left) skew-symmetric tensor $\delta\tilde{\boldsymbol{\theta}} \doteq \delta\mathbf{R}\mathbf{R}^T$ (in the sense explained for the weak form AMB equation), and are treated in two different ways:

- remain unconstrained, as in the Cosserat-type continuum. Then the extended configuration space is defined as

  $$\mathcal{C}_{\mathrm{ext}} \doteq \{(\boldsymbol{\chi}, \mathbf{R}) : \ B \rightarrow R^3 \times \mathrm{SO}(3)\}. \tag{4.2}$$

  Note that $\boldsymbol{\chi}$ does not belong to the classical configuration space. This approach to rotations is quite popular in shells, which can be treated as pseudo-Cosserat surfaces, see e.g. [244, 52, 200] and the papers cited therein.

- are constrained, either by the polar decomposition of $\mathbf{F}$ equation (3.2) or the RC equation (3.8). Then the extended configuration space is defined as

$$\mathcal{C}_{\text{ext}} \doteq \{(\boldsymbol{\chi}, \mathbf{R}) : \ B \rightarrow R^3 \times \mathrm{SO}(3) \quad | \quad \boldsymbol{\chi} \in \mathcal{C}\}, \tag{4.3}$$

where $\mathcal{C}$ is the classical configuration space. Note that $\boldsymbol{\chi}$ is required to belong to $\mathcal{C}$, i.e. it is identical as for the classical non-polar Cauchy continuum, see [128, 238, 74, 175, 13]. This approach is used in [252, 253, 254], to define the second-order kinematics of shells.

The basic formulation of this chapter is given for the nominal stress from which the formulations for other types of stress are derived. The formulations based on the Biot stress, see [191, 42, 249], and the formulations based on the second Piola–Kirchhoff stress, see [99, 214], are presented. Several variational principles are also summarized in [9].

Four-field (4-F) formulation exploits the polar decomposition equation, while the three-field (3-F) formulations are based on the RC equation. Two-field (2-F) formulations are obtained by regularization of the 3-F functionals, except the one for unconstrained rotations.

Finally, we note that both approaches, i.e. with constrained and unconstrained rotations, can be applied to shells. The 3-F and 2-F formulations are used in subsequent chapters as the basis for derivation of shell equations.

4.1 Governing equations

Balance equations and boundary conditions. The local balance equations and the boundary conditions are

1. linear momentum balance (LMB):

$$\mathrm{Div}\mathbf{P} + \rho_{\mathrm{R}}\mathbf{b} = \mathbf{0} \quad \text{in} \quad \mathrm{B}, \tag{4.4}$$

where $\mathbf{P}$ is the nominal stress tensor (its transpose is the first Piola–Kirchhoff stress), ρ_R is the mass density for the reference (initial) configuration, and $\mathbf{b}$ is the body force.

2. angular momentum balance (AMB):

$$\mathbf{F} \times \mathbf{P} = \mathbf{0} \qquad \text{or} \qquad \mathrm{skew}(\mathbf{P}\mathbf{F}^T) = \mathbf{0} \quad \text{in} \quad \mathrm{B}, \tag{4.5}$$

where $\mathbf{F} = \mathrm{Grad}\boldsymbol{\chi}$ and $\det \mathbf{F} > 0$.

3. boundary conditions (BC):

$$\boldsymbol{\chi} = \hat{\boldsymbol{\chi}} \quad \text{on} \quad \partial_\chi \mathrm{B} \qquad \text{and} \qquad \mathbf{Pn} = \hat{\mathbf{p}} \quad \text{on} \quad \partial_\sigma \mathrm{B}, \tag{4.6}$$

where $\partial_\chi \mathrm{B}$ and $\partial_\sigma \mathrm{B}$ denote disjoint parts of the boundary $\partial \mathrm{B}$ on which the deformation and traction boundary conditions are specified. The outward normal vector is denoted by $\mathbf{n}$ and $\hat{\mathbf{p}}$ is the external load (surface traction) which we assume as not depending on deformation.

Weak form of basic equations. The weak form of eqs. (4.4)–(4.6) is obtained by calculating their scalar products with the respective admissible fields and integrating over the volume B or the surface traction BC area $\partial_\sigma \mathrm{B}$ of the initial configuration.

LMB. For eq. (4.4), we calculate the volume integral of its scalar product with the kinematically admissible variation of deformation $\delta\boldsymbol{\chi}$, i.e. such that $\delta\boldsymbol{\chi} = \mathbf{0}$ on $\partial_u \mathrm{B}$,

$$\int_B (\mathrm{Div}\mathbf{P} + \rho_\mathrm{R}\mathbf{b}) \cdot \delta\boldsymbol{\chi} \, \mathrm{d}V = 0. \tag{4.7}$$

Using the formula for the divergence of a product of two tensors, e.g. [33] eq. (5.5.19), we obtain

$$\mathrm{Div}\mathbf{P} \cdot \delta\boldsymbol{\chi} = \mathrm{Div}(\mathbf{P}^T \delta\boldsymbol{\chi}) - \mathbf{P} \cdot \nabla\delta\boldsymbol{\chi}. \tag{4.8}$$

For the first r.h.s. term, we use the divergence theorem, e.g. [33] eq. (5.8.11),

$$\int_B \mathrm{Div}(\mathbf{P}^T \delta\boldsymbol{\chi}) \, \mathrm{d}V = \int_{\partial B} (\mathbf{P}^T \delta\boldsymbol{\chi}) \cdot \mathbf{n} \, \mathrm{d}A = \int_{\partial B} (\mathbf{Pn}) \cdot \delta\boldsymbol{\chi} \, \mathrm{d}A. \tag{4.9}$$

For the second term, we note that $\nabla\delta\boldsymbol{\chi} = \delta\mathbf{F}$. Then the weak form of the LMB is

$$\int_B (\mathbf{P} \cdot \delta\mathbf{F} - \rho_R \mathbf{b} \cdot \delta\boldsymbol{\chi}) \, \mathrm{d}V - \int_{\partial B} (\mathbf{Pn}) \cdot \delta\boldsymbol{\chi} \, \mathrm{d}A. \tag{4.10}$$

AMB. For eq. (4.5), we calculate a volume integral of its scalar product with a skew-symmetric (left) tensor $\delta\tilde{\boldsymbol{\theta}}$,

$$\int_B \mathrm{skew}(\mathbf{PF}^T) \cdot \delta\tilde{\boldsymbol{\theta}} \, \mathrm{d}V = 0. \tag{4.11}$$

If $\delta\tilde{\boldsymbol{\theta}}$ generates rotations, i.e. $\{\delta\tilde{\boldsymbol{\theta}} : \ \delta\mathbf{R} \doteq \delta\tilde{\boldsymbol{\theta}}\,\mathbf{R}\}$, which we can assume for the extended configuration space but not for the classical one, the weak form AMB becomes

$$\int_B \operatorname{skew}(\mathbf{P}\mathbf{F}^T) \cdot (\mathbf{R}^T \delta\mathbf{R})\, \mathrm{d}V = 0. \tag{4.12}$$

BCD. For the displacement BC, eq. (4.6), we calculate a surface integral of a scalar product with $\delta(\mathbf{Pn})$,

$$\int_{\partial_\chi \mathrm{B}} (\boldsymbol{\chi} - \hat{\boldsymbol{\chi}}) \cdot \delta(\mathbf{Pn})\, \mathrm{d}A = 0. \tag{4.13}$$

BCT. For the traction BC, eq. (4.6), we calculate a surface integral of a scalar product with a kinematically admissible variation $\delta\boldsymbol{\chi}$,

$$\int_{\partial_\sigma \mathrm{B}} (\mathbf{Pn} - \hat{\mathbf{p}}) \cdot \delta\boldsymbol{\chi}\, \mathrm{d}A = 0. \tag{4.14}$$

Remark. Note that, compared to the classical 1-F formulation in terms of $\boldsymbol{\chi}$ only, the weak form AMB equation is different while the other equations are the same. To explain the expression that $\delta\tilde{\boldsymbol{\theta}}$ *generates* rotations, we transform $\delta\mathbf{R} \doteq \delta\tilde{\boldsymbol{\theta}}\,\mathbf{R}$ by using $\delta(\ ) = \dot{(\ )}\,\delta t$, where the superimposed dot denotes the time-derivative. This yields a differential equation, $\dot{\mathbf{R}} - \dot{\tilde{\boldsymbol{\theta}}}\,\mathbf{R} = \mathbf{0}$, to which we append the initial condition $\mathbf{R}(t = 0) = \mathbf{R}_0$. From this equation we can calculate (*generate*) $\mathbf{R}$ for an assumed $\dot{\tilde{\boldsymbol{\theta}}}$; for details see Sect. 9.4.

Virtual work of stress, strain energy, constitutive law. Below, the VW of the nominal stress $\mathbf{P}$ is transformed to four equivalent forms. Next, the corresponding strain energy functionals are defined and the respective constitutive laws are derived.

a. Strain energy $\mathcal{W}(\mathbf{U})$. The VW of the nominal stress $\mathbf{P} \cdot \delta\mathbf{F}$ can be expressed as

$$\mathbf{P} \cdot \delta\mathbf{F} = \operatorname{sym}(\mathbf{R}^T\mathbf{P}) \cdot \delta\mathbf{U}, \tag{4.15}$$

where $\mathbf{R}$ and $\mathbf{U}$ are obtained from the polar decomposition equation $\mathbf{F} = \mathbf{RU}$. Taking a variation of this equation, we have $\delta\mathbf{F} = \delta\mathbf{R}(\mathbf{R}^T\mathbf{R})\mathbf{U} + \mathbf{R}\delta\mathbf{U}$, where $\delta\mathbf{R}\mathbf{R}^T \doteq \delta\tilde{\boldsymbol{\theta}}$, and $\delta\tilde{\boldsymbol{\theta}} = -\delta\tilde{\boldsymbol{\theta}}^T$, i.e. is skew-symmetric. Then

$$\mathbf{P} \cdot \delta\mathbf{F} = \mathbf{P} \cdot (\delta\tilde{\boldsymbol{\theta}}\mathbf{F}) + \mathbf{P} \cdot (\mathbf{R}\delta\mathbf{U}) = (\mathbf{P}\mathbf{F}^T) \cdot \delta\tilde{\boldsymbol{\theta}} + \mathrm{sym}(\mathbf{R}^T\mathbf{P}) \cdot \delta\mathbf{U},$$

and the first term vanishes as a scalar product of a symmetric $\mathbf{P}\mathbf{F}^T$ (which is a consequence of the AMB: $\mathrm{skew}(\mathbf{P}\mathbf{F}^T) = \mathbf{0}$) and a skew-symmetric $\delta\tilde{\boldsymbol{\theta}}$.

The strain deduced from the r.h.s. of eq. (4.15) as the work conjugate to $\mathrm{sym}(\mathbf{R}^T\mathbf{P})$, is the right stretch strain,

$$\mathbf{H} \doteq (\mathbf{F}^T\mathbf{F})^{1/2} - (\mathbf{I}^T\mathbf{I})^{1/2}, \tag{4.16}$$

where $\mathbf{I}$ is consistent with $\mathbf{F}$, see eq. (5.17).

Assume that the strain energy density per unit non-deformed volume, $\mathcal{W}$, is a function of $\mathbf{U}$. $\mathcal{W}(\mathbf{U})$ satisfies the material objectivity (frame indifference) requirement, because $\mathbf{U}$ is a polynomial of $\mathbf{C}$, i.e. $\mathbf{U} = \mathbf{C}^{\frac{1}{2}} = a_0\mathbf{I} + a_1\mathbf{C} + a_2\mathbf{C}^2$, as discussed below eq. (3.2). A variation of the strain energy is

$$\delta\mathcal{W}(\mathbf{U}) = \partial_U\mathcal{W}(\mathbf{U}) \cdot \delta\mathbf{U}. \tag{4.17}$$

The term $\mathrm{sym}(\mathbf{R}^T\mathbf{P}) \cdot \delta\mathbf{U}$ can be treated as $\delta\mathcal{W}$ and, hence, from eqs. (4.15) and (4.17), we obtain the constitutive law

$$\mathrm{sym}(\mathbf{R}^T\mathbf{P}) = \partial_U\mathcal{W}(\mathbf{U}). \tag{4.18}$$

This CL is used in the 4-F formulation for the nominal stress.

b. Strain energy $\mathcal{W}(\mathbf{C})$. The VW of the nominal stress $\mathbf{P} \cdot \delta\mathbf{F}$ can be expressed as

$$\mathbf{P} \cdot \delta\mathbf{F} = \tfrac{1}{2}\mathbf{S} \cdot \delta\mathbf{C}, \tag{4.19}$$

where $\mathbf{S}$ is the second Piola-Kirchhoff stress tensor and $\mathbf{C} \doteq \mathbf{F}^T\mathbf{F}$ is the right Cauchy–Green deformation tensor. The above formula is obtained by using $\mathbf{P} = \mathbf{F}\mathbf{S}$ for which the AMB, $\mathrm{skew}(\mathbf{P}\mathbf{F}^T) = \mathrm{skew}(\mathbf{F}\mathbf{S}\mathbf{F}^T) = \mathbf{0}$, implies $\mathbf{S} = \mathbf{S}^T$. Equation (4.19) is obtained by the following transformations:

$$(\mathbf{F}\mathbf{S}) \cdot \delta\mathbf{F} = \mathbf{S} \cdot (\mathbf{F}^T\delta\mathbf{F}) = \mathbf{S} \cdot \mathrm{sym}(\mathbf{F}^T\delta\mathbf{F}) = \mathbf{S} \cdot \delta(\tfrac{1}{2}\mathbf{F}^T\mathbf{F}) = \tfrac{1}{2}\mathbf{S} \cdot \delta\mathbf{C}.$$

The strain deduced from the r.h.s. of eq. (4.19) as the work conjugate to $\mathbf{S}$, is the Green strain,

$$\mathbf{E} \doteq \tfrac{1}{2}(\mathbf{F}^T\mathbf{F} - \mathbf{I}^T\mathbf{I}). \tag{4.20}$$

This strain can be obtained from the change of the square of the length of an infinitesimal line element, $\mathrm{d}\mathbf{x} = (\partial \mathbf{x}/\partial \mathbf{y})\,\mathrm{d}\mathbf{y} = \mathbf{F}\,\mathrm{d}\mathbf{y}$,

$$\mathrm{d}\mathbf{x}\cdot\mathrm{d}\mathbf{x} - \mathrm{d}\mathbf{y}\cdot\mathrm{d}\mathbf{y} = (\mathbf{F}\mathrm{d}\mathbf{y})\cdot(\mathbf{F}\mathrm{d}\mathbf{y}) - (\mathbf{I}\mathrm{d}\mathbf{y})\cdot(\mathbf{I}\mathrm{d}\mathbf{y}) = 2\mathrm{d}\mathbf{y}\cdot(\mathbf{E}\,\mathrm{d}\mathbf{y}). \tag{4.21}$$

Note that $\mathbf{I}$ is consistent with $\mathbf{F}$, see eq. (5.17).

Assume that the strain energy density per unit non-deformed volume, $\mathcal{W}$, is a function of $\mathbf{C}$. To satisfy the frame indifference requirement, $\mathcal{W}$ must remain the same for the observer transformation $\mathbf{x}^+ = \mathbf{O}\mathbf{x} + \mathbf{c}$, where $\mathbf{O} \in \mathrm{SO}(3)$, ([239] p. 44). The observer transformation yields $\mathbf{F}^+ = \mathbf{O}\mathbf{F}$ and the right Cauchy–Green tensor is invariant, i.e. $\mathbf{C}^+ = (\mathbf{F}^+)^T\mathbf{F}^+ = \mathbf{F}^T\mathbf{O}^T\mathbf{O}\mathbf{F} = \mathbf{F}^T\mathbf{F} = \mathbf{C}$. If $\mathcal{W}$ is a function of $\mathbf{C}$, then $\mathcal{W}(\mathbf{C}^+) = \mathcal{W}(\mathbf{C})$, and this requirement is satisfied. A variation of the strain energy is as follows

$$\delta\mathcal{W}(\mathbf{C}) = \partial_C\mathcal{W}(\mathbf{C})\cdot\delta\mathbf{C}. \tag{4.22}$$

The term $\frac{1}{2}\mathbf{S}\cdot\delta\mathbf{C}$ can be treated as $\delta\mathcal{W}$ and, hence, from eqs. (4.19) and (4.22), we obtain the constitutive law

$$\mathbf{S} = 2\,\partial_C\mathcal{W}(\mathbf{C}). \tag{4.23}$$

This CL is used in the formulations for the second Piola–Kirchhoff stress.

c. Strain energy $\mathcal{W}(\mathbf{Q}^T\mathbf{F})$. The VW of the nominal stress $\mathbf{P}\cdot\delta\mathbf{F}$ can be expressed as

$$\mathbf{P}\cdot\delta\mathbf{F} = (\mathbf{Q}^T\mathbf{P})\cdot\delta(\mathbf{Q}^T\mathbf{F}), \tag{4.24}$$

where $\mathbf{Q} \in \mathrm{SO}(3)$, and $(\mathbf{Q}^T\mathbf{F})$ is non-symmetric.

Proof. First,

$$\mathbf{P}\cdot\delta\mathbf{F} = \mathrm{tr}(\mathbf{Q}\mathbf{Q}^{\mathrm{T}}\mathbf{P}\delta\mathbf{F}^{\mathrm{T}}) = \mathrm{tr}(\mathbf{Q}^{\mathrm{T}}\mathbf{P}\delta\mathbf{F}^{\mathrm{T}}\mathbf{Q}) = (\mathbf{Q}^{\mathrm{T}}\mathbf{P})\cdot(\mathbf{Q}^{\mathrm{T}}\delta\mathbf{F}).$$

Next, we use $\mathbf{Q}^T\delta\mathbf{F} = \delta(\mathbf{Q}^T\mathbf{F}) - \delta\mathbf{Q}^T\mathbf{F}$. Then,

$$(\mathbf{Q}^T\mathbf{P})\cdot(\mathbf{Q}^T\delta\mathbf{F}) = (\mathbf{Q}^T\mathbf{P})\cdot\delta(\mathbf{Q}^T\mathbf{F}) - (\mathbf{Q}^T\mathbf{P})\cdot(\delta\mathbf{Q}^T\mathbf{F}),$$

where the 2nd component,

$$(\mathbf{Q}^T\mathbf{P})\cdot(\delta\mathbf{Q}^T\mathbf{F}) = \mathrm{tr}(\mathbf{Q}^{\mathrm{T}}\mathbf{P}\mathbf{F}^{\mathrm{T}}\delta\mathbf{Q}) = \mathrm{tr}(\delta\mathbf{Q}\mathbf{Q}^{\mathrm{T}}\mathbf{P}\mathbf{F}^{\mathrm{T}}) = \delta\tilde{\boldsymbol{\theta}}\cdot(\mathbf{P}\mathbf{F}^{\mathrm{T}}) = \mathbf{0},$$

as $\delta \mathbf{Q}\mathbf{Q}^T \doteq \delta\tilde{\boldsymbol{\theta}}$ is skew-symmetric and $\mathbf{P}\mathbf{F}^T$ is symmetric as a consequence of the AMB: $\text{skew}(\mathbf{P}\mathbf{F}^T) = \mathbf{0}$. This ends the proof. □

The strain deduced from the r.h.s. of eq. (4.24), as the work conjugate to $(\mathbf{Q}^T\mathbf{P})$, is the *non-symmetric relaxed* right stretch strain

$$\tilde{\mathbf{H}}_n \doteq \mathbf{Q}^T\mathbf{F} - \mathbf{I}^T\mathbf{I}, \tag{4.25}$$

where $\mathbf{I}$ is consistent with $\mathbf{F}$, see eq. (5.17).

Assume that the strain energy density per unit non-deformed volume, $\mathcal{W}$, is a function of $\mathbf{Q}^T\mathbf{F}$. Note that if $\text{skew}(\mathbf{Q}^T\mathbf{F}) \to \mathbf{0}$, then $\mathbf{Q}^T\mathbf{F} \to \mathbf{U}$ and $\mathcal{W}(\mathbf{Q}^T\mathbf{F}) \to \mathcal{W}(\mathbf{U})$ which satisfies the material objectivity (frame indifference) requirement, as discussed earlier. A variation of the strain energy is

$$\delta\mathcal{W}(\mathbf{Q}^T\mathbf{F}) = \partial_{Q^TF}\mathcal{W}(\mathbf{Q}^T\mathbf{F}) \cdot \delta(\mathbf{Q}^T\mathbf{F}). \tag{4.26}$$

The term $(\mathbf{Q}^T\mathbf{P}) \cdot \delta(\mathbf{Q}^T\mathbf{F})$ can be treated as $\delta\mathcal{W}$ and, hence, from eqs. (4.24) and (4.26), we obtain the constitutive law

$$(\mathbf{Q}^T\mathbf{P}) = \partial_{Q^TF}\mathcal{W}(\mathbf{Q}^T\mathbf{F}). \tag{4.27}$$

We note that the above CL is applicable only to the unconstrained formulation, with rotations restricted neither by the polar decomposition equation nor by the RC equation.

d. Strain energy $\mathcal{W}(\text{sym}(\mathbf{Q}^T\mathbf{F}))$. The sum of the VW of the nominal stress and the weak form of the RC equation can be expressed as

$$\begin{aligned}\mathbf{P} \cdot \delta\mathbf{F} &+ \delta\text{skew}(\mathbf{Q}^T\mathbf{P}) \cdot \text{skew}(\mathbf{Q}^T\mathbf{F}) \\ &= \text{sym}(\mathbf{Q}^T\mathbf{P}) \cdot \delta\text{sym}(\mathbf{Q}^T\mathbf{F}) + \delta[\text{skew}(\mathbf{Q}^T\mathbf{P}) \cdot \text{skew}(\mathbf{Q}^T\mathbf{F})],\end{aligned} \tag{4.28}$$

where we applied eq. (4.24) to the first component and the split into symmetric and skew-symmetric parts,

$$(\mathbf{Q}^T\mathbf{P}) \cdot \delta(\mathbf{Q}^T\mathbf{F}) = \text{sym}(\mathbf{Q}^T\mathbf{P}) \cdot \text{sym}\delta(\mathbf{Q}^T\mathbf{F}) + \text{skew}(\mathbf{Q}^T\mathbf{P}) \cdot \text{skew}\delta(\mathbf{Q}^T\mathbf{F}).$$

Besides, commuting of the operations of taking a symmetric (or skew) part and taking a variation, i.e. $\text{sym}\delta(\cdot) = \delta\text{sym}(\cdot)$ and $\text{skew}\delta(\cdot) = \delta\text{skew}(\cdot)$, is accounted for.

The strain deduced from the first term on the r.h.s. of eq. (4.28), as the work conjugate to $\text{sym}(\mathbf{Q}^T\mathbf{P})$, is the *symmetric relaxed* right stretch strain,

$$\tilde{\mathbf{H}} \doteq \text{sym}(\mathbf{Q}^T\mathbf{F}) - \text{sym}(\mathbf{I}^T\mathbf{I}), \tag{4.29}$$

where $\mathbf{I}$ is consistent with $\mathbf{F}$, see eq. (5.17).

Assume that the strain energy density per unit non-deformed volume, $\mathcal{W}$, is a function of $\text{sym}(\mathbf{Q}^T\mathbf{F})$. Note that if $\text{skew}(\mathbf{Q}^T\mathbf{F}) \to \mathbf{0}$, then $\text{sym}(\mathbf{Q}^T\mathbf{F}) \to \mathbf{U}$ and $\mathcal{W}(\text{sym}(\mathbf{Q}^T\mathbf{F})) \to \mathcal{W}(\mathbf{U})$, which satisfies the material objectivity (frame indifference) requirement, as discussed earlier. The variation of the strain energy is

$$\delta\mathcal{W}(\tilde{\mathbf{U}}) = \partial_{\tilde{U}}\mathcal{W}(\tilde{\mathbf{U}}) \cdot \delta\tilde{\mathbf{U}}, \tag{4.30}$$

where $\tilde{\mathbf{U}} \doteq \text{sym}(\mathbf{Q}^T\mathbf{F})$ is the *relaxed* right stretch tensor. The first term of eq. (4.28), $\text{sym}(\mathbf{Q}^T\mathbf{P}) \cdot \delta\text{sym}(\mathbf{Q}^T\mathbf{F})$, can be treated as $\delta\mathcal{W}$ and, hence, from this first term and eq. (4.30), we obtain the constitutive law

$$\text{sym}(\mathbf{Q}^T\mathbf{P}) = \partial_{\tilde{U}}\mathcal{W}(\tilde{\mathbf{U}}). \tag{4.31}$$

This CL is used in the 3-F formulation for the nominal stress.

Using the Biot stress $\mathbf{T}_s^B \doteq \text{sym}(\mathbf{Q}^T\mathbf{P})$ of eq. (4.50), we can rewrite eq. (4.31) as follows:

$$\mathbf{T}_s^B = \partial_{\tilde{U}}\mathcal{W}(\tilde{\mathbf{U}}). \tag{4.32}$$

This CL is used in the formulations for the Biot stress.

4.2 4-F formulation for nominal stress

In this section, we describe a four-field formulation including rotations derived from the balance equations in terms of the nominal stress, see [74, 10], which has the following features:

- the rotations $\mathbf{Q}$ are constrained by the polar decomposition equation (3.2),
- the strain energy and the CL are defined for the right stretch strain of eq. (3.12).

To the set of governing equations (4.4)–(4.6), we append the following equations:

1. Polar decomposition equation:

$$\mathbf{F} - \mathbf{R}\mathbf{U} = \mathbf{0}, \tag{4.33}$$

2. Constitutive law of eq. (4.18):

$$\mathrm{sym}(\mathbf{R}^T\mathbf{P}) = \frac{\partial \mathcal{W}(\mathbf{U})}{\partial \mathbf{U}}, \tag{4.34}$$

which all furnish a mixed formulation in terms of four fields $\{\boldsymbol{\chi}, \mathbf{R}, \mathbf{U}, \mathbf{P}\}$.

Weak form of basic equations. A weak form of the governing equations, (4.4)–(4.6), is given by eqs. (4.10) and (4.12)–(4.14). For the polar decomposition equation, (4.33), we calculate a volume integral of a scalar product of this equation with $\delta\mathbf{P}$,

$$\int_B (\mathbf{F} - \mathbf{R}\mathbf{U}) \cdot \delta\mathbf{P}\, \mathrm{d}V = 0. \tag{4.35}$$

VW equation. Adding the above weak form (scalar) equations, we obtain the VW equation

$$\int_B \{\mathbf{P} \cdot \delta\mathbf{F} + \delta\,[\mathbf{P} \cdot (\mathbf{F} - \mathbf{R}\mathbf{U})]\}\ \mathrm{d}V - \delta F_{\mathrm{ext}} = 0, \tag{4.36}$$

where

$$\delta F_{\mathrm{ext}} \doteq \delta F_b + \delta F_\sigma + \delta F_\chi, \tag{4.37}$$

$$\delta F_b \doteq \int_B \rho_R \mathbf{b} \cdot \delta\boldsymbol{\chi}\, \mathrm{d}V, \qquad \delta F_\sigma \doteq \int_{\partial_\sigma \mathrm{B}} (\mathbf{P}\mathbf{n} - \hat{\mathbf{p}}) \cdot \delta\boldsymbol{\chi}\, \mathrm{d}A,$$

$$\delta F_\chi \doteq \int_{\partial_\chi \mathrm{B}} (\boldsymbol{\chi} - \hat{\boldsymbol{\chi}}) \cdot \delta(\mathbf{P}\mathbf{n})\, \mathrm{d}A.$$

Proof. The integrand of eq. (4.36) is obtained as follows. Adding the scalar equations (4.10) and (4.12)–(4.14), we obtain

$$\mathbf{P} \cdot \delta\mathbf{F} + \delta\mathbf{P} \cdot (\mathbf{F} - \mathbf{R}\mathbf{U}) + \mathrm{skew}(\mathbf{P}\mathbf{F}^T) \cdot (\delta\mathbf{R}^T\mathbf{R}), \tag{4.38}$$

which can be transformed to the following equivalent form

$$\mathbf{P} \cdot \delta\mathbf{F} + \delta\,[\mathbf{P} \cdot (\mathbf{F} - \mathbf{R}\mathbf{U})]\,, \tag{4.39}$$

as follows. Note that the first terms of both equations are identical. The second term of eq. (4.39) can be rewritten as

$$\delta[\mathbf{P} \cdot (\mathbf{F} - \mathbf{R}\mathbf{U})] = \delta\mathbf{P} \cdot (\mathbf{F} - \mathbf{R}\mathbf{U}) + \mathbf{P} \cdot \delta\mathbf{F} - \mathbf{P} \cdot (\delta\mathbf{R}\mathbf{U}) - \mathbf{P} \cdot (\mathbf{R}\delta\mathbf{U}), \tag{4.40}$$

where the first term is equal to the second term of eq. (4.38). The second and fourth terms cancel out because

$$\begin{aligned}\mathbf{P}\cdot(\mathbf{R}\delta\mathbf{U}) &= \mathrm{tr}(\mathbf{P}\delta\mathbf{U}\mathbf{R}^{\mathrm{T}}) = \mathrm{tr}(\mathbf{R}^{\mathrm{T}}\mathbf{P}\delta\mathbf{U}) = (\mathbf{R}^{\mathrm{T}}\mathbf{P})\cdot\delta\mathbf{U}\\ &= \mathrm{sym}(\mathbf{R}^{T}\mathbf{P})\cdot\delta\mathbf{U} = \mathbf{P}\cdot\delta\mathbf{F},\end{aligned}$$

where the last form was obtained on use of eq. (4.15). The third term is equal to the third term of eq. (4.39) because

$$\begin{aligned}\mathbf{P}\cdot(\delta\mathbf{R}\mathbf{U}) &= \mathbf{P}\cdot(\delta\mathbf{R}\mathbf{R}^{T}\mathbf{F}) = \mathrm{tr}(\mathbf{P}\mathbf{F}^{\mathrm{T}}\mathbf{R}\delta\mathbf{R}^{\mathrm{T}})\\ &= (\mathbf{P}\mathbf{F}^{T})\cdot(\delta\mathbf{R}\mathbf{R}^{T}) = -\mathrm{skew}(\mathbf{P}\mathbf{F}^{T})\cdot(\mathbf{R}^{T}\delta\mathbf{R}),\end{aligned}$$

which ends the proof. □

Four-field potential. On use of eqs. (4.15) and (4.18), we have $\mathbf{P}\cdot\delta\mathbf{F} = \mathrm{sym}(\mathbf{R}^{T}\mathbf{P})\cdot\delta\mathbf{U} = \partial_{U}\mathcal{W}(\mathbf{U})\cdot\delta\mathbf{U}$. Thus, from eq. (4.36) we can deduce the four-field functional

$$F_4^P(\boldsymbol{\chi},\mathbf{R},\mathbf{U},\mathbf{P}) \doteq \int_B [\mathcal{W}(\mathbf{U}) + \mathbf{P}\cdot(\mathbf{F}-\mathbf{R}\mathbf{U})]\,\mathrm{d}V - F_{\mathrm{ext}}, \tag{4.41}$$

where $\mathbf{P}$ is a Lagrange multiplier for the polar decomposition equation (4.33). Besides, the functional of external forces

$$F_{\mathrm{ext}} \doteq F_b + F_\sigma + F_\chi, \tag{4.42}$$

where the functionals for the body force, the (deformation independent) external loads and the displacement boundary conditions are defined as

$$F_b \doteq \int_B \rho_R\mathbf{b}\cdot\boldsymbol{\chi}\,\mathrm{d}V,\quad F_\sigma \doteq \int_{\partial_\sigma \mathrm{B}} \hat{\mathbf{p}}\cdot\boldsymbol{\chi}\,\mathrm{d}A,\quad F_\chi \doteq \int_{\partial_\chi \mathrm{B}} (\mathbf{P}\mathbf{n})\cdot(\boldsymbol{\chi}-\hat{\boldsymbol{\chi}})\,\mathrm{d}A.$$

Remark. In this formulation, the right stretch $\mathbf{U}$ is not a function of $\boldsymbol{\chi}$ but an independent tensorial variable. It must be parameterized in a way ensuring that it is symmetric and positive definite; the latter can be achieved by expressing $\mathbf{U}$ in terms of its principal values, taken as squares of some parameters, and a rotation tensor. We see that $\mathbf{U}$ introduces six additional variables in a complicated form, and that's why other simpler formulations were developed; they are presented in the following sections.

4.3 3-F formulation for nominal stress

In this section, we describe a three-field formulation including rotations, in terms of $\{\chi, \mathbf{Q}, \mathbf{T}_a\}$, which has the following features:

- the rotations $\mathbf{Q}$ are constrained by the Rotation Constraint (RC), eq. (3.8),
- the strain energy and the CL are defined for the *relaxed* right stretch, eq. (3.12).

To the set of governing equations (4.4)–(4.6), we append the following equations:

1. Rotation Constraint:

$$\mathfrak{C} \doteq \text{skew}(\mathbf{Q}^T\mathbf{F}) = \mathbf{0}, \tag{4.43}$$

2. Constitutive Law of eq. (4.31):

$$\text{sym}(\mathbf{Q}^T\mathbf{P}) = \frac{\partial \mathcal{W}(\tilde{\mathbf{U}})}{\partial \tilde{\mathbf{U}}}, \qquad \tilde{\mathbf{U}} = \text{sym}(\mathbf{Q}^T\mathbf{F}), \tag{4.44}$$

which furnish a formulation in terms of three fields $\{\chi, \mathbf{Q}, \mathbf{P}\}$. Comparing with the four-field formulation of the previous section, the right stretch tensor $\mathbf{U}$ is not present.

Strain energy and constitutive law. If $\mathbf{Q} = \mathbf{R}$, where $\mathbf{R} \in \text{SO}(3)$ satisfies the polar decomposition equation, then, by eq. (4.15), $\delta\mathcal{W} = \mathbf{P} \cdot \delta\mathbf{F} = \text{sym}(\mathbf{R}^T\mathbf{P}) \cdot \delta\mathbf{U}$, i.e. the tensor $\text{sym}(\mathbf{R}^T\mathbf{P})$ is work-conjugate to $\mathbf{U}$. Let us assume the existence of the strain energy $\mathcal{W}$ in terms of the *relaxed* stretch strain $\tilde{\mathbf{U}} = \text{sym}(\mathbf{Q}^T\mathbf{F})$. Using $\tilde{\mathbf{U}}$ in place of $\mathbf{U}$ in eq. (4.34), we obtain the constitutive law (4.18).

Weak form of basic equations. A weak form of the governing equations (4.4)–(4.6), yields eqs. (4.10) and (4.12)–(4.14). For the RC, eq. (4.43), we calculate a volume integral of a scalar product of this equation with a skew-symmetric tensor $\delta\text{skew}(\mathbf{Q}^T\mathbf{P})$,

$$\int_B \text{skew}(\mathbf{Q}^T\mathbf{F}) \cdot \delta\text{skew}(\mathbf{Q}^T\mathbf{P})\, \mathrm{d}V = 0. \tag{4.45}$$

The reason for using here a variation of $\text{skew}(\mathbf{Q}^T\mathbf{P})$ will become obvious in the sequel.

VW equation. Adding the scalar eq. (4.10), (4.13)–(4.14) and (4.45), we obtain

$$\int_B \left[\mathbf{P} \cdot \delta\mathbf{F} + \delta\text{skew}(\mathbf{Q}^T\mathbf{P}) \cdot \text{skew}(\mathbf{Q}^T\mathbf{F})\right] \, \mathrm{d}V - \delta F_{\text{ext}} = 0, \tag{4.46}$$

where δF_{ext} is defined in eq. (4.37). The integrand can be further transformed to the form given by eq. (4.28), i.e.

$$\int_B \left\{\text{sym}(\mathbf{Q}^T\mathbf{P}) \cdot \text{sym}\delta(\mathbf{Q}^T\mathbf{F}) + \delta[\text{skew}(\mathbf{Q}^T\mathbf{P}) \cdot \text{skew}(\mathbf{Q}^T\mathbf{F})]\right\} \, \mathrm{d}V \\ - \delta F_{\text{ext}} = 0. \tag{4.47}$$

Note that the AMB, eq. (4.5), was exploited in the derivation of eq. (4.28), and earlier of eq. (4.24), but its weak form of eq. (4.12) is not present in the integrand of eq. (4.46).

Three-field potential. On the basis of eq. (4.47), by using the CL of eq. (4.32), we can define the three-field potential

$$F_3^P(\boldsymbol{\chi}, \mathbf{Q}, \mathbf{P}) \doteq \int_B \left[\mathcal{W}(\text{sym}(\mathbf{Q}^T\mathbf{F})) + \text{skew}(\mathbf{Q}^T\mathbf{P}) \cdot \text{skew}(\mathbf{Q}^T\mathbf{F})\right] \, \mathrm{d}V - F_{\text{ext}}, \tag{4.48}$$

where F_{ext} is defined in eq. (4.42). This also proves that the use of $\delta\text{skew}(\mathbf{Q}^T\mathbf{P})$ in eq. (4.45) was indeed correct.

Remark 1. The right stretch $\mathbf{U}$ can also be eliminated from the four-field formulation in another way. Note that we can rewrite the Lagrange term of the functional of eq. (4.41) as $\mathbf{P} \cdot (\mathbf{F} - \mathbf{R}\mathbf{U}) = (\mathbf{R}^T\mathbf{P}) \cdot (\mathbf{R}^T\mathbf{F} - \mathbf{U})$, and further split it into a symmetric part and a skew part,

$$(\mathbf{R}^T\mathbf{P}) \cdot (\mathbf{R}^T\mathbf{F} - \mathbf{U}) = \text{sym}(\mathbf{R}^T\mathbf{P}) \cdot \left[\text{sym}(\mathbf{R}^T\mathbf{F}) - \mathbf{U}\right] \\ + \text{skew}(\mathbf{R}^T\mathbf{P}) \cdot \text{skew}(\mathbf{R}^T\mathbf{F}). \tag{4.49}$$

If we assume that $\mathbf{U} \doteq \text{sym}(\mathbf{R}^T\mathbf{F})$, i.e. adopting the *relaxed* right stretch of eq. (3.12), then the first term of eq. (4.49) vanishes, and $F_4^P(\boldsymbol{\chi}, \mathbf{R}, \mathbf{U}, \mathbf{P})$ of eq. (4.41) reduces to the three-field functional of eq. (4.48), with $\mathbf{R}$ in place of $\mathbf{Q}$.

Remark 2. If we use in eq. (4.47) the CL $\operatorname{sym}(\mathbf{Q}^T\mathbf{P}) = \partial_{\tilde{U}}\mathcal{W}$ of eq. (4.31), then the nominal stress $\mathbf{P}$ remains only in the term $\operatorname{skew}(\mathbf{Q}^T\mathbf{P})$. Hence, we can define a skew-symmetric tensor $\mathbf{T}_a \doteq \operatorname{skew}(\mathbf{Q}^T\mathbf{P})$ with only three components and abandon using $\mathbf{P}$ with nine components. That is the basic motivation behind using the Biot stress in the next section.

4.4 3-F and 2-F formulations for Biot stress

In this section, we describe a three-field formulation in terms of $\{\boldsymbol{\chi}, \mathbf{Q}, \mathbf{T}_a\}$, developed in [42, 191]. This formulation can be obtained from the three-field formulation for the nominal stress tensor, which is described in the previous section, just by introducing the definition of the Biot stress. A two-field formulation, which is valid only for an isotropic material, is also presented.

Biot stress. Define the tensor $\mathbf{T} \doteq \mathbf{Q}^T\mathbf{P}$, where $\mathbf{Q} \in SO(3)$, and split it into the symmetric and skew-symmetric parts, $\mathbf{T} = \mathbf{T}_s^B + \mathbf{T}_a$, where

$$\mathbf{T}_s^B \doteq \operatorname{sym}\mathbf{T} = \operatorname{sym}(\mathbf{Q}^T\mathbf{P}), \qquad \mathbf{T}_a \doteq \operatorname{skew}\mathbf{T} = \operatorname{skew}(\mathbf{Q}^T\mathbf{P}). \tag{4.50}$$

The symmetric part $\mathbf{T}_s^B$ is called the Biot stress, or the Biot–Lure stress, or the Jaumann stress. Having $\mathbf{T}_s^B$, $\mathbf{T}_a$, and $\mathbf{Q}$, we can uniquely calculate $\mathbf{P}$.

VW equation. Introducing the definitions of $\mathbf{T}_s^B$ and $\mathbf{T}_a$ of eq. (4.50) into eq. (4.47), we obtain the VW in the form

$$\int_B \left\{\mathbf{T}_s^B \cdot \operatorname{sym}\delta(\mathbf{Q}^T\mathbf{F}) + \delta[\mathbf{T}_a \cdot \operatorname{skew}(\mathbf{Q}^T\mathbf{F})]\right\} \, \mathrm{d}V - \delta F_{\text{ext}} = 0, \tag{4.51}$$

where δF_{ext} is defined in eq. (4.37), but with $\mathbf{P}$ replaced by $\mathbf{QT}$.

Three-field potential. For the symmetric $\mathbf{T}_s^B$ we can use the CL, eq. (4.32), i.e. $\mathbf{T}_s^B = \partial_{\tilde{U}}\mathcal{W}$. On the basis of this CL and eq. (4.51), we can define the three-field potential

$$F_3^B(\boldsymbol{\chi}, \mathbf{Q}, \mathbf{T}_a) \doteq \int_B \left[\mathcal{W}(\operatorname{sym}(\mathbf{Q}^T\mathbf{F})) + \mathbf{T}_a \cdot \operatorname{skew}(\mathbf{Q}^T\mathbf{F})\right] \, \mathrm{d}V - F_{\text{ext}}, \tag{4.52}$$

in which $\mathbf{T}_a$ is the Lagrange multiplier for the RC equation. Besides, F_{ext} is defined in eq. (4.42), but with $\mathbf{P}$ replaced by $\mathbf{QT}$.

Euler–Lagrange equations. Because of this new variable, $\mathbf{T}_a$, we have to check whether the Euler–Lagrange equations for F_3^B yield the governing equations (4.4)–(4.6) and (4.43). Using eq. (4.30) and (4.32), we obtain the following variations of the strain energy (4.52):

$$\delta_\chi \mathcal{W}(\mathrm{sym}(\mathbf{Q}^T\mathbf{F})) = \mathbf{T}_s^B \cdot \delta_\chi \tilde{\mathbf{U}} = \mathbf{T}_s^B \cdot (\mathbf{Q}^T \delta\mathbf{F}) = (\mathbf{Q}\mathbf{T}_s^B) \cdot \delta\mathbf{F},$$
$$\delta_Q \mathcal{W}(\mathrm{sym}(\mathbf{Q}^T\mathbf{F})) = \mathbf{T}_s^B \cdot \delta_Q \tilde{\mathbf{U}} = \mathbf{T}_s^B \cdot (\delta\mathbf{Q}^T \mathbf{F}) = -\delta\tilde{\boldsymbol{\theta}} \cdot \mathrm{skew}(\mathbf{Q}\mathbf{T}_s^B\mathbf{F}^T),$$

where $\delta\mathbf{Q} \doteq \delta\tilde{\boldsymbol{\theta}}\,\mathbf{Q}$. The variations of the RC term are

$$\begin{aligned} \delta_\chi[\mathbf{T}_a \cdot \mathrm{skew}(\mathbf{Q}^T\mathbf{F})] &= \delta_\chi[(\mathbf{Q}\mathbf{T}_a) \cdot \mathbf{F}] = (\mathbf{Q}\mathbf{T}_a) \cdot \delta\mathbf{F}, \\ \delta_{T_a}[\mathbf{T}_a \cdot \mathrm{skew}(\mathbf{Q}^T\mathbf{F})] &= \delta\mathbf{T}_a \cdot \mathrm{skew}(\mathbf{Q}^T\mathbf{F}), \\ \delta_Q[\mathbf{T}_a \cdot \mathrm{skew}(\mathbf{Q}^T\mathbf{F})] &= (\delta\mathbf{Q}\mathbf{T}_a) \cdot \mathbf{F} = \mathrm{tr}(\delta\tilde{\boldsymbol{\theta}}\mathbf{Q}\mathbf{T}_a\mathbf{F}^{\mathrm{T}}) \\ &= -\delta\tilde{\boldsymbol{\theta}} \cdot \mathrm{skew}(\mathbf{Q}\mathbf{T}_a\mathbf{F}^T). \end{aligned} \tag{4.53}$$

Hence, the first variation of F_3^P of eq. (4.48) is

$$\delta F_3^B(\boldsymbol{\chi}, \mathbf{Q}, \mathbf{T}_a) = \int_B \left[\mathbf{A} \cdot \delta\mathbf{F} + \delta\mathbf{T}_a \cdot \mathrm{skew}(\mathbf{Q}^T\mathbf{F}) - \delta\tilde{\boldsymbol{\theta}} \cdot \mathrm{skew}(\mathbf{A}\mathbf{F}^T)\right] \mathrm{d}V - \delta F_{\mathrm{ext}}, \tag{4.54}$$

where $\mathbf{A} \doteq \mathbf{Q}(\mathbf{T}_s^B + \mathbf{T}_a) = \mathbf{Q}\mathbf{T} = \mathbf{P}$. We see that δF_3^B is identical as a sum of eqs. (4.10), (4.12)–(4.14) and (4.45), which now is rewritten as $\int_B \mathrm{skew}(\mathbf{Q}^T\mathbf{F}) \cdot \delta\mathbf{T}_a \,\mathrm{d}V = 0$. Hence, the Euler–Lagrange equation are identical to eqs. (4.4)–(4.6) and (4.43), and hence F_3^B is a correct potential for the formulation including rotations.

Remark. Another form of elimination of $\mathbf{U}$ from the four-field functional of eq. (4.41), is to use the Legendre transformation

$$\mathcal{W}(\mathbf{U}) - \mathbf{T}_s^B \cdot \mathbf{U} = -\mathcal{W}_c(\mathbf{T}_s^B), \tag{4.55}$$

where $\mathcal{W}_c$ is the complementary energy density, which requires the constitutive relation to be invertible, $\partial\mathcal{W}_c/\partial\mathbf{T}_s^B = \mathbf{U}$. This approach is described in [9], eq. (3.36).

AMB for isotropic material. For an isotropic material, we can show that the AMB equation is satisfied when the skew-symmetric stress vanishes, i.e. $\mathbf{T}_a = \mathbf{0}$. Rewrite the AMB eq. (4.5), as

$$\mathbf{Q}\mathbf{T}\mathbf{F}^T - \mathbf{F}\mathbf{T}^T\mathbf{Q}^T = \mathbf{0}. \tag{4.56}$$

If the RC is satisfied, then we have $\mathbf{F} = \mathbf{Q}\mathbf{F}^T\mathbf{Q}$ and $\mathbf{Q}^T\mathbf{F} = \mathbf{U}$. Using them in the AMB, we obtain $\mathbf{Q}\,(\mathbf{T}\mathbf{U} - \mathbf{U}\mathbf{T}^T)\,\mathbf{Q}^T = \mathbf{0}$ and the split $\mathbf{T} = \mathbf{T}_s^B + \mathbf{T}_a$ yields

$$\mathbf{T}_a\mathbf{U} + \mathbf{U}\mathbf{T}_a = \mathbf{T}_s^B\mathbf{U} - \mathbf{U}\mathbf{T}_s^B. \tag{4.57}$$

For an isotropic material, $\mathbf{T}_s^B$ and $\mathbf{U}$ are a work-conjugate pair, so they are co-axial and commute. Hence, the r.h.s. of eq. (4.57) vanishes and the AMB is reduced to

$$\mathbf{T}_a\mathbf{U} + \mathbf{U}\mathbf{T}_a = \mathbf{0}. \tag{4.58}$$

Note that $\mathbf{U}$ is symmetric and positive definite, while $\mathbf{T}_a$ is skew-symmetric, hence the assumptions of Lemma 3.1 in [214] are satisfied. Using this lemma, eq. (4.58) is satisfied only when $\mathbf{T}_a = \mathbf{0}$, which completes the proof. □

When the RC is not satisfied or the material is not isotropic, then $\mathbf{T}_a \neq \mathbf{0}$ and must remain in the functional.

Two-field functional for isotropic material. To obtain a two-field functional which does not depend on $\mathbf{T}_a^B$, we regularize F_3^B of eq. (4.52) in $\mathbf{T}_a$ as follows

$$\tilde{F}_3^B(\boldsymbol{\chi}, \mathbf{Q}, \mathbf{T}_a) \doteq F_3^B(\boldsymbol{\chi}, \mathbf{Q}, \mathbf{T}_a) - \frac{1}{2\gamma}\int_B \mathbf{T}_a \cdot \mathbf{T}_a \, \mathrm{d}V, \tag{4.59}$$

where $\gamma \in (0, \infty)$ is the regularization parameter. In the volume integral in $\tilde{F}_3^B$, which is affected by the regularization, the integrand is

$$\mathcal{W}(\mathrm{sym}(\mathbf{Q}^T\mathbf{F})) + \mathbf{T}_a \cdot \mathrm{skew}(\mathbf{Q}^T\mathbf{F}) - \frac{1}{2\gamma}\mathbf{T}_a \cdot \mathbf{T}_a. \tag{4.60}$$

A variation of $\tilde{F}_3^B$ w.r.t. $\mathbf{T}_a$ yields the Euler–Lagrange equation: $\gamma\,\mathrm{skew}(\mathbf{Q}^T\mathbf{F}) - \mathbf{T}_a = 0$, for $\delta\mathbf{T}_a$ in B. From this equation, we calculate $\mathbf{T}_a$ and use it in eq. (4.60), which becomes

$$\mathcal{W}(\mathrm{sym}(\mathbf{Q}^T\mathbf{F})) + \frac{\gamma}{2}\mathrm{skew}(\mathbf{Q}^T\mathbf{F}) \cdot \mathrm{skew}(\mathbf{Q}^T\mathbf{F}), \tag{4.61}$$

in which the second term is the RC equation $\mathrm{skew}(\mathbf{Q}^T\mathbf{F}) = \mathbf{0}$ imposed by the penalty method. Then, the two-field functional, not depending on $\mathbf{T}_a$, is defined as

$$\tilde{F}_2^B(\boldsymbol{\chi}, \mathbf{Q}) \doteq \int_B \left[\mathcal{W}(\mathrm{sym}(\mathbf{Q}^T\mathbf{F})) + \frac{\gamma}{2}\,\mathrm{skew}(\mathbf{Q}^T\mathbf{F}) \cdot \mathrm{skew}(\mathbf{Q}^T\mathbf{F})\right] \mathrm{d}V - F_{\mathrm{ext}}. \tag{4.62}$$

The corresponding VW equation is

$$\int_B \left[\mathbf{T}_s^B \cdot \delta\mathrm{sym}(\mathbf{Q}^T\mathbf{F}) \;+\; \gamma\,\mathrm{skew}(\mathbf{Q}^T\mathbf{F}) \cdot \delta\mathrm{skew}(\mathbf{Q}^T\mathbf{F})\right]\,\mathrm{d}V - \delta F_{\mathrm{ext}} = 0. \tag{4.63}$$

This equation can be used only for isotropic material.

4.5 3-F and 2-F formulations for second Piola–Kirchhoff stress

In this section, we assume that the strain energy $\mathcal{W}$ is a function of the right Cauchy–Green tensor $\mathbf{C}$, and we obtain the formulations with rotations in terms of the second Piola–Kirchhoff stress $\mathbf{S}$. The governing equations for such a formulation are obtained by using $\mathbf{P} = \mathbf{FS}$ in eqs. (4.4)–(4.6), and by appending the RC of eq. (4.43). From the outset, we assume that $\mathbf{S} = \mathbf{S}^T$, i.e. that the LMB of eq. (4.5) is satisfied, as in [214]. The CL for $\mathbf{S}$ is given by eq. (4.23).

Weak form of basic equations. We modify the VW of eq. (4.47) as follows: (i) we use $\mathbf{P} = \mathbf{FS}$ in the term

$$\delta[\mathrm{skew}(\mathbf{Q}^T\mathbf{P}) \cdot \mathrm{skew}(\mathbf{Q}^T\mathbf{F})] = \delta[\mathrm{skew}(\mathbf{Q}^T\mathbf{FS}) \cdot \mathrm{skew}(\mathbf{Q}^T\mathbf{F})],$$

(ii) we use the strain energy $\mathcal{W}(\mathbf{C})$ in terms of the right Cauchy–Green tensor $\mathbf{C}$,

$$\partial_{\tilde{U}}\mathcal{W}(\tilde{U}) \cdot \mathrm{sym}\delta(\mathbf{Q}^T\mathbf{F}) = \partial_C\mathcal{W}(\mathbf{C}) \cdot \mathrm{sym}\delta(\mathbf{F}^T\mathbf{F}),$$

where eqs. (4.19) and (4.22) were used. This yields the VW equation,

$$\int_B \left\{\partial_C\mathcal{W}(\mathbf{C}) \cdot \mathrm{sym}\delta(\mathbf{F}^T\mathbf{F}) + \delta[\mathbf{T}_a \cdot \mathrm{skew}(\mathbf{Q}^T\mathbf{F})]\right\}\,\mathrm{d}V - \delta F_{\mathrm{ext}} = 0, \tag{4.64}$$

where $\mathbf{T}_a \doteq \mathrm{skew}(\mathbf{Q}^T\mathbf{FS})$ is used to change the variables, i.e. instead of $\mathbf{S}$ with six components, we use $\mathbf{T}_a$ with only three components. δF_{ext} is defined in eq. (4.37), but with $\mathbf{P}$ replaced by $\mathbf{FS}$.

Three-field potential. From eq. (4.64), we can deduce the three-field potential

$$F_3^{\mathrm{2PK}}(\boldsymbol{\chi}, \mathbf{Q}, \mathbf{T}_a) \doteq \int_B \left[\mathcal{W}(\mathbf{F}^T\mathbf{F}) + \mathbf{T}_a \cdot \mathrm{skew}(\mathbf{Q}^T\mathbf{F})\right]\,\mathrm{d}V - F_{\mathrm{ext}}, \tag{4.65}$$

where $\mathbf{T}_a$ is the Lagrange multiplier for the RC equation. Besides, F_{ext} is defined in eq. (4.42) but with $\mathbf{P}$ replaced by $\mathbf{FS}$.

Euler–Lagrange equations. Because of this new variable, $\mathbf{T}_a$, we have to check whether the Euler-Lagrange equations for F_3^{2PK} of eq. (4.65) yield the governing equations (4.4)–(4.6) and (4.43).

By using eqs. (4.19) and (4.23), we obtain a variation of the strain energy $\delta_\chi \mathcal{W}(\mathbf{F}^T\mathbf{F}) = (\mathbf{FS}) \cdot \delta\mathbf{F}$. The variations of the RC term are given by eq. (4.53). Hence,

$$\delta F_3^{\text{2PK}}(\boldsymbol{\chi}, \mathbf{Q}, \mathbf{T}_a) = \int_B \left[\mathbf{A} \cdot \delta\mathbf{F} + \delta\mathbf{T}_a \cdot \text{skew}(\mathbf{Q}^T\mathbf{F}) - \delta\tilde{\boldsymbol{\theta}} \cdot \text{skew}(\mathbf{Q}\mathbf{T}_a\mathbf{F}^T) \right] \, \mathrm{d}V - \delta F_{\text{ext}}, \tag{4.66}$$

where $\mathbf{A} \doteq \mathbf{FS} + \mathbf{QT}_a$ and $\delta\tilde{\boldsymbol{\theta}} \doteq \delta\mathbf{Q}\mathbf{Q}^T$. The term $\mathbf{A} \cdot \delta\mathbf{F}$ can be transformed further. Using the formula for the divergence of a product of two tensors, see [33] eq. (5.5.19), and $\delta\mathbf{F} = \nabla\delta\mathbf{u}$, we obtain

$$\text{Div}\mathbf{A} \cdot \nabla\delta\mathbf{u} = \text{Div}(\mathbf{A}^T\delta\mathbf{u}) - \mathbf{A} \cdot \nabla\delta\mathbf{u}.$$

The second term contributes to the equilibrium equation, while the first term is transformed on use of the divergence theorem, see [33] eq. (5.8.11), as follows

$$\int_B \text{Div}(\mathbf{A}^T\delta\mathbf{u}) \, \mathrm{d}V = \int_{\partial B} (\mathbf{A}^T\delta\mathbf{u}) \cdot \mathbf{n} \, \mathrm{d}A = \int_{\partial B} (\mathbf{An}) \cdot \delta\mathbf{u} \, \mathrm{d}A.$$

We see that this term contributes to the traction BC. Finally, the following Euler–Lagrange equations are obtained

$$\begin{aligned} \text{Div}\mathbf{A} + \rho_R\mathbf{b} = \mathbf{0} \quad &\text{in} \quad \text{B}, \\ \text{skew}(\mathbf{Q}\mathbf{T}_a\mathbf{F}^T) = \mathbf{0} \quad &\text{in} \quad \text{B}, \\ \text{skew}(\mathbf{Q}^T\mathbf{F}) = \mathbf{0} \quad &\text{in} \quad \text{B}, \\ \mathbf{An} = \hat{\mathbf{p}} \quad &\text{on} \quad \partial_\sigma\text{B}. \end{aligned} \tag{4.67}$$

These equations will be equal to the governing equations (4.4), (4.6) and (4.43) when $\mathbf{T}_a = \mathbf{0}$, as then the second of the above equations is trivially satisfied and $\mathbf{A} = \mathbf{FS} = \mathbf{P}$. The proof that $\mathbf{T}_a = \mathbf{0}$ is given below.

Proof. Eq.$(4.67)_2$ is post-multiplied by $\mathbf{Q}$, and transformed as follows:

$$2\,\text{skew}(\mathbf{Q}\mathbf{T}_a\mathbf{F}^T)\,\mathbf{Q} = \mathbf{Q}\mathbf{T}_a\mathbf{F}^T\mathbf{Q} - \mathbf{F}\mathbf{T}_a^T\mathbf{Q}^T\mathbf{Q} = \mathbf{Q}\mathbf{T}_a\mathbf{F}^T\mathbf{Q} + \mathbf{F}\mathbf{T}_a. \tag{4.68}$$

From eq. $(4.67)_3$, we have $\mathbf{F}^T\mathbf{Q} = \mathbf{Q}^T\mathbf{F}$ and, on the left polar decomposition $\mathbf{F} = \mathbf{V}\mathbf{Q}$, where $\mathbf{V}$ is the left stretching tensor, we obtain

$$\mathbf{Q}\mathbf{T}_a\mathbf{Q}^T\mathbf{V}\mathbf{Q}+\mathbf{V}\mathbf{Q}\mathbf{T}_a = \mathbf{T}_a^*\mathbf{V}\mathbf{Q}+\mathbf{V}\mathbf{Q}\mathbf{Q}^T\mathbf{T}_a^*\mathbf{Q} = (\mathbf{T}_a^*\mathbf{V}+\mathbf{V}\mathbf{T}_a^*)\,\mathbf{Q}, \quad (4.69)$$

where $\mathbf{T}_a^* \doteq \mathbf{Q}\mathbf{T}_a\mathbf{Q}^T$ is the forward-rotated $\mathbf{T}_a$. Hence, eq. $(4.67)_2$ yields

$$\mathbf{T}_a^*\,\mathbf{V} + \mathbf{V}\,\mathbf{T}_a^* = \mathbf{0}. \quad (4.70)$$

Because $\mathbf{T}_a^*$ is skew-symmetric and $\mathbf{V}$ is symmetric and positive definite, the assumptions of Lemma 3.1 in [214] are satisfied. With this lemma, the above equation is satisfied only when $\mathbf{T}_a^* = \mathbf{0}$. Hence, $\mathbf{T}_a = \mathbf{Q}^T\mathbf{T}_a^*\mathbf{Q} = \mathbf{0}$, which ends the proof. □

Two-field functional. We can regularize the functional (4.65) in $\mathbf{T}_a$ as follows:

$$\tilde{F}_3^{\mathrm{2PK}}(\boldsymbol{\chi}, \mathbf{Q}, \mathbf{T}_a) = F_3^{\mathrm{2PK}}(\boldsymbol{\chi}, \mathbf{Q}, \mathbf{T}_a) - \frac{1}{2\gamma}\int_B \mathbf{T}_a \cdot \mathbf{T}_a \,\mathrm{d}V, \quad (4.71)$$

where $\gamma \in (0,\infty)$ is the regularization parameter. It can be shown that the correct Euler–Lagrange equations of $\tilde{F}_3^{\mathrm{2PK}}$ are obtained not only when $\gamma \to \infty$, but for any value of γ. A variation of $\tilde{F}_3^{\mathrm{2PK}}$ w.r.t. $\mathbf{T}_a$ yields the following Euler–Lagrange equation for $\delta\mathbf{T}_a$ in B,

$$\mathrm{skew}(\mathbf{Q}^T\mathbf{F}) - \frac{1}{\gamma}\mathbf{T}_a = 0. \quad (4.72)$$

From this equation we calculate $\mathbf{T}_a = \gamma\,\mathrm{skew}(\mathbf{Q}^T\mathbf{F})$, and use it in eq. (4.71). Then we can define a two-field functional

$$\tilde{F}_2^{\mathrm{2PK}}(\boldsymbol{\chi}, \mathbf{Q}) \doteq \int_B \left[\mathcal{W}(\mathbf{F}^T\mathbf{F}) + \frac{\gamma}{2}\mathrm{skew}(\mathbf{Q}^T\mathbf{F}) \cdot \mathrm{skew}(\mathbf{Q}^T\mathbf{F})\right] \mathrm{d}V - F_{\mathrm{ext}}, \quad (4.73)$$

with the penalty term for the RC equation. We have to check that the Euler–Lagrange equations for F_2^{2PK} yield the governing equations (4.4), (4.6) and (4.43); the proof is given in [214], eqs. (22)–(25). This functional is typically used in numerical implementations.

Remark. In this formulation, the rotations $\mathbf{Q}$ appear only in the RC, but not in the other governing equations. Hence, we can first solve the problem for $\boldsymbol{\chi}$ and determine $\mathbf{Q}$ afterwards, which can be done in two ways, using either the RC equation or the polar decomposition of $\mathbf{F}$, as discussed earlier. This method cannot be used in the Reissner-type shells, where $\mathbf{Q}$ appears also in the governing equations.

4.6 2-F formulation with unconstrained rotations

In this section, we describe a two-field formulation in terms of $\{\boldsymbol{\chi}, \mathbf{Q}\}$, which has the following features:

- neither the polar decomposition equation (3.2), nor the RC equation (3.8) are used to constrain rotations $\mathbf{Q}$.
- the strain energy and the CL are defined for the *non-symmetric relaxed* right stretch eq. (3.12).

To the set of governing equations, eqs. (4.4)–(4.6), we only append the constitutive law, eq. (4.27),

$$(\mathbf{Q}^T\mathbf{P}) = \partial_{Q^TF}\mathcal{W}(\mathbf{Q}^T\mathbf{F}), \tag{4.74}$$

where $\mathbf{Q}^T\mathbf{F}$ is non-symmetric.

VW equation. Adding weak forms of the governing equations, i.e. eqs. (4.10), and (4.13)–(4.14), and applying eq. (4.24), we obtain

$$\int_B (\mathbf{Q}^T\mathbf{P}) \cdot \delta(\mathbf{Q}^T\mathbf{F})\,\mathrm{d}V - \delta F_{\text{ext}} = 0, \tag{4.75}$$

where δF_{ext} is defined in eq. (4.37). Note that the AMB, eq. (4.12), was exploited in derivation of eq. (4.24) and, hence, it does not appear explicitly in eq. (4.75).

Two-field potential. Using eq. (4.74), we obtain

$$(\mathbf{Q}^T\mathbf{P}) \cdot \delta(\mathbf{Q}^T\mathbf{F}) = \partial_{Q^TF}\mathcal{W}(\mathbf{Q}^T\mathbf{F}) \cdot \delta(\mathbf{Q}^T\mathbf{F}).$$

Hence, on the basis of this equation and eq. (4.75), we can define a two-field potential

$$F_2^*(\boldsymbol{\chi}, \mathbf{Q}) \doteq \int_B \mathcal{W}(\mathbf{Q}^T\mathbf{F})\,\mathrm{d}V - F_{\text{ext}}, \tag{4.76}$$

where F_{ext} is defined in eq. (4.42).

Remark. Note that $F_2^*(\boldsymbol{\chi}, \mathbf{Q})$ can be additionally constrained by the RC equation, $\operatorname{skew}(\mathbf{Q}^T\mathbf{F}) = \mathbf{0}$, by using the penalty method. Then,

$$F_2^{**}(\boldsymbol{\chi}, \mathbf{Q}) \doteq \int_B \mathcal{W}(\mathbf{Q}^T\mathbf{F}) + \frac{\gamma}{2}\operatorname{skew}(\mathbf{Q}^T\mathbf{F}) \cdot \operatorname{skew}(\mathbf{Q}^T\mathbf{F})\,\mathrm{d}V - F_{\text{ext}}, \tag{4.77}$$

where $\gamma \in (0, \infty)$ is the penalty parameter. Note that the argument of $\mathcal{W}$ is different to that in eq. (4.62).