STUDYING PROBLEMS IN ELASTICITY AND PLASTICITY USING A QR DECOMPOSITION OF THE DEFORMATION GRADIENT

A Dissertation

by

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ABSTRACT

With the recent developments of **QR** kinematics and the associated constitutive model, in this thesis, we address some of the fundamental issues in **QR** kinematics and extend this method to study some problems in elasto-plasticity. In this framework, the matrix of the deformation gradient is decomposed into an orthogonal rotation $\boldsymbol{\mathcal{R}}$ and an upper-triangular matrix $\boldsymbol{\mathcal{U}}$, called the Laplace stretch. The **QR** decomposition can be achieved using different techniques, of which a Gram-Schmidt procedure is most suitable for our application. A Gram-Schmidt procedure requires the specification of a particular coordinate direction and a specific coordinate plane, which includes this particular coordinate direction, given some coordinate systems of interest. Unfortunately, this coordinate direction and associated coordinate plane are not known *a priori*, because they require information from both the triad of base vectors and the deformation in question. This issue is resolved by introducing a strategy whereby that edge of a representative cube undergoing the least amount of transverse shear under a given deformation, and the adjoining coordinate plane that experiences the least amount of in-plane shear are selected. Next, a compatibility condition for the Laplace stretch is derived, whenever a right Cauchy-Green tensor $\mathbf{C} = \mathbf{F}^T\mathbf{F}$ is prescribed. Here, we choose the right Cauchy-Green tensor as our primary kinematic variable and show that a vanishing of the Riemann curvature tensor imposes restrictions on the spatial variations of certain elements of the Laplace stretch $\boldsymbol{\mathcal{U}}$. A natural extension of our work on compatibility is to study the incompatibility of a pertient space when the **QR** kinematics is applied to elastoplasticity. Using the property that the set of all upper-triangular matrices form a group under multiplication, Freed *et al.* (2019) [36] proposed an elastic-plastic decomposition of Laplace stretch, i.e., $\boldsymbol{\mathcal{U}} = \boldsymbol{\mathcal{U}}^e\,\boldsymbol{\mathcal{U}}^p$. Using this decomposition, we study the geometric dislocation density tensor and Burgers vector. The geometric dislocation density tensor $\tilde{\mathbf{G}}$ is obtained using the classical argument of failure of a Burgers circuit in a suitable configuration $\tilde{\kappa}_p$ where the deformation of a body is solely due to the movement of dislocations. The geometric features of space $\tilde{\kappa}_p$ are explored and it has been shown that the derived geometric dislocation tensor is related to the torsion of $\tilde{\kappa}_p$. The total dislocation

density can be additively decomposed into the dislocation density due to plastic "straining" and a term representing the incompatibility of rotation field. The latter of which is physically similar to Nye's definition of dislocation density tensor. Based on this kinematics, a constitutive model has been developed for isotropic, elastic-plastic materials. A maximum rate of dissipation criterion has been used in deriving the constitutive equations as this criterion is valid for a wider class of materials. Two cases of plastic deformation – volume-preserving and dilatant-pressure dependent deformations have been considered. As illustration of the proposed model, the classical J_2 plasticity and Drucker-Prager model has been derived. The concept of plastic spin has also been investigated in this framework. It has been shown that the intermediate configuration $\tilde{\kappa}_p$ acts as a macroscopic manifestation of the material substructure. Expressions for a substructural spin and a material spin have been obtained using appropriate physical arguments based on this configuration. An internal state variable has been considered to represent the macroscopic manifestation of the microstructural properties. Considering the orientational properties of this internal variable with respect to the material substructure, an expression for the plastic spin has been obtained and its implication in the context of single crystal plasticity has been shown. Finally, this plastic spin has been incorporated into a constitutive model by means of an appropriate definition of the co-rotational rate of the internal state variable.

DEDICATION

To all my teachers, including my parents.

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1. INTRODUCTION

In recent years, an alternative **QR** decomposition of the deformation gradient **F** has been proposed which has several advantages over the traditional polar decomposition. The polar decomposition decomposes the deformation gradient into an orthogonal rotation tensor **R** and a symmetric stretch tensor, either **U** or **V**. Despite being a well-established theory, when it comes to the ease of application, the polar decomposition is not without its shortcomings. For instance,

- The invariants of the stretch tensor lack direct physical meanings.
- Computation of the rotation tensor is cumbersome as it requires inversion of the stretch tensor and involves complex eigenvalue analysis.
- The Cauchy stress is related to the invariants of stretch tensor through the derivatives of strain energy in a complicated manner [88].
- The covariance between invariants hinders one's ability to parametrize material model [20].
- It is not possible to obtain a unique deformation gradient from a prescribed Cauchy-Green tensor [8] , etc.

In order to avoid these issues, an alternative **QR** decomposition was put forward [63, 64, 88] which decomposes the deformation gradient into an orthogonal rotation $\boldsymbol{\mathcal{R}}$ and an upper-triangular matrix $\boldsymbol{\mathcal{U}}$, called the Laplace stretch [36]. The primary attraction of this new decomposition is its utility regarding experiments. Due to the direct physical interpretation of the components of Laplace stretch, an experimenter can directly and unambiguously measure the deformations in all six degrees of freedom within a specific coordinate frame [34]. In our work, the **QR** kinematics is employed to study some problems in elasticity and plasticity.

1.1 Background and literature review

QR decomposition has been a well adopted technique in the mathematics community for over a century. The idea of this procedure was first introduced by Laplace (1820) where he introduced successive orthogonal projections to solve a least squares problem to estimate the masses of Jupiter and Saturn. Gram (1879) used this technique in his work on the series expansions of real functions. This algorithm became popular when Schmidt (1907) used this technique to solve integral equations. Although the techniques in these pioneering works are essentially the same, their algorithms are different. A review of Gram-Schmidt factorization can be found in Leon *et al.* (2013) [55]. As mentioned earlier, in this decomposition, any matrix with positive determinant is decomposed into a proper orthogonal matrix and an upper-triangular matrix. Many different algorithms exist in the literature to perform this decomposition, viz., Gram-Schmidt factorization, Givens rotation method, Householder reflection method etc. of which the Gram-Schmidt process is best suited for our application. In Gram-Schmidt factorization, an orthogonal set of base vectors are obtained by using successive orthogonal projections of a given set of base vectors [1]. It is in this coordinate frame, spanned by the newly obtained orthogonal bases, where a given matrix with positive determinant takes on the form of an upper-triangular matrix.

McLellan (1976) [63] was the first to introduce this technique into the physics literature when he applied a Gram-Schmidt factorization to the matrix of the deformation gradient and decomposed it into an orthogonal matrix $\boldsymbol{\mathcal{R}}$, inverse of which $\boldsymbol{\mathcal{R}}^T$ transforms an Eulerian triad into a set of bases $\tilde{e}_i$ that spans experimenter's frame of reference and an upper-triangular matrix, $\boldsymbol{\mathcal{U}}$, known as Laplace stretch [36]. He [64] also showed that this decomposition has an added advantage over the classical polar decomposition, as upper-triangular matrices with positive determinant form a group under multiplication[2]. This feature allowed him to further decompose the upper-triangular matrix $\boldsymbol{\mathcal{U}}$ into a diagonal matrix whose diagonal elements represent elongations along the coordinate directions, and an unit upper-triangular matrix whose off-diagonal elements represent three simple shears acting perpendicular to one another, thereby resulting in an Iwasawa (1949) [44] matrix decomposition of the deformation gradient. He applied this decomposition in his work on the thermodynamic stability of crystalline phases. Later, Souchet (1993) [87] introduced a lower-triangular decomposition of the deformation gradient. Boulanger and Hayes [10] have shown that

[1]Note that this given set of base vectors need not be orthogonal.

[2]Note that a set of symmetric matrices is not closed under multiplication, and hence does not form a group.

triangular decompositions of the deformation gradient are special cases of their more general class of extended polar decompositions [9].

Srinivasa (2012) [88] showed that this decomposition has some more advantages over the classical polar decomposition of $\mathbf{F}$. Of which, the most important is the direct physical meaning of the components of $\boldsymbol{\mathcal{U}}$, and hence its utility regarding experiments. The coordinate frame in which a **QR** decomposition of the deformation gradient is performed, when aligned with a laboratory apparatus, enables one to measure the components $\mathcal{U}_{ij}$ unambiguously from experiments. Therefore, this coordinate frame is termed as experimenter's frame of reference. **QR** kinematics have been further explored by Freed and Srinivasa (2015) [34]. Lembo (2017) [53] attempted the problem of finding a compatibility condition for Laplace stretch by following a procedure similar to Shield's (1973) [83] work on compatibility for a polar decomposition of $\mathbf{F}$. Freed and Zamani (2018) [37] investigated **QR** kinematics for a locally convected coordinate system.

Advances in the research on **QR** kinematics paved way for an alternative constitutive theory. Traditionally, tensor invariants are employed in the construction of constitutive theories throughout mechanics. Despite of its elegance, the theory falls short from an experimental point of view as the covariance between invariants hinders one to be able to parametrize a material model [20]. In order to avoid this issue, Freed *et al*. (2017) [33] developed a constitutive theory that uses scalar conjugate stress/strain base pairs. This model is particularly useful for 2-D biological membranes. This work was further extended to three-dimensional isotropic materials by Freed (2017) [32] and anisotropic materials by Erel *et al*. (2019) [27]. Rajagopal and Srinivasa (2016) [76] employed this kinematics to implicit constitutive theory for three-dimensional elastic bodies. Based on their kinematics described in a locally convected coordinate system, Freed and Zamani (2019) [35] developed constitutive relations for elastic bodies that takes into account Kelvin-Poisson-Poynting effects. Clayton and Freed (2020) [17] developed constitutive models for viscoelastic materials based on this kinematics.

The upper-triangular decomposition was extended to elasto-plasticity when Ghosh and Srinivasa (2014) [39] used it in their work on shape-memory alloys. In this paper, the plastic part of the deformation gradient arising from a Kröner [49]–Lee [52] decomposition is further decomposed into a proper orthogonal matrix and an upper-triangular plastic stretch, while the elastic part of deformation gradient remains as a full matrix, thus $\mathbf{F} = \mathbf{F}^e \boldsymbol{\mathcal{R}} \boldsymbol{\mathcal{U}}^p$ [3]. Freed *et al.* [36] used a different approach to employ an upper-triangular decomposition for elasto-plasticity. They first employed Gram-Schmidt factorization to a deformation gradient with the resulting upper-triangular Laplace stretch being decomposed into elastic and plastic parts. The latter decomposition is possible due to the fact that any upper-triangular matrix with positive determinant forms a group under multiplication.[4] Moreover, this renders the elastic-plastic decomposition of Laplace stretch unique and thus, the issue of non-uniqueness of the intermediate configuration, arising in is suppressed at the kinematics level.

1.2 Preliminaries

Before going to the main objective of this dissertation, in this section, we briefly discuss an overview of the prior research mentioned in § 1.1.

1.2.1 QR kinematics

Consider a simply connected body embedded in a three-dimensional Euclidean point space. Motion $\boldsymbol{\mathcal{X}}(\boldsymbol{X}, t)$ is a homeomorphism that maps points in an undeformed configuration $\kappa_r(\mathcal{B})$ into points in a current configuration $\kappa_t(\mathcal{B})$. Position vectors of a material point in the undeformed and current configurations are denoted by $\boldsymbol{X}$ and $\boldsymbol{x}$, respectively. An assumption of simple-connectedness of the body ensures the applicability of Stokes' theorem. The deformation gradient $\mathbf{F} = \partial \boldsymbol{\mathcal{X}}(\boldsymbol{X}, t)/\partial \boldsymbol{X}$ is a linear transformation that maps tangent vectors at a point in the body in $\kappa_r(\mathcal{B})$ into tangent vectors at its corresponding point in $\kappa_t(\mathcal{B})$.

We choose a Cartesian coordinate system $\boldsymbol{E}_I$ to represnt the deformation gradient $\mathbf{F}$ in matrix

[3]Note that $\boldsymbol{\mathcal{R}}$ is different from the rotation tensor $\mathbf{R}$ obtained from polar decomposition of $\mathbf{F}$.

[4]Note that in traditional Kröner–Lee decomposition, one can have multiple intermediate configurations up to a finite rigid rotation. The issue of non-uniqueness is resolved at the constitutive level by imposing an invariance requirement under rigid body rotation.

form. In this coordinate system, the matrix of the deformation gradient can be written as

$$F^i_J = \left[\begin{array}{c|c|c} \boldsymbol{f}_1 & \boldsymbol{f}_2 & \boldsymbol{f}_3 \end{array} \right] \tag{1.1}$$

where $\boldsymbol{f}_I = F^j_I \, \boldsymbol{E}_j$ are the columns of the matrix of the deformation gradient. Now we apply the Gram-Schmidt procedure on this matrix to obtain the bases of our physical frame of reference as

$$\begin{aligned} \tilde{\boldsymbol{e}}_1 &= \frac{\boldsymbol{f}_1}{\|\boldsymbol{f}_1\|}; \\ \tilde{\boldsymbol{e}}_2 &= \frac{\boldsymbol{f}_2 - (\boldsymbol{f}_1 \cdot \boldsymbol{f}_2)\, \boldsymbol{f}_1}{\|\boldsymbol{f}_2 - (\boldsymbol{f}_1 \cdot \boldsymbol{f}_2)\, \boldsymbol{f}_1\|}; \\ \tilde{\boldsymbol{e}}_3 &= \frac{\boldsymbol{f}_3 - (\boldsymbol{f}_1 \cdot \boldsymbol{f}_3)\, \boldsymbol{f}_1 - (\boldsymbol{f}_2 \cdot \boldsymbol{f}_3)\, \boldsymbol{f}_2}{\|\boldsymbol{f}_3 - (\boldsymbol{f}_1 \cdot \boldsymbol{f}_3)\, \boldsymbol{f}_1 - (\boldsymbol{f}_2 \cdot \boldsymbol{f}_3)\, \boldsymbol{f}_2\|}. \end{aligned} \tag{1.2}$$

The new set of bases $\{\tilde{\boldsymbol{e}}_i\}$ aligns with our laboratory apparatus. In this coordinate system, one can decompose $\mathbf{F}$ into an orthogonal matrix $\boldsymbol{\mathcal{R}}$ and an upper-triangular matrix $\boldsymbol{\mathcal{U}}$ called the Laplace stretch [36]. The components of these matrices are described by

$$\mathcal{R}_{IJ} = \left[\begin{array}{c|c|c} \tilde{\boldsymbol{e}}_1 & \tilde{\boldsymbol{e}}_2 & \tilde{\boldsymbol{e}}_3 \end{array} \right]; \quad \mathcal{U}^i_J = \begin{bmatrix} a & a\gamma & a\beta \\ 0 & b & b\alpha \\ 0 & 0 & c \end{bmatrix} \tag{1.3}$$

where a, b, c are three, independent extensions along the coordinate axes of our laboratory frame, and α, β, γ represent three, independent shears acting perpendicular to each other. Note that a, b, c are positive, whereas α, β, γ can be positive, zero or negative. The inverse of Laplace stretch is readily available and has components of

$$\mathcal{U}^{-1}{}^J_i = \begin{bmatrix} \frac{1}{a} & -\frac{\gamma}{b} & -\frac{\beta - \alpha\gamma}{c} \\ 0 & \frac{1}{b} & -\frac{\alpha}{c} \\ 0 & 0 & \frac{1}{c} \end{bmatrix}. \tag{1.4}$$

The physical components of Laplace stretch, when expressed in terms of the columns of the matrix of the deformation gradient, have three orthogonal elongations that are quantified via

$$a = \|\boldsymbol{f}_1\| \tag{1.5a}$$

$$b = \sqrt{\|\boldsymbol{f}_2\|^2 - (\boldsymbol{f}_1 \cdot \boldsymbol{f}_2)^2 / \|\boldsymbol{f}_1\|^2} \tag{1.5b}$$

$$c = \sqrt{\|\boldsymbol{f}_3\|^2 - \frac{(\boldsymbol{f}_1 \cdot \boldsymbol{f}_3)^2}{\|\boldsymbol{f}_1\|^2} - \frac{\left((\boldsymbol{f}_2 \cdot \boldsymbol{f}_3) - (\boldsymbol{f}_1 \cdot \boldsymbol{f}_2)(\boldsymbol{f}_1 \cdot \boldsymbol{f}_3)/\|\boldsymbol{f}_1\|^2\right)^2}{\|\boldsymbol{f}_2\|^2 - (\boldsymbol{f}_1 \cdot \boldsymbol{f}_2)^2/\|\boldsymbol{f}_1\|^2}} \tag{1.5c}$$

and three orthogonal shears that are quantified via

$$\alpha = \frac{(\boldsymbol{f}_2 \cdot \boldsymbol{f}_3) - (\boldsymbol{f}_1 \cdot \boldsymbol{f}_2)(\boldsymbol{f}_1 \cdot \boldsymbol{f}_3)/\|\boldsymbol{f}_1\|^2}{\|\boldsymbol{f}_2\|^2 - (\boldsymbol{f}_1 \cdot \boldsymbol{f}_2)^2/\|\boldsymbol{f}_1\|^2} \tag{1.5d}$$

$$\beta = \frac{\boldsymbol{f}_1 \cdot \boldsymbol{f}_3}{\|\boldsymbol{f}_1\|^2} \tag{1.5e}$$

$$\gamma = \frac{\boldsymbol{f}_1 \cdot \boldsymbol{f}_2}{\|\boldsymbol{f}_1\|^2} \tag{1.5f}$$

wherein $\|\boldsymbol{f}_1\| = \sqrt{\boldsymbol{f}_1 \cdot \boldsymbol{f}_1} = \sqrt{F_{11}^2 + F_{21}^2 + F_{31}^2}$, etc.

The right Cauchy-Green tensor $\mathbf{C} := \mathbf{F}^T\mathbf{F}$ is related to Laplace stretch through a Cholesky factorization of $\mathbf{C}$ [88] and this factorization is unique, viz.,

$$\mathbf{C} = \boldsymbol{\mathcal{U}}^T \boldsymbol{\mathcal{U}}. \tag{1.6}$$

Srinivasa (2012) [88] showed that it is also possible to determine a unique $\boldsymbol{\mathcal{U}}$ generated from a given Cauchy-Green tensor $\mathbf{C}$ through its Cholesky factorization. The Laplace stretch, written in terms of the given components $\mathbf{C}_{IJ}$ for the right Cauchy-Green tensor, becomes:

$$[\mathcal{U}_{ij}] = \begin{bmatrix} \sqrt{C_{11}} & \dfrac{C_{12}}{\mathcal{U}_{11}} & \dfrac{C_{13}}{\mathcal{U}_{11}} \\ 0 & \sqrt{C_{22} - \mathcal{U}_{12}^2} & \dfrac{C_{23} - \mathcal{U}_{12}\mathcal{U}_{13}}{\mathcal{U}_{22}} \\ 0 & 0 & \sqrt{C_{33} - \mathcal{U}_{13}^2 - \mathcal{U}_{23}^2} \end{bmatrix}. \tag{1.7}$$

This Cholesky factorization proves that a Laplace stretch tensor can be *uniquely* determined from a right Cauchy-Green tensor.

Laplace stretch can be further decomposed into a diagonal matrix and two unit upper-triangular matrices [34]. This is a direct consequence of the Iwasawa matrix decomposition of a deformation gradient [44, 37]:

$$\mathcal{U}^i_J = \begin{bmatrix} a & a\gamma & a\beta \\ 0 & b & b\alpha \\ 0 & 0 & c \end{bmatrix} = \begin{bmatrix} a & 0 & 0 \\ 0 & b & 0 \\ 0 & 0 & c \end{bmatrix} \begin{bmatrix} 1 & 0 & \beta \\ 0 & 1 & \alpha \\ 0 & 0 & 1 \end{bmatrix} \begin{bmatrix} 1 & \gamma & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 1 \end{bmatrix} = \Lambda\, \mathcal{U}^{\alpha\beta}\, \mathcal{U}^{\gamma} \tag{1.8}$$

where the physical meaning of Λ, $\mathcal{U}^{\alpha\beta}$ and $\mathcal{U}^{\gamma}$ is explained through Fig. 1.1. Note that the final deformation of the unit cube is slightly different from the one described in Eqn. (1.3). The reason behind this minor difference is that in Fig. 1.1, the deformation is shown in an oblique, convected bases whereas in Eqn. (1.3), the Laplace stretch is described in an orthonormal bases obtained by using Gram-Schmidt procedure.

In an experimenter's frame of reference, a body subjected to a deformation of $\mathcal{U}^{\gamma}$ undergoes a simple shearing between parallel X_1X_3 planes along the $\tilde{e}_1$ direction. $\mathcal{U}^{\alpha\beta}$ causes a shearing between parallel X_1X_2 planes along the direction $\beta\tilde{e}_1 + \alpha\tilde{e}_2$. The deformation Λ denotes an extension of the body in all three directions. Thus, the deformation of a body in all six degrees of freedom is *completely* specified by Laplace stretch.

The diagonal component of Laplace stretch in Eqn. (1.8), Λ can further be decomposed into one dilatation and three squeeze modes, resulting in

$$\Lambda^i_J = \underbrace{\sqrt[3]{abc}\begin{bmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 1 \end{bmatrix}}_{\text{dilatation}} \times \underbrace{\begin{bmatrix} \sqrt[3]{a/b} & 0 & 0 \\ 0 & \sqrt[3]{b/a} & 0 \\ 0 & 0 & 1 \end{bmatrix}}_{\text{1-2 planar squeeze}} \times \underbrace{\begin{bmatrix} 1 & 0 & 0 \\ 0 & \sqrt[3]{b/c} & 0 \\ 0 & 0 & \sqrt[3]{c/b} \end{bmatrix}}_{\text{2-3 planar squeeze}} \times \underbrace{\begin{bmatrix} \sqrt[3]{a/c} & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & \sqrt[3]{c/a} \end{bmatrix}}_{\text{3-1 planar squeeze}}. \tag{1.9}$$

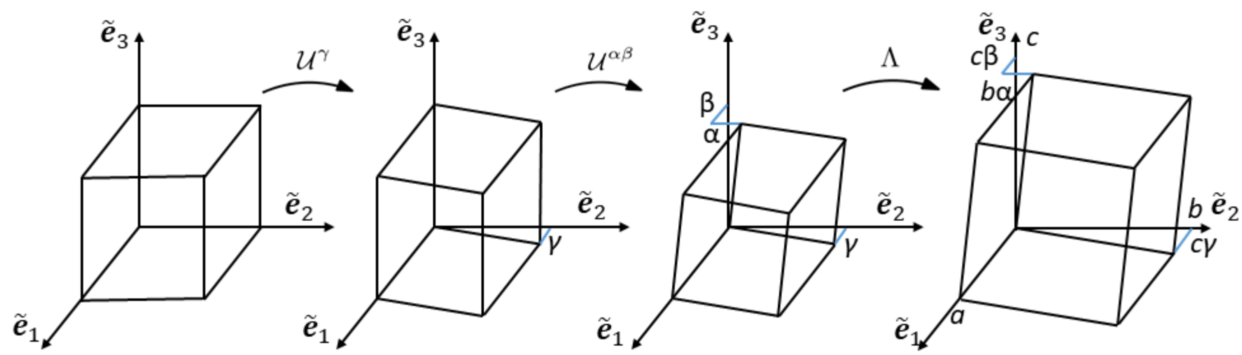

Figure 1.1: The distorion of an unit cube into an oblique rectangular prism through various components of Laplace stretch $\boldsymbol{\mathcal{U}}$. The component γ causes a simple shear between X_1X_3 planar sheets in the $\tilde{\mathrm{e}}_1$ direction. The components α and β are the shearing along the $\tilde{\mathrm{e}}_1$ and $\tilde{\mathrm{e}}_2$ directions, respectively, between parallel X_1X_2 planes. Parameters a, b and c denote elongations along the $\tilde{\mathrm{e}}_1$, $\tilde{\mathrm{e}}_2$ and $\tilde{\mathrm{e}}_3$ directions, respectively.

1.2.2 Kinetics

Based on the **QR** kinematics, it is possible to describe the kinetics of the body in terms of scalar, conjugate, thermodynamic stress/strain base pairs. Let us first define the velocity gradient associated with a Laplace stretch as $\boldsymbol{\mathcal{L}} := \dot{\boldsymbol{\mathcal{U}}}\,\boldsymbol{\mathcal{U}}^{-1}$. Let $\mathbf{S}$ and $\mathbf{E}$ denote the symmetric, second, Piola-Kirchhoff stress and the Green strain, respectively. The rate of work done on an internal mass element is therefore given by [32]

$$\dot{W} := \mathrm{tr}(\mathbf{S}\,\dot{\mathbf{E}}) = \mathrm{tr}(\boldsymbol{\mathcal{S}}\,\boldsymbol{\mathcal{L}}) \tag{1.10}$$

where $\boldsymbol{\mathcal{S}}$ is the Kirchhoff stress in our physical frame of reference $\tilde{\kappa}_t$, which is related to Eulerian Kirchhoff stress $\mathrm{S} := \det(\mathbf{F})\,\boldsymbol{\sigma}$ through the relation $\boldsymbol{\mathcal{S}} := \boldsymbol{\mathcal{U}}\,\mathrm{S}\,\boldsymbol{\mathcal{U}}^T$ where $\boldsymbol{\sigma}$ denotes Cauchy stress. The stress tensor $\boldsymbol{\mathcal{S}}$ is symmetric because the second Piola-Kirchhoff stress is symmetric.

Using the kinematic quantities described in Eqns. (1.8 and 1.9), the stress power can be expressed in terms of seven, conjugate, stress/strain, base pairs. Each of these base pairs describes a specific deformation mode.

Pressure and dilatation:

$$\text{Dilatation,} \qquad \delta := \tfrac{1}{3}\ln(abc), \quad \dot{\delta} = \frac{1}{3}\left(\frac{\dot{a}}{a} + \frac{\dot{b}}{b} + \frac{\dot{c}}{c}\right)$$
$$\text{Pressure,} \qquad \pi := \mathcal{S}_{11} + \mathcal{S}_{22} + \mathcal{S}_{33} \tag{1.11a}$$

Squeeze:

1-2 planar squeeze

$$\text{Strain,} \qquad \varepsilon_1 := \tfrac{1}{3}\ln(a/b), \quad \dot{\varepsilon_1} = \frac{1}{3}\left(\frac{\dot{a}}{a} - \frac{\dot{b}}{b}\right)$$
$$\text{Conjugate stress,} \qquad \sigma_1 := \mathcal{S}_{11} - \mathcal{S}_{22} \tag{1.11b}$$

2-3 planar squeeze

$$\text{Strain,} \qquad \varepsilon_2 := \tfrac{1}{3}\ln(b/c), \quad \dot{\varepsilon_2} = \frac{1}{3}\left(\frac{\dot{b}}{b} - \frac{\dot{c}}{c}\right)$$
$$\text{Conjugate stress,} \qquad \sigma_2 := \mathcal{S}_{22} - \mathcal{S}_{33} \tag{1.11c}$$

3-1 planar squeeze

$$\text{Strain,} \qquad \varepsilon_3 := \tfrac{1}{3}\ln(c/a), \quad \dot{\varepsilon_3} = \frac{1}{3}\left(\frac{\dot{c}}{c} - \frac{\dot{a}}{a}\right)$$
$$\text{Conjugate stress,} \qquad \sigma_3 := \mathcal{S}_{33} - \mathcal{S}_{11} \tag{1.11d}$$

Note that the stresses $\sigma_1, \sigma_2, \sigma_3$, their corresponding conjugate strains, and their rates are not independent; specifically, any one of these stress/strain pairs for squeeze can be expressed as a linear combination of the other two, e.g., $\sigma_3 = -(\sigma_1 + \sigma_2)$ and $\varepsilon_3 = -(\varepsilon_1 + \varepsilon_2)$. The stress/strain base pairs given in Eqns. (1.11a–1.11d) come from the extensional part of the Laplace stretch, $\mathbf{\Lambda}$, whereas the remaining three stress/strain base pairs correspond to the three shear deformations, and are given as

Shear:

Out-of plane shears:

$$\text{Strain, } \gamma_1 := \alpha \quad \text{Conjugate stress, } \tau_1 := \frac{b}{c}\mathcal{S}_{23}; \tag{1.11e}$$

$$\text{Strain, } \gamma_2 := \beta \quad \text{Conjugate stress, } \tau_2 := \frac{a}{c}\mathcal{S}_{13}; \tag{1.11f}$$

In-plane shear:

$$\text{Strain, } \gamma_3 := \gamma \quad \text{Conjugate stress, } \tau_3 := \frac{a}{b}\mathcal{S}_{12} - \alpha\frac{a}{c}\mathcal{S}_{13}. \tag{1.11g}$$

Note that a coupling exists between the in-plane and an out-of-plane shear. Now, using the stress/strain base pairs given in Eqns. (1.11a–1.11g), the stress power can be rewritten as

$$\dot{W} = \pi\dot{\delta} + \sum_{i=1}^{3} \sigma_i \dot{\varepsilon}_i + \sum_{i=1}^{3} \tau_i \dot{\gamma}_i. \tag{1.12}$$

Therefore, instead of the traditionally used tensor invariants, here we can use the list of scalar variables $l_{\mathcal{U}}$ defined as

$$l_{\mathcal{U}} := \{\delta \quad \varepsilon_1 \quad \varepsilon_2 \quad \varepsilon_3 \quad \gamma_1 \quad \gamma_2 \quad \gamma_3\} \tag{1.13}$$

as our primary kinematic variables. In a similar way, we can also define a list of kinematic variables containing the rate of strain attributes as

$$l_{\dot{\mathcal{U}}} := \{\dot{\delta} \quad \dot{\varepsilon}_1 \quad \dot{\varepsilon}_2 \quad \dot{\varepsilon}_3 \quad \dot{\gamma}_1 \quad \dot{\gamma}_2 \quad \dot{\gamma}_3\} \ . \tag{1.14}$$

Because, e.g., strain measure ε_3 and its rate $\dot{\varepsilon}_3$ can be expressed as a linear combination of the other two squeeze strains and strain-rates, one may have a natural propensity to exclude them from lists $l_{\mathcal{U}}$ and $l_{\dot{\mathcal{U}}}$, respectively. However, if this were to be done, then it would become particularly difficult to track the appropriate strains and strain-rates arising within a constitutive relation given a particular function, e.g., the Helmholtz potential or the dissipation function used in subsequent analysis. Keeping this in mind, we will include all three squeeze strains ε_i and their rates $\dot{\varepsilon}_i$ in our lists of kinematic variables. The stress attributes conjugate to the strain attributes $l_{\mathcal{U}}$, can be listed as

$$l_\sigma := \{\pi \quad \sigma_1 \quad \sigma_2 \quad \sigma_3 \quad \tau_1 \quad \tau_2 \quad \tau_3\} \ . \tag{1.15}$$

Now, it is possible to establish bijective maps between these base pairs and the components of Kirchhoff stress $\boldsymbol{\mathcal{S}}$, and the components of a velocity gradient expressed in terms of Laplace stretch $\boldsymbol{\mathcal{L}}$ [32]. For an isotropic material, the stress/strain components are related to the components of Kirchhoff stress $\boldsymbol{\mathcal{S}}$ and the velocity gradient $\boldsymbol{\mathcal{L}}$ through

$$\begin{Bmatrix} \dot{\delta} \\ \dot{\varepsilon}_1 \\ \dot{\varepsilon}_2 \\ \dot{\gamma}_1 \\ \dot{\gamma}_2 \\ \dot{\gamma}_3 \end{Bmatrix} = \begin{bmatrix} 1/3 & 1/3 & 1/3 & 0 & 0 & 0 \\ 1/3 & -1/3 & 0 & 0 & 0 & 0 \\ 0 & 1/3 & -1/3 & 0 & 0 & 0 \\ 0 & 0 & 0 & c/b & 0 & 0 \\ 0 & 0 & 0 & 0 & c/a & b\gamma_1/a \\ 0 & 0 & 0 & 0 & 0 & b/a \end{bmatrix} \begin{Bmatrix} \mathcal{L}_{11} \\ \mathcal{L}_{22} \\ \mathcal{L}_{33} \\ \mathcal{L}_{23} \\ \mathcal{L}_{13} \\ \mathcal{L}_{12} \end{Bmatrix} \tag{1.16}$$

and

$$\begin{Bmatrix} \pi \\ \sigma_1 \\ \sigma_2 \\ \tau_1 \\ \tau_2 \\ \tau_3 \end{Bmatrix} = \begin{bmatrix} 1 & 1 & 1 & 0 & 0 & 0 \\ 1 & -1 & 0 & 0 & 0 & 0 \\ 0 & 1 & -1 & 0 & 0 & 0 \\ 0 & 0 & 0 & b/c & 0 & 0 \\ 0 & 0 & 0 & 0 & a/c & 0 \\ 0 & 0 & 0 & 0 & -a\gamma_1/c & a/b \end{bmatrix} \begin{Bmatrix} \mathcal{S}_{11} \\ \mathcal{S}_{22} \\ \mathcal{S}_{33} \\ \mathcal{S}_{23} \\ \mathcal{S}_{13} \\ \mathcal{S}_{12} \end{Bmatrix} . \tag{1.17}$$

These maps are not necessarily unique. It is interesting to note that in this framework, an anisotropic material response does not enter into the constitutive model directly through the material parameters. Instead, the anisotropy is enfolded in the encoding/decoding map that relates the components of the velocity gradient $\boldsymbol{\mathcal{L}}$ and the strain rate attributes, and the components of the Kirchhoff stress $\boldsymbol{\mathcal{S}}$ and the stress attributes. For an anisotropic, elastic materials the relationship between the components of $\boldsymbol{\mathcal{L}}$ and the strain rate attributes is given as

$$\begin{Bmatrix} \dot{\delta} \\ \dot{\varepsilon}_1 \\ \dot{\varepsilon}_2 \\ \dot{\gamma}_1 \\ \dot{\gamma}_2 \\ \dot{\gamma}_3 \end{Bmatrix} = \begin{bmatrix} vw/3u & uw/3v & uv/3w & 0 & 0 & 0 \\ vw/3u & -uw/3v & 0 & 0 & 0 & 0 \\ 0 & uw/3v & -uv/3w & 0 & 0 & 0 \\ 0 & 0 & 0 & c/b & 0 & 0 \\ 0 & 0 & 0 & 0 & c/a & b\gamma_1/a \\ 0 & 0 & 0 & 0 & 0 & b/a \end{bmatrix} \begin{Bmatrix} \mathcal{L}_{11} \\ \mathcal{L}_{22} \\ \mathcal{L}_{33} \\ \mathcal{L}_{23} \\ \mathcal{L}_{13} \\ \mathcal{L}_{12} \end{Bmatrix} \tag{1.18}$$

whereas the stress attributes are related to the components of $\boldsymbol{\mathcal{S}}$ via

$$\begin{Bmatrix} \pi \\ \sigma_1 \\ \sigma_2 \\ \tau_1 \\ \tau_2 \\ \tau_3 \end{Bmatrix} = \begin{bmatrix} u/vw & v/uw & w/uv & 0 & 0 & 0 \\ u/vw & -v/uw & 0 & 0 & 0 & 0 \\ 0 & v/uw & -w/uv & 0 & 0 & 0 \\ 0 & 0 & 0 & b/c & 0 & 0 \\ 0 & 0 & 0 & 0 & a/c & 0 \\ 0 & 0 & 0 & 0 & -a\gamma_1/c & a/b \end{bmatrix} \begin{Bmatrix} \mathcal{S}_{11} \\ \mathcal{S}_{22} \\ \mathcal{S}_{33} \\ \mathcal{S}_{23} \\ \mathcal{S}_{13} \\ \mathcal{S}_{12} \end{Bmatrix} \tag{1.19}$$

where u, v and w are anisotropy parameters representing strength of anisotropy along the directions $\tilde{\boldsymbol{e}}_1$, $\tilde{\boldsymbol{e}}_2$ and $\tilde{\boldsymbol{e}}_3$ over the other directions respectively. For an isotropic material, each of these parameters equals to one.

1.2.3 Elastic-plastic decomposition of Laplace stretch

Following the Kröner[49] – Lee[52] decomposition $\mathbf{F} = \mathbf{F}^e\mathbf{F}^p$, Freed *et al.* (2019) [36] proposed an extension of the upper-triangular decomposition to elasto-plasticity. In this work, first a $\mathbf{QR}$ decomposition of the deformation gradient is performed resulting in an orthogonal rotation tensor $\boldsymbol{\mathcal{R}}$ and the Laplace stretch $\boldsymbol{\mathcal{U}}$, and then this Laplace stretch is further decomposed into elastic and plastic parts, thus,

$$\mathbf{F} = \boldsymbol{\mathcal{R}}\boldsymbol{\mathcal{U}}^e\boldsymbol{\mathcal{U}}^p. \tag{1.20}$$

Both $\boldsymbol{\mathcal{U}}^e$ and $\boldsymbol{\mathcal{U}}^p$ are upper-triangular matrices. When written in matrices, the plastic part of Laplace stretch has components of

$$\boldsymbol{\mathcal{U}}^{pi}{}_J = \begin{bmatrix} a^p & a^p\gamma^p & a^p\beta^p \\ 0 & b^p & b^p\alpha^p \\ 0 & 0 & c^p \end{bmatrix} \tag{1.21}$$

where a^p, b^p, c^p are three inelastic elongation ratios and $\alpha^p, \beta^p, \gamma^p$ are three magnitudes of shear that ideally remain upon a removal of tractions.

Because the set of upper-triangular matrices with positive diagonal elements forms a group under multiplication, the elastic part of Laplace stretch also belongs to this group. In matrix form, the elastic part therefore has components of

$$\boldsymbol{\mathcal{U}}^{ei}{}_J = \begin{bmatrix} a^e & a^e\gamma^e & a^e\beta^e \\ 0 & b^e & b^e\alpha^e \\ 0 & 0 & c^e \end{bmatrix} \tag{1.22}$$

where a^e, b^e, c^e are three elastic elongation ratios and $\alpha^e, \beta^e, \gamma^e$ are three magnitudes of elastic shear.

The components of Laplace stretch and its elastic and plastic parts are related through

$$\begin{aligned} a &= a^e a^p \quad & \alpha &= c^p\alpha^e/b^p + \alpha^p \\ b &= b^e b^p \quad & \beta &= c^p\beta^e/a^p + b^p\gamma^e\alpha^p/a^p + \beta^p \\ c &= c^e c^p \quad & \gamma &= b^p\gamma^e/a^p + \gamma^p \end{aligned} \tag{1.23}$$

Similarly, components of $\boldsymbol{\mathcal{U}}^e$ and $\boldsymbol{\mathcal{U}}^p$ can be expressed in terms of their other corresponding counterparts. Upon unloading $\boldsymbol{\mathcal{U}} \to \boldsymbol{\mathcal{U}}^p$ as $\boldsymbol{\mathcal{U}}^e \to \mathbf{I}$. Thus, the knowledge of any two kinematic quantities is sufficient to determine the third.

Like the total Laplace stretch $\boldsymbol{\mathcal{U}}$, its inelastic part $\boldsymbol{\mathcal{U}}^p$ can also be measured from what would ideally be an homogeneous deformation in a configuration where all external tractions associated with $\boldsymbol{\mathcal{U}}$ have been removed, i.e., the body is subjected to an elastic unloading [¶]. It is a common notion that the elastic components of Kröner – Lee decomposition $\mathbf{F}^e$ for a single crystal can be measured from experiments using methods like high resolution – electron backscatter diffraction (HR-EBSD), a common technique to measure the changes in length of a crystal along the coordinate directions and the crystallographic angles (e.g., Jiang *et al.* (2016) [45]). With these measurements, the components of elastic deformation gradient $\mathbf{F}^e$ is determined. The components of the total deformation gradient $\mathbf{F}$ can be measured from techniques like digital image correlation (DIC) etc. Once these two quantities are measured, the inelastic component of $\mathbf{F}$ can be easily measured by employing $\mathbf{F}^p = \mathbf{F}^{e-1}\mathbf{F}$. However, such measurement suffers from a theoretical issue. By measuring changes in length along crystallographic directions and crystallographic angles in a single crystal, what one really measures is the displacement field and thereby, its gradient. The deformation gradient is eventually obtained by adding $\mathbf{I}$ to the measured displacement gradient. A similar technique is used to determine the total deformation gradient $\mathbf{F}$ from DIC experiments. In DIC measurement, this technique works because the total deformation is compatible, which enables one to define a global deformation map $\boldsymbol{x}(\boldsymbol{X}, t)$ between the undeformed configuration κ_r and the deformed configuration κ_t of the body. Hence, it is possible to define a displacement field by using the definition: $\boldsymbol{u}(\boldsymbol{X}, t) = \boldsymbol{x}(\boldsymbol{X}, t) - \boldsymbol{X}$. However, it is universally accepted that neither the elastic component $\mathbf{F}^e$ nor the inelastic component of deformation gradient $\mathbf{F}^p$ is compatible which implies that it is not possible to define a global deformation map between the undeformed configuration κ_r and the intermediate configuration κ_p. In this case, such a definition of displacement field becomes invalid. Therefore, the measurement of components of $\mathbf{F}^e$ (and thus, $\mathbf{F}^p$) is unsound from a theoretical point of view.

This theoretical problem is resolved whenever an elastic-plastic decomposition of the Laplace stretch is used owing to the physical meaning of the components of Laplace stretch. Note that one does not require to define a deformation map and thereby, a displacement field in order to provide a

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physical meaning of the components of Laplace stretch. The physical interpretation of the Laplace stretch and its components is valid irrespective of the compatibility of deformation. Therefore, *in an experimenter's frame of reference*, if one measures the changes in crystallographic lengths and angles, the measured quantities directly and unambiguously correspond to the components of elastic Laplace stretch $\boldsymbol{\mathcal{U}}^e$. The only caveat is: how can one obtain the crystallographic deformations in the experimenter's frame of reference? This can be done by performing Gram-Schmidt procedure on the total deformation gradient $\mathbf{F}$, measured from DIC experiments. Therefore, the elastic Laplace stretch $\boldsymbol{\mathcal{U}}^e$ can be measured, in principle, by the following steps:

1. Measure total deformation gradient $\mathbf{F}$ from DIC experiments.

2. Perform Gram-Schmidt procedure to find the rotation tensor $\boldsymbol{\mathcal{R}}$. The rotation tensor $\boldsymbol{\mathcal{R}}$ takes part in coordinate transformation.

3. Fix a coordinate system and perform HR-EBSD experiments to measure the changes in crystallographic lengths along that coordinate direction and crystallographic angles.

4. Transform the measured elastic changes in crystallographic lengths and angles in experimenter's frame of reference by applying $\boldsymbol{\mathcal{R}}$. The transformed elastic deformation should correspond to the components of $\boldsymbol{\mathcal{U}}^e$.

The measurement of $\boldsymbol{\mathcal{U}}^e$ is unambiguous up to an homogeneous rotation field $\boldsymbol{\mathcal{R}}$.

Comparing with the traditional Kröner–Lee decomposition, one can express Lee's elastic and plastic deformation gradients in terms of $\boldsymbol{\mathcal{U}}^e$ and $\boldsymbol{\mathcal{U}}^p$ plus the elastic and plastic components of the rotation tensor, viz., $\boldsymbol{\mathcal{R}}^e$ and $\boldsymbol{\mathcal{R}}^p$ where $\boldsymbol{\mathcal{R}} = \boldsymbol{\mathcal{R}}^p\boldsymbol{\mathcal{R}}^e$ and $\mathbf{F}^p = \boldsymbol{\mathcal{R}}^p\boldsymbol{\mathcal{U}}^p$. Lee's elastic deformation gradient $\mathbf{F}^e$ can then be expressed as

$$\mathbf{F}^e = \boldsymbol{\mathcal{R}}^p\boldsymbol{\mathcal{R}}^e\boldsymbol{\mathcal{U}}^e\boldsymbol{\mathcal{R}}^{pT} \tag{1.24}$$

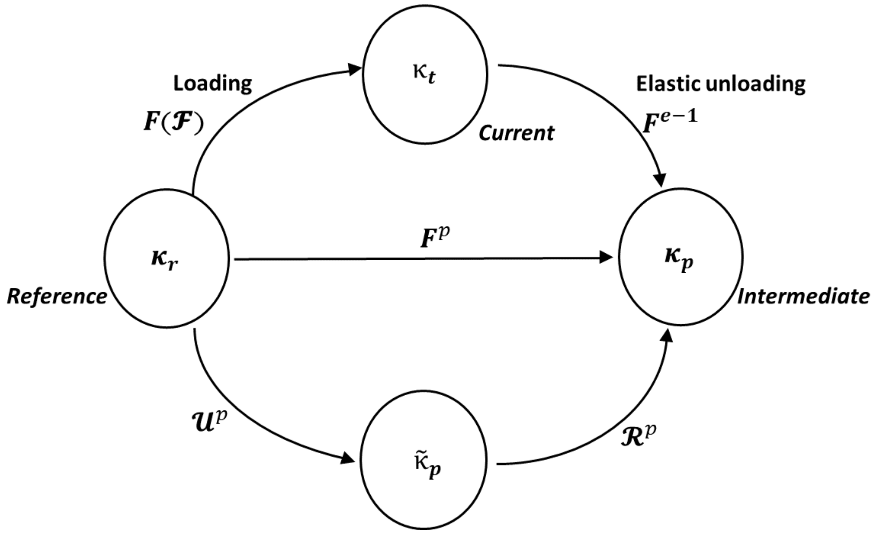

Figure 1.2: Configurations of the body associated with plastic deformation and the maps showing elastic-plastic loading and elastic unloading of the body.

and as such, the total deformation gradient can be expressed as

$$\mathbf{F} = \boldsymbol{\mathcal{R}}^p \boldsymbol{\mathcal{R}}^e \boldsymbol{\mathcal{U}}^e \boldsymbol{\mathcal{U}}^p \tag{1.25}$$

where $\boldsymbol{\mathcal{R}} = \boldsymbol{\mathcal{R}}^p \boldsymbol{\mathcal{R}}^e$ and $\boldsymbol{\mathcal{U}} = \boldsymbol{\mathcal{U}}^e \boldsymbol{\mathcal{U}}^p$.

It is important to understand the geometric significance of the elasti-plastic decomposition of Laplace stretch for the further development of this dissertation. Physically it is not possible for a body in an undeformed or reference configuration κ_r to undergo only plastic deformation and thereby reach the intermediate configuration κ_p.[5] However, if a body undergoes elasto-plastic deformation, i.e., goes from a reference configuration κ_r to the current configuration κ_t through $\mathbf{F}$ (or $\boldsymbol{\mathcal{F}}$), and then is subjected to an elastic unloading by applying $\mathbf{F}^{e-1}$, it is possible to measure a deformation of the body due to only plastic deformation. Hence, in this state of the body, closure failure of an arbitrary line integral provides the measure of lattice defects, i.e., dislocations in the sense of Burgers. This process is shown in Fig. 1.2.

[5]Although it is indeed possible for bodies made up of a rigid plastic material to undergo a plastic only deformation, such a constitutive relation is too restrictive.

Consider an infinitesimal fiber $\mathbf{d}\boldsymbol{X}$ in the reference configuration κ_r. The deformed fiber in a current configuration κ_t is denoted by $\mathbf{d}\boldsymbol{x}$ so that

$$\mathbf{d}\boldsymbol{x} = \mathbf{F}\,\mathbf{d}\boldsymbol{X} = \boldsymbol{\mathcal{R}}^p\boldsymbol{\mathcal{R}}^e\boldsymbol{\mathcal{U}}^e\boldsymbol{\mathcal{U}}^p\,\mathbf{d}\boldsymbol{X}. \tag{1.26}$$

An elastic unloading of the fiber takes it from κ_t to an intermediate configuration κ_p. In this configuration, the deformation of the body is solely due to movement of dislocations. Here $\mathbf{d}\boldsymbol{x}^{\boldsymbol{p}}$ denotes an infinitesimal fiber of the body subjected to an elastic unloading, i.e.,

$$\mathbf{d}\boldsymbol{x}^p = \mathbf{F}^{e-1}\,\mathbf{d}\boldsymbol{x} \tag{1.27}$$

where $\mathbf{F}^e$ denotes Lee's elastic deformation gradient. $\mathbf{F}^e$ is related to $\boldsymbol{\mathcal{U}}^e$ and a rotation tensor through Eqn. (1.24). Using this relation, one can easily arrive at

$$\mathbf{d}\boldsymbol{x}^p = \boldsymbol{\mathcal{R}}^p\boldsymbol{\mathcal{U}}^p\,\mathbf{d}\boldsymbol{X}. \tag{1.28}$$

At this point, it is important to understand the role of rotation tensor $\boldsymbol{\mathcal{R}}$. The inverse to this rotation tensor, i.e., $\boldsymbol{\mathcal{R}}^T$, rotates an Eulerian triad into the experimenter's frame of reference, and hence plays an important role in coordinate transformation. If $\boldsymbol{e}_i$ and $\tilde{\boldsymbol{e}}_I$ denote Cartesian bases for the Eulerian and experimenter's frames of reference, respectively, then $\boldsymbol{e}_i = \boldsymbol{\mathcal{R}}\tilde{\boldsymbol{e}}_I$ [34]. In view of the physical meaning of the components of Laplace stretch, it is clearly understood that deformation of a body in all six degrees of freedom is completely described by the six components of $\boldsymbol{\mathcal{U}}$, as shown in §1.2.1. However, the components of $\boldsymbol{\mathcal{U}}$ are not all independent, and their dependence has an important consequence as will be discussed later.

Therefore, plastic deformation of the body is completely described by the inelastic part of Laplace stretch $\boldsymbol{\mathcal{U}}^p$ in an experimenter's frame of reference, per Eqn. (1.21). Let the configuration of a body, subjected only to $\boldsymbol{\mathcal{U}}^p$, be denoted by $\tilde{\kappa}_p$ with $\mathbf{d}\tilde{\boldsymbol{x}}^p$ denoting an infinitesimal fiber of the body in this configuration so that

$$\mathrm{d}\tilde{\boldsymbol{x}}^p = \boldsymbol{\mathcal{U}}^p \,\mathrm{d}\boldsymbol{X} = \boldsymbol{\mathcal{R}}^{pT} \,\mathrm{d}\boldsymbol{x}^p. \tag{1.29}$$

This configuration of the body is particularly important because it is in this configuration where the deformation of the body is purely due to the plastic component of Laplace stretch $\boldsymbol{\mathcal{U}}^p$. Due to the “deformation gradient-like" nature of the Laplace stretch, the plastic deformation caused by a movement of dislocations is *fully* characterized in this configuration.

It is worth noting that because the matrix of $\boldsymbol{\mathcal{U}}^p$ is also upper-triangular, a decomposition similar to Eqns. (1.8 and 1.9) can be performed on $\boldsymbol{\mathcal{U}}^p$ with a superscript 'p' denoting the plastic part. Therefore, the matrix of $\boldsymbol{\mathcal{U}}^p$ can be decomposed as

$$\mathcal{U}^{pi}{}_J = \underbrace{\begin{bmatrix} a^p & 0 & 0 \\ 0 & b^p & 0 \\ 0 & 0 & c^p \end{bmatrix}}_{\Lambda^p} \underbrace{\begin{bmatrix} 1 & 0 & \beta^p \\ 0 & 1 & \alpha^p \\ 0 & 0 & 1 \end{bmatrix}}_{\mathcal{U}^{\alpha^p\beta^p}} \underbrace{\begin{bmatrix} 1 & \gamma^p & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 1 \end{bmatrix}}_{\mathcal{U}^{\gamma^p}} \tag{1.30}$$

with

$$\begin{aligned} \Lambda^{pi}{}_J = & \underbrace{\sqrt[3]{a^p b^p c^p} \begin{bmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 1 \end{bmatrix}}_{\text{dilatation}} \times \underbrace{\begin{bmatrix} \sqrt[3]{a^p/b^p} & 0 & 0 \\ 0 & \sqrt[3]{b^p/a^p} & 0 \\ 0 & 0 & 1 \end{bmatrix}}_{\text{1-2 planar squeeze}} \\ & \times \underbrace{\begin{bmatrix} 1 & 0 & 0 \\ 0 & \sqrt[3]{b^p/c^p} & 0 \\ 0 & 0 & \sqrt[3]{c^p/b^p} \end{bmatrix}}_{\text{2-3 planar squeeze}} \times \underbrace{\begin{bmatrix} \sqrt[3]{a^p/c^p} & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & \sqrt[3]{c^p/a^p} \end{bmatrix}}_{\text{3-1 planar squeeze}}. \end{aligned} \tag{1.31}$$

To describe the kinetics, first two sets of kinematic variables and their rates, similar to the ones described in § 1.2.2 can be defined for the elastic and plastic components of Laplace stretch. These lists of variables are given as

$$l_{\mathcal{U}^p} := \{\delta^p \quad \varepsilon_1^p \quad \varepsilon_2^p \quad \varepsilon_3^p \quad \gamma_1^p \quad \gamma_2^p \quad \gamma_3^p\} \tag{1.32}$$

$$l_{\mathcal{U}^e} := \{\delta^e \quad \varepsilon_1^e \quad \varepsilon_2^e \quad \varepsilon_3^e \quad \gamma_1^e \quad \gamma_2^e \quad \gamma_3^e\} \tag{1.33}$$

and

$$l_{\dot{\mathcal{U}}^p} := \{\dot{\delta}^p \quad \dot{\varepsilon}_1^p \quad \dot{\varepsilon}_2^p \quad \dot{\varepsilon}_3^p \quad \dot{\gamma}_1^p \quad \dot{\gamma}_2^p \quad \dot{\gamma}_3^p\} \tag{1.34}$$

$$l_{\dot{\mathcal{U}}^e} := \{\dot{\delta}^e \quad \dot{\varepsilon}_1^e \quad \dot{\varepsilon}_2^e \quad \dot{\varepsilon}_3^e \quad \dot{\gamma}_1^e \quad \dot{\gamma}_2^e \quad \dot{\gamma}_3^e\} \tag{1.35}$$

$$\tag{1.36}$$

where the elastic strain attributes are defined as

$$\begin{gathered}\delta^e = \tfrac{1}{3}\ln(a^e b^e c^e), \quad \varepsilon_1^e = \tfrac{1}{3}\ln(a^e/b^e), \quad \varepsilon_2^e = \tfrac{1}{3}\ln(b^e/c^e), \quad \varepsilon_3^e = \tfrac{1}{3}\ln(c^e/a^e), \\ \gamma_1^e = \alpha^e, \quad \gamma_2^e = \beta^e, \quad \gamma_3^e = \gamma^e\end{gathered} \tag{1.37}$$

and their plastic counterparts are given as

$$\begin{gathered}\delta^p = \tfrac{1}{3}\ln(a^p b^p c^p), \quad \varepsilon_1^p = \tfrac{1}{3}\ln(a^p/b^p), \quad \varepsilon_2^p = \tfrac{1}{3}\ln(b^p/c^p), \quad \varepsilon_3^p = \tfrac{1}{3}\ln(c^p/a^p), \\ \gamma_1^p = \alpha^p, \quad \gamma_2^p = \beta^p, \quad \gamma_3^p = \gamma^p.\end{gathered} \tag{1.38}$$

Using relationships between components of the total Laplace stretch and those of their elastic and plastic counterparts, given in Eqn. (1.23), one can establish a relationship between the total strain attributes and their elastic and plastic components; specifically,

$$\begin{aligned}
\delta &= \delta^e + \delta^p, \\
\varepsilon_i &= \varepsilon_i^e + \varepsilon_i^p \ (i = 1, 2, 3), \\
\gamma_1 &= \exp(-3\varepsilon_1^p)\, \gamma_1^e + \gamma_1^p, \\
\gamma_2 &= \exp(3\varepsilon_3^p)\, \gamma_2^e + \gamma_2^p + \gamma_1^p\, (\gamma_3 - \gamma_3^p), \\
\gamma_3 &= \exp(-3\varepsilon_1^p)\, \gamma_3^e + \gamma_3^p.
\end{aligned} \tag{1.39}$$

Traditionally, an additive decomposition of the total strain into its elastic and plastic components is more commonly used in a small displacement-gradient theory; whereas, a multiplicative decomposition of a kinematic quantity, such as a deformation gradient, is typically used in a finite deformation setting.[6] Here, interestingly, an additive decomposition of the total strain results in as a direct consequence of the multiplicative elastic-plastic decomposition of the Laplace stretch, without any assumption of a small displacement gradient. This key feature of **QR** kinematics is extremely useful when constructing constitutive models for elastic-plastic materials due to its similarity with small strain theory. Such an additive elastic-plastic decomposition of total strain was also achieved by Miehe (1998) [65] for a finite deformation theory through the assumption of a plastic metric. Note that although the additive decompositions of the dilatational strain δ and the squeeze strains ε_i are rather straightforward, such is not the case for the shear strains γ_i. Specifically, the elastic components of the shear strains appear as a product with a function of the squeeze strains. Although this fact does not pose much of a problem in our subsequent derivations, one must be vigilant whenever one is dealing with the shear terms.

If $\boldsymbol{\mathcal{L}}^p$ denotes a plastic velocity gradient, defined as $\boldsymbol{\mathcal{L}}^p := \dot{\boldsymbol{\mathcal{U}}}^p\, \boldsymbol{\mathcal{U}}^{p-1}$, then it is possible to establish a bijective map between the elements of the matrix of $\boldsymbol{\mathcal{L}}^p$ and the list of variables $l_{\dot{\mathcal{U}}^p}$.

[6] Although an additive elastic-plastic decomposition of the rate of deformation tensor is quite commonly used in finite deformation theory, e.g., Nemat-Nasser (1982) [69].

Such a map is not, in general, unique. For an isotropic material, this map can be written as

$$\begin{pmatrix} \dot{\delta}^p \\ \dot{\varepsilon}_1^p \\ \dot{\varepsilon}_2^p \\ \dot{\gamma}_1^p \\ \dot{\gamma}_2^p \\ \dot{\gamma}_3^p \end{pmatrix} = \begin{bmatrix} 1/3 & 1/3 & 1/3 & 0 & 0 & 0 \\ 1/3 & -1/3 & 0 & 0 & 0 & 0 \\ 0 & 1/3 & -1/3 & 0 & 0 & 0 \\ 0 & 0 & 0 & c^p/b^p & 0 & 0 \\ 0 & 0 & 0 & 0 & c^p/a^p & b^p\alpha^p/a^p \\ 0 & 0 & 0 & 0 & 0 & b^p/a^p \end{bmatrix} \begin{pmatrix} \mathcal{L}_{11}^p \\ \mathcal{L}_{22}^p \\ \mathcal{L}_{33}^p \\ \mathcal{L}_{23}^p \\ \mathcal{L}_{13}^p \\ \mathcal{L}_{12}^p \end{pmatrix}. \tag{1.40}$$

Therefore, one can potentially replace $\boldsymbol{\mathcal{L}}^p$ by the list of plastic conjugate strain rates $l_{\dot{\mathcal{U}}^p}$. Similar to Eqn. (1.18), for an anisotropic material, the plastic strain rate attributes are related to the components of the plastic velocity gradient through

$$\begin{Bmatrix} \dot{\delta}^p \\ \dot{\varepsilon}_1^p \\ \dot{\varepsilon}_2^p \\ \dot{\gamma}_1^p \\ \dot{\gamma}_2^p \\ \dot{\gamma}_3^p \end{Bmatrix} = \begin{bmatrix} vw/3u & uw/3v & uv/3w & 0 & 0 & 0 \\ vw/3u & -uw/3v & 0 & 0 & 0 & 0 \\ 0 & uw/3v & -uv/3w & 0 & 0 & 0 \\ 0 & 0 & 0 & c^p/b^p & 0 & 0 \\ 0 & 0 & 0 & 0 & c^p/a^p & b^p\gamma_1^p/a^p \\ 0 & 0 & 0 & 0 & 0 & b^p/a^p \end{bmatrix} \begin{Bmatrix} \mathcal{L}_{11}^p \\ \mathcal{L}_{22}^p \\ \mathcal{L}_{33}^p \\ \mathcal{L}_{23}^p \\ \mathcal{L}_{13}^p \\ \mathcal{L}_{12}^p \end{Bmatrix}. \tag{1.41}$$

For convenience, we define another list of variables $l_{\dot{\mathcal{U}}^p}$ containing the plastic strain rate attributes as

$$l_{\dot{\mathcal{U}}^p} := \{\ \dot{\delta}^p \quad \dot{\varepsilon}_1^p \quad \dot{\varepsilon}_2^p \quad \dot{\varepsilon}_3^p \quad \dot{\gamma}_1^p \quad \dot{\gamma}_2^p \quad \dot{\gamma}_3^p\ \}. \tag{1.42}$$

1.3 Motivation and scope of the current work

Based on this interesting development on **QR** framework, the main objective of this dissertation is to explore some persisting problems in elasticity and inelasticity using this framework.

In the Gram-Schmidt process, a set of orthonormal base vectors $\tilde{\boldsymbol{e}}_i$, $i = 1, 2, 3$, arise from a rectangular triad of reference base vectors $\boldsymbol{E}_i$ by applying Laplace's technique of successive orthogonal projections. To obtain $\tilde{e}_i$ in three-dimensional space, one needs to select its 1 coordinate direction and its 12 coordinate plane prior to determining its other coordinate directions, because the 1 coordinate direction and 12 coordinate plane remain invariant under transformations of Laplace stretch [64]. The question to be addressed is: How does one index an observer's basis so that the 1 coordinate direction and the 12 coordinate plane are prescribed in a meaningful way? For example, do the $\tilde{e}_i$ arise from an $\boldsymbol{E}_i$ obtained from a mapping of $(\boldsymbol{E}_1, \boldsymbol{E}_2, \boldsymbol{E}_3) \mapsto (\boldsymbol{\mathcal{E}}_1, \boldsymbol{\mathcal{E}}_2, \boldsymbol{\mathcal{E}}_3)$, or do they arise from an $\boldsymbol{\mathcal{E}}_i$ obtained from a mapping of $(\boldsymbol{E}_1, \boldsymbol{E}_3, \boldsymbol{E}_2) \mapsto (\boldsymbol{\mathcal{E}}_1, \boldsymbol{\mathcal{E}}_2, \boldsymbol{\mathcal{E}}_3)$, or do they arise from one of the four other possible mappings? Only mapping $(\boldsymbol{E}_1, \boldsymbol{E}_2, \boldsymbol{E}_3) \mapsto (\boldsymbol{\mathcal{E}}_1, \boldsymbol{\mathcal{E}}_2, \boldsymbol{\mathcal{E}}_3)$ has been used to date. Considering all six potential re-labelings of an observer's coordinate axes, we develop a strategy to obtain a unique, consistent description for Laplace stretch.

With the issue of arbitrariness of the Laplace stretch resolved, we explore the compatibility condition for **QR** kinematics whenever a right Cauchy-Green tensor $\mathbf{C}$ is prescribed. This problem has been previously attempted by Lembo (2017) [53] where he adopted a procedure similar to that of Shield's (1973) [83] and employed it to a **QR** decomposition of $\mathbf{F}$, viz., $\mathbf{F} = \boldsymbol{\mathcal{R}}\boldsymbol{\mathcal{U}}$ in our notation. He considered the rotation tensor to be the primary variable [12, 54], and then determined a partial differential equation that solves for the rotation tensor $\boldsymbol{\mathcal{R}}$. He showed that the integrability condition for this partial differential equation is equivalent to a vanishing of the Riemann curvature tensor. Finally, a compatibility condition for Laplace stretch was obtained from the integrability of its *deformation gradient*. However, *uniqueness* of the deformation gradient obtained from the relation $\mathbf{C} = \mathbf{F}^T\mathbf{F}$ is questionable [8]. Therefore, we choose the Cauchy-Green tensor $\mathbf{C}$ to be the fundamental kinematic variable [5, 16] to derive a compatibility condition without any conflict on the issue of non-uniqueness of $\mathbf{F}$. The compatibility conditions derived herein restrict a dependence of components for $\boldsymbol{\mathcal{U}}$ on the spatial variables.

The compatibility of a deformation manifests that the deformed configuration of the body is a Euclidean space. In fact, one can assign a global deformation map between points in the undeformed and deformed configurations only when the deformation is compatible. The elastic-plastic decomposition of the Laplace stretch introduces an intermediate, relaxed configuration $\tilde{\kappa}_p$ in addition to an undeformed (reference) configuration $\kappa_r(\mathcal{B})$ and a deformed (current) configuration $\kappa_t(\mathcal{B})$. In an experimenter's frame of reference, the plastic component of Laplace stretch $\boldsymbol{\mathcal{U}}^p$ maps tangent vectors at a material point in $\kappa_r(\mathcal{B})$ to that at its corresponding point in an intermediate configuration, whereas its elastic component $\boldsymbol{\mathcal{U}}^e$ maps tangent vectors at a material point in $\tilde{\kappa}_p(\mathcal{B})$ to vectors in the tangent space of the current configuration $\tilde{\kappa}_t(\mathcal{B})$. It is to note that the intermediate, relaxed configuration $\tilde{\kappa}_p(\mathcal{B})$ is not a Euclidean space. This feature of $\tilde{\kappa}_p$ is attributed to the dislocations that cause plastic flow [71, 7, 11, 24, 1, 15, 42]. Therefore, we explore the geometric features of the space $\tilde{\kappa}_p$ next and characterize the geometrically necessary dislocations exploiting the incompatibility of this space.

Although we are now able to characterize microscopic defects such as dislocations using an elastic-plastic decomposition of Laplace stretch, the question of under what loading condition this decomposition is done and an evolution equation of elastic and plastic Laplace stretch are still not resolved. Therefore, our next objective is to develop a constitutive model for elastic-plastic materials based on these kinematics. A constitutive model for elastic-plastic materials is developed using scalar, conjugate, stress/strain, base pairs in a finite deformation setting. A maximum rate of dissipation criterion has been used in deriving our constitutive equations, as this criterion is valid for a wider class of materials. Two constitutive assumptions—one for a Helmholtz potential, and one for the rate of dissipation function—are required for our constitutive construction. This model does not presuppose the existence of a yield surface. In fact, it is shown that whether a material exhibits a yielding or a creep-like behavior depends upon the differentiability of the rate of dissipation function.

Another important problem in plasticity that remains to be explored in the context of this framework is the concept of plastic spin and its incorporation in constitutive modeling. We show that the intermediate configuration $\tilde{\kappa}_p$ acts as a material substructure. When incorporating internal variables that represent a macroscopic manifestation of the microstructural properties, one must define an appropriate rate of these variables that co-rotates with this material substructure. Thus, the plastic spin implicitly enters into the constitutive model through a proper definition of the co-rotational rate of internal variables. Traditionally, a plastically-induced anisotropy is introduced in the constitutive model as one of the internal variables. However, in our framework, material anisotropy enters into the model thorugh encoding/decoding maps between the stress/strain attributes and the components of Kirchhoff stress and velocity gradient, respectively. Therefore, in this case, a plastically-induced anisotropy is incorporated by considering the anisotropy parameters as variables evolving with the plastic deformation process.

The rest of the dissertation is organized as follows. In chapter 2, the issue with non-uniqueness of coordinate frame choices for upper-triangular decomposition is outlined and a strategy to resolve this issue is developed. In chapter 3, a detailed derivation of the compatibility condition for $\boldsymbol{\mathcal{U}}$ is provided for a prescribed right Cauchy-Green tensor $\mathbf{C}$. This condition is comprised of five equations that arise because of specified couplings between three orthogonal shears with two orthogonal elongations. These couplings are not arbitrary; they are very specific and a consequence of Gram-Schmidt factorization. In chapter 4, a measure of incompatibility for the intermediate configuration $\tilde{\kappa}_p$ is attained and the Burgers vector and geometric dislocation tensor are derived. Derivation of a dislocation density involves the traditional argument of closure failure of a Burgers circuit [13] in an appropriate configuration ($\tilde{\kappa}_p$). In chapter 5, a constitutive model for elastic-plastic materials based on the **QR** kinematics has been developed. The concept of plastic spin and its role in constitutive modeling have been discussed in chapter 6. Finally, the proposal is summarized and drawn to conclusion with a list of possible future works.

2. COORDINATE INDEXING FOR AN UNAMBIGUOUS REPRESENTATION OF LAPLACE STRETCH *

The most suitable method to obtain a Laplace stretch from a prescribed deformation gradient is a Gram-Schmidt procedure in which a new set of base vectors are obtained through Laplace's successive orthogonal projections. This new set of vectors are related to the columns of the matrix of the deformation gradient through Eqn. (1.2). However, this procedure requires specification of a particular coordinate direction (1 coordinate direction) and a particular coordinate plane (12 coordinate plane) containing this coordinate direction. Tacit in Eqn. (1.2) is the assumption that the Lagrangian base vector $\boldsymbol{E}_1$ is chosen as the 1 coordinate direction and $\boldsymbol{E}_1 \times \boldsymbol{E}_2$ is chosen as the 12 coordinate plane. However, this need not be the case always. Although one can readily compute the base vectors $\{\tilde{e}_i\}$ and the components of Laplace stretch whenever a 1 coordinate direction and a 12 coordinate plane are prescribed, these two features of the coordinate system are not, in general, known *a priori* to us. For an experimenter, a coordinate triad $(\boldsymbol{E}_1, \boldsymbol{E}_2, \boldsymbol{E}_3)$ is typically specified to align with their laboratory apparatus. The experimenter is free to index this triad to their advantage, using any of six potential indexing patterns, e.g., $(\boldsymbol{E}_2, \boldsymbol{E}_3, \boldsymbol{E}_1) \mapsto (\boldsymbol{\mathcal{E}}_1, \boldsymbol{\mathcal{E}}_2, \boldsymbol{\mathcal{E}}_3)$ wherein $(\boldsymbol{\mathcal{E}}_1, \boldsymbol{\mathcal{E}}_2, \boldsymbol{\mathcal{E}}_3)$ is a re-indexed Lagrangian basis $(\boldsymbol{E}_1, \boldsymbol{E}_2, \boldsymbol{E}_3)$. The quandary is that the components of Laplace stretch obtained in these six coordinate systems will likely be quite different, especially when shears are involved.

Because the components of Laplace stretch have physical meanings, any variation in these components due to a change in coordinate indexing would be non-physical. Thus, any constitutive model[32, 33, 35] that uses Laplace stretch as a kinematic variable will be invalid. Therefore, in this chapter, we address this issue of coordinate indexing and put forward a strategy to resolve it.

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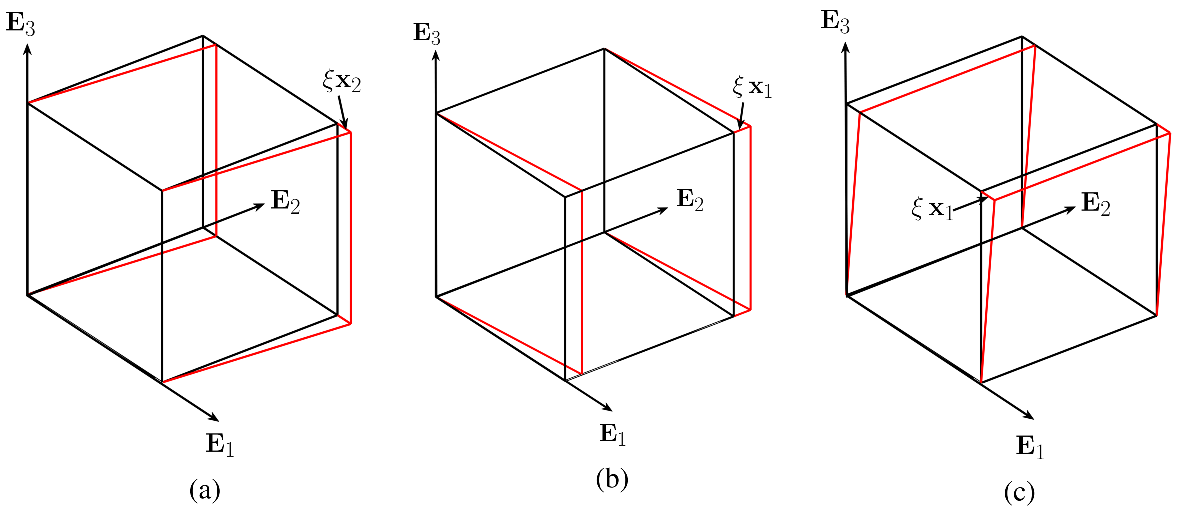

Figure 2.1: Deformations of a unit cube subjected to shears of like magnitude, but acting in three different directions. In all three cases, the magnitude of shear ξ is the same, whereas the extent of shear depends upon the elongations along other directions. (a) This cube is subjected to a shear of ξx_2 within the 12 plane; (b) This cube is subjected to a shear of ξx_1 within the 12 plane; and (c) This cube is subjected to a shear of ξx_3 within the 13 plane.

2.1 Ambiguity regarding choice of coordinate system

To demonstrate this problem, let us consider a unit cube subjected to simple shears of like magnitude ξ, but acting in three different directions, as shown in Fig. 2.1. Let us select a Lagrangian basis $\{\boldsymbol{E}_i\}$ placed at a corner of the cube with its three coordinate directions running along the edges of this cube. The three cases shown in Fig. 2.1 represent three shears applied in three different directions. The deformation gradients in these three cases are

$$F_{ij(a)} = \begin{bmatrix} 1 & \xi & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 1 \end{bmatrix}, \quad F_{ij(b)} = \begin{bmatrix} 1 & 0 & 0 \\ \xi & 1 & 0 \\ 0 & 0 & 1 \end{bmatrix}, \quad F_{ij(c)} = \begin{bmatrix} 1 & 0 & \xi \\ 0 & 1 & 0 \\ 0 & 0 & 1 \end{bmatrix} \tag{2.1}$$

respectively.

In all three cases, we consider the 1 coordinate direction in our physical frame of reference to lie along the $\boldsymbol{E}_1$ direction, and the 12 coordinate plane to be that plane containing line directions $\boldsymbol{E}_1$ and $\boldsymbol{E}_2$ in the reference state. From these two choices, one can fix the other two coordinate directions of our physical frame of reference by using Eqn. (1.2). Next, we compute the components of Laplace stretch for these three deformations by using Eqn. (1.5).

a) Whenever the unit cube is subjected to a shear ξ along the $\boldsymbol{E}_1$ direction and within the $\boldsymbol{E}_1 \times \boldsymbol{E}_2$ plane, i.e., the plane whose normal aligns with direction $\boldsymbol{E}_3$ in the undeformed configuration shown in Fig. 2.1^a, the deformation gradient becomes upper triangular, and thus, the Laplace stretch is the same as the deformation gradient. Components of the Laplace stretch are therefore given as

$$\mathcal{U}_{ij(a)} = \begin{bmatrix} 1 & \xi & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 1 \end{bmatrix}. \tag{2.2a}$$

b) In case (b), where the unit cube is subjected to a shear ξ along the $\boldsymbol{E}_2$ direction and within the $\boldsymbol{E}_1 \times \boldsymbol{E}_2$ plane, the deformation gradient becomes lower triangular in construction, as shown in Eqn. (2.1)^b. Thus, the components of Laplace stretch take on the form of

$$\mathcal{U}_{ij(b)} = \begin{bmatrix} \sqrt{1+\xi^2} & \xi & 0 \\ 0 & 1/\sqrt{1+\xi^2} & 0 \\ 0 & 0 & 1 \end{bmatrix}. \tag{2.2b}$$

c) Whenever the cube is subjected to a shear of ξ, as shown in Fig. 2.1^c, the deformation gradient again becomes upper triangular. In this case, the components of Laplace stretch are written as

$$\mathcal{U}_{ij(c)} = \begin{bmatrix} 1 & 0 & \xi \\ 0 & 1 & 0 \\ 0 & 0 & 1 \end{bmatrix}. \tag{2.2c}$$

It is worth noting that physically, cases (a), (b) and (c) represent the same deformation, but along different directions and across different planes. However, the Laplace stretches found for these three cases are starkly different. Particularly, Eqn. (2.2b) shows that there is an elongation and a contraction along the $\tilde{\boldsymbol{e}}_1$ and $\tilde{\boldsymbol{e}}_2$ directions, respectively, which is physically inconsistent with the other two cases. Moreover, even though Eqns. (2.2a) and (2.2c) show that the Laplace stretch for cases (a) and (c) are consistent in representing the given deformation, the stretch components $\mathcal{U}_{ij(b)}$ and $\mathcal{U}_{ij(c)}$ are different. The Laplace stretches arising in all three cases, however, ought to be the same, because they represent the same physical deformation. This inconsistency is ascribed to a non-uniqueness associated with the choice of selecting a 1 coordinate direction and a 12 coordinate plane used to construct the basis for this physical frame of reference through successive orthogonal projections. For example, in case (c), if the 13 plane of the cube containing $\boldsymbol{E}_1$ and $\boldsymbol{E}_3$ were chosen to be the 12 coordinate plane for the physical frame of reference, then $\mathcal{U}_{ij(a)}$ and $\mathcal{U}_{ij(c)}$ would have been exactly the same.

This non-uniqueness allows two observers using different coordinate systems to observe different deformations, and hence, any constitutive model based upon such a Laplace stretch would be faulty. This issue of non-uniqueness, and its subsequent inconsistency associated with the physical meanings belonging to the components of Laplace stretch, motivated us to develop a systematic means for selecting the 1 coordinate direction and the 12 coordinate plane, which are invariant under transformations of the Laplace stretch [64]. The result is the unique selection of a basis $\{\boldsymbol{\mathcal{E}}_i\}$ that generates a unique representation for Laplace stretch, irrespective of the deformation, i.e., the scheme produces a representation for the Laplace stretch that remains invariant with different assignments for the set of base vectors $\{\boldsymbol{E}_i\}$.

2.2 Remedy

The main feature of a physical coordinate system with corresponding base vectors $\{\tilde{e}_i\}$ that comprise the columns of rotation $\boldsymbol{\mathcal{R}} = \left[\, \tilde{e}_1 \,\middle|\, \tilde{e}_2 \,\middle|\, \tilde{e}_3 \,\right]$ associated with a Laplace stretch $\boldsymbol{\mathcal{U}}$ is: the 1 coordinate direction and the 12 coordinate plane remain invariant under transformations of Laplace stretch over a deformation history [64]. Our conjecture is: *Select a base vector $\boldsymbol{E}_i \mapsto \boldsymbol{\mathcal{E}}_1$ from the set of Lagrangian base vectors $(\boldsymbol{E}_1, \boldsymbol{E}_2, \boldsymbol{E}_3)$ whose edge of a representative cube along the selected direction experiences minimal transverse shear. Then select a base vector $\boldsymbol{E}_j \mapsto \boldsymbol{\mathcal{E}}_2$, $j \neq i$, from those Lagrangian base vectors $(\boldsymbol{E}_1, \boldsymbol{E}_2, \boldsymbol{E}_3)$ whose 12 coordinate plane containing*

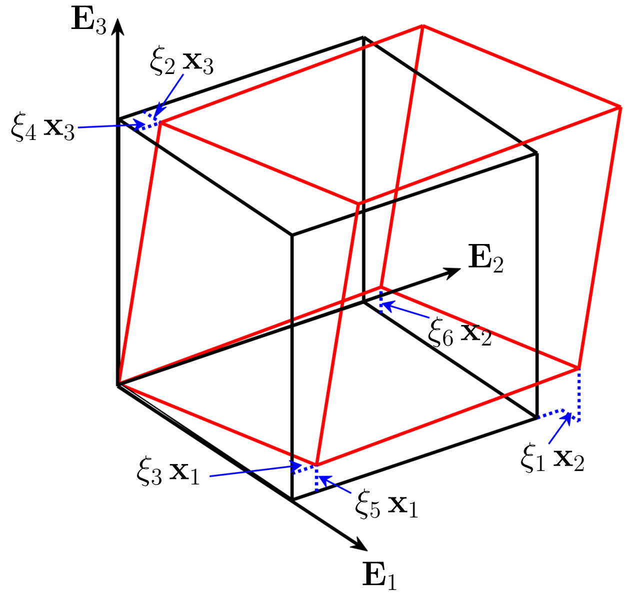

Figure 2.2: The deformed shape of a unit cube subjected to an arbitrary deformation. Variables x_1, x_2, x_3 represent elongations along the sides of the cube, whereas variables $\xi_m, m = 1, ..., 6$ represent the magnitudes of shear.

$\boldsymbol{\mathcal{E}}_1$ and $\boldsymbol{\mathcal{E}}_2$ experiences minimal in-plane shear, with $\boldsymbol{\mathcal{E}}_3$ taking on the remaining Lagrangian base vector $\boldsymbol{E}_k$, $k \neq i, j$. With base vectors $(\boldsymbol{\mathcal{E}}_1, \boldsymbol{\mathcal{E}}_2, \boldsymbol{\mathcal{E}}_3)$ now in hand, re-indexed from the Lagrangian bases $(\boldsymbol{E}_1, \boldsymbol{E}_2, \boldsymbol{E}_3)$, one can determine components for the deformation gradient $\mathcal{F}_{ij}$ evaluated in this re-indexed basis $\{\boldsymbol{\mathcal{E}}_i\}$ because $\mathbf{F} = F_{ij}\, \boldsymbol{E}_i \otimes \boldsymbol{E}_j = \mathcal{F}_{ij}\, \boldsymbol{\mathcal{E}}_i \otimes \boldsymbol{\mathcal{E}}_j$. Out of here a Gram-Schmidt decomposition can then be constructed, viz., $\mathcal{F}_{ij} = \mathcal{R}_{ik}\mathcal{U}_{kj}$, where $\mathcal{R}_{ij}$ and $\mathcal{U}_{ij}$ no longer depend on an observer's choice for a coordinate system $(\boldsymbol{E}_1, \boldsymbol{E}_2, \boldsymbol{E}_3)$, but upon the systematic re-indexed coordinate frame $(\boldsymbol{\mathcal{E}}_1, \boldsymbol{\mathcal{E}}_2, \boldsymbol{\mathcal{E}}_3)$. It is worth noting that we have not changed orientation of the Lagrangian triad, we are only changing how its base vectors are to be indexed. This conjecture solves our dilemma of non-uniqueness.

To demonstrate this procedure for acquiring a unique coordinate system $\{\tilde{e}_i\}$, consider a unit cube subjected to an arbitrary general deformation, as shown in Fig. 2.2. A Lagrangian triad $\{\boldsymbol{E}_i\}$ is placed at one corner of the cube whose coordinate directions are along the sides of this undeformed cube. Variables x_1, x_2, x_3 represent elongations that are projections of the deformed parallelepiped unto the coordinate base vectors $\{\boldsymbol{E}_i\}$ aligned with the cube's edges, whereas variables $\xi_m, m = 1, \ldots, 6$, represent six shear components associated with this deformation. Thus, the deformation gradient considered is given by

$$F_{ij} = \begin{bmatrix} F_{11} & F_{12} & F_{13} \\ F_{21} & F_{22} & F_{23} \\ F_{31} & F_{32} & F_{33} \end{bmatrix} = \begin{bmatrix} x_1 & \xi_1 x_2 & \xi_2 x_3 \\ \xi_3 x_1 & x_2 & \xi_4 x_3 \\ \xi_5 x_1 & \xi_6 x_2 & x_3 \end{bmatrix} \tag{2.3}$$

where in terms of the components of the deformation gradient $\mathbf{F}$, the magnitudes of shear ξ_m's can be written as

$$\begin{aligned} \xi_1 &= F_{12}/F_{22}, \quad \xi_2 = F_{13}/F_{33}, \quad \xi_3 = F_{21}/F_{11}, \\ \xi_4 &= F_{23}/F_{33}, \quad \xi_5 = F_{31}/F_{11}, \quad \xi_6 = F_{32}/F_{22}. \end{aligned} \tag{2.4}$$

all of which are evaluated in the user's Lagrangian basis $\{\boldsymbol{E}_i\}$.

2.2.1 Choosing the 1 coordinate direction in our physical frame of reference

From Fig. 2.2, it is evident that the side of the cube that was along the $\boldsymbol{E}_1$ direction in its undeformed configuration is subjected to two possible shear components, viz., F_{21} and F_{31}, and an elongation component F_{11}. Therefore, the 1 coordinate direction is subjected to a transverse shear in an amount of

$$\mathcal{G}_1 = \frac{\sqrt{F_{21}^2 + F_{31}^2}}{F_{11}} \tag{2.5a}$$

while, similarly, the 2 and 3 coordinate directions are subjected to transverse shears of

$$\mathcal{G}_2 = \frac{\sqrt{F_{12}^2 + F_{32}^2}}{F_{22}} \tag{2.5b}$$

and

$$\mathcal{G}_3 = \frac{\sqrt{F_{13}^2 + F_{23}^2}}{F_{33}} \tag{2.5c}$$

respectively. Therefore, among the transverse shears $\mathcal{G}_1$, $\mathcal{G}_2$ and $\mathcal{G}_3$, if $\mathcal{G}_i$ is the minimum, then $\boldsymbol{E}_i \mapsto \boldsymbol{\mathcal{E}}_1$ is to be selected as the 1 coordinate direction in our re-indexed frame of reference.

2.2.2 Choosing the 12 coordinate plane in our physical frame of reference

Once the 1 coordinate direction is determined, there are two potential planes that one can select to be the 12 coordinate plane. Among the six distorted planes of the parallelepiped, it is reasonable to consider only the three planes that contain the origin. This is due to the fact that information regarding the deformation of any one plane in a deformed parallelepiped is retained by the plane that was initially parallel to it. Let π_i denote the distorted plane whose normal was along the $\boldsymbol{E}_i$ direction in the undeformed configuration of the cube.

Before providing a general technique to select our 12 coordinate plane, we first focus on the simplest possible case where the edge of the cube that was initially along the direction $\boldsymbol{E}_1$ is found to undergo the least amount of transverse shear (i.e., $\mathcal{G}_1$ is minimum so that $\boldsymbol{E}_1 \mapsto \boldsymbol{\mathcal{E}}_1$). In this case, the two, potential, 12 coordinate planes are π_2 and π_3. In order to compare in-plane shears in these two planes, we need to first re-index the deformation gradient $\mathbf{F}$ by applying the linear transformation $\boldsymbol{\mathcal{F}} = \mathbf{P}^{\mathsf{T}}\mathbf{F}\mathbf{P}$ where $\mathbf{P}$ is an orthogonal tensor that re-labels the coordinate directions, with $\boldsymbol{\mathcal{F}}$ being the re-indexed deformation gradient. This process is depicted in Fig. 2.3. It is this re-indexed deformation gradient to which the Gram-Schmidt process is to be applied, viz., $\boldsymbol{\mathcal{F}} = \boldsymbol{\mathcal{R}}\boldsymbol{\mathcal{U}}$.

By re-indexing, the 1 coordinate direction of $\boldsymbol{\mathcal{E}}_1$ resides in column vector $\boldsymbol{f}_1$ with the additional information needed to establish the 12 coordinate plane residing in column vector $\boldsymbol{f}_2$, while column vector $\boldsymbol{f}_3$ contains information regarding the normal to this 12 plane. If the π_3 plane is chosen as the 12 coordinate plane, then no re-indexing of the deformation gradient is required because the π_3 plane already contains the line directions $\boldsymbol{E}_1$ and $\boldsymbol{E}_2$ in the undeformed cube. Therefore, the re-indexing tensor $\mathbf{P}_1$ is the identity tensor because $(\boldsymbol{E}_1, \boldsymbol{E}_2, \boldsymbol{E}_3) \mapsto (\boldsymbol{\mathcal{E}}_1, \boldsymbol{\mathcal{E}}_2, \boldsymbol{\mathcal{E}}_3)$, which is the

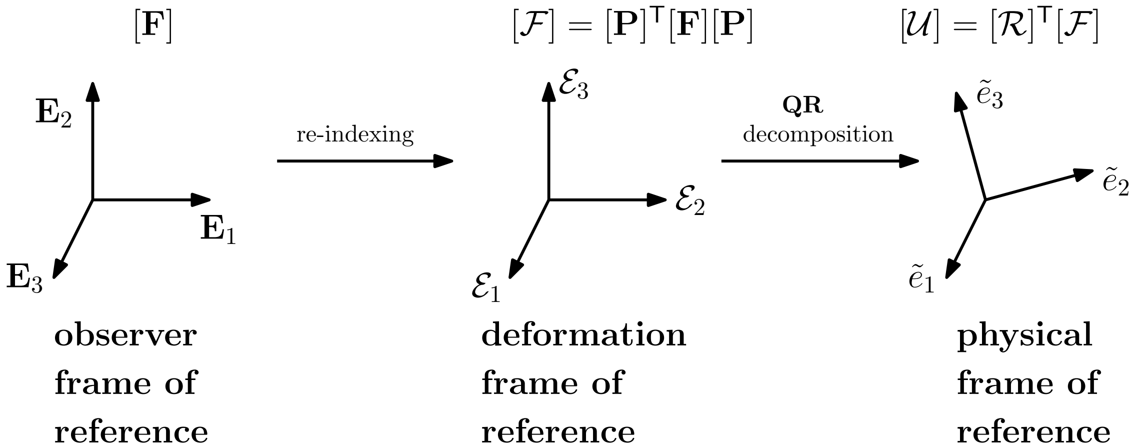

Figure 2.3: Frames of reference associated with the various coordinate systems. There is no rotation taking place between the observer and deformation frames of reference. Only a relabeling of indical orientation occurs here. There is a potential rotation that can arise between the deformation and physical frames of reference. This is a Gram-Schmidt rotation.

default condition, and therefore the re-indexed deformation gradient remains

$$\mathcal{F}_{ij} = \begin{bmatrix} F_{11} & F_{12} & F_{13} \\ F_{21} & F_{22} & F_{23} \\ F_{31} & F_{32} & F_{33} \end{bmatrix} = \begin{bmatrix} x_1 & \xi_1 x_2 & \xi_2 x_3 \\ \xi_3 x_1 & x_2 & \xi_4 x_3 \\ \xi_5 x_1 & \xi_6 x_2 & x_3 \end{bmatrix} = \left[\; \boldsymbol{f}_1 \; \middle| \; \boldsymbol{f}_2 \; \middle| \; \boldsymbol{f}_3 \; \right]. \tag{2.6}$$

Consequently, one can find the Laplace stretch $\boldsymbol{\mathcal{U}}$ using Eqn. (1.5), with the six physical attributes of Laplace stretch having three elongations of

$$a = \|\boldsymbol{f}_1\| \tag{2.7a}$$

$$b = \sqrt{\|\boldsymbol{f}_2\|^2 - (\boldsymbol{f}_1 \cdot \boldsymbol{f}_2)^2 / \|\boldsymbol{f}_1\|^2} \tag{2.7b}$$

$$c = \sqrt{\|\boldsymbol{f}_3\|^2 - \frac{(\boldsymbol{f}_1 \cdot \boldsymbol{f}_3)^2}{\|\boldsymbol{f}_1\|^2} - \frac{\left((\boldsymbol{f}_2 \cdot \boldsymbol{f}_3) - (\boldsymbol{f}_1 \cdot \boldsymbol{f}_2)(\boldsymbol{f}_1 \cdot \boldsymbol{f}_3)/\|\boldsymbol{f}_1\|^2\right)^2}{\|\boldsymbol{f}_2\|^2 - (\boldsymbol{f}_1 \cdot \boldsymbol{f}_2)^2 / \|\boldsymbol{f}_1\|^2}} \tag{2.7c}$$

and three shears of

$$\alpha = \frac{(\boldsymbol{f}_2 \cdot \boldsymbol{f}_3) - (\boldsymbol{f}_1 \cdot \boldsymbol{f}_2)(\boldsymbol{f}_1 \cdot \boldsymbol{f}_3)/\left\|\boldsymbol{f}_1\right\|^2}{\left\|\boldsymbol{f}_2\right\|^2 - (\boldsymbol{f}_1 \cdot \boldsymbol{f}_2)^2/\left\|\boldsymbol{f}_1\right\|^2} \tag{2.7d}$$

$$\beta = \frac{\boldsymbol{f}_1 \cdot \boldsymbol{f}_3}{\left\|\boldsymbol{f}_1\right\|^2} \tag{2.7e}$$

$$\gamma = \frac{\boldsymbol{f}_1 \cdot \boldsymbol{f}_2}{\left\|\boldsymbol{f}_1\right\|^2} \tag{2.7f}$$

On the other hand, if the π_2 plane is chosen to be the 12 coordinate plane, then one would find that $(\boldsymbol{E}_1, \boldsymbol{E}_2, \boldsymbol{E}_3) \mapsto (\boldsymbol{\mathcal{E}}_1, \boldsymbol{\mathcal{E}}_3, \boldsymbol{\mathcal{E}}_2)$ and the re-indexing tensor becomes

$$[\mathbf{P}_2] = \begin{bmatrix} 1 & 0 & 0 \\ 0 & 0 & 1 \\ 0 & 1 & 0 \end{bmatrix} \tag{2.8}$$

so that the re-indexed deformation gradient, found by applying the orthogonal tensor $\mathbf{P}_2$ through $\boldsymbol{\mathcal{F}} = \mathbf{P}_2^{\mathsf{T}} \mathbf{F} \mathbf{P}_2$, is given as

$$\mathcal{F}_{ij} = \begin{bmatrix} F_{11} & F_{13} & F_{12} \\ F_{31} & F_{33} & F_{32} \\ F_{21} & F_{23} & F_{22} \end{bmatrix} = \begin{bmatrix} x_1 & \xi_2 x_3 & \xi_1 x_2 \\ \xi_5 x_1 & x_3 & \xi_6 x_2 \\ \xi_3 x_1 & \xi_4 x_3 & x_2 \end{bmatrix} = \left[\ \bar{\boldsymbol{f}}_1 \ \middle|\ \bar{\boldsymbol{f}}_2 \ \middle|\ \bar{\boldsymbol{f}}_3\ \right]. \tag{2.9}$$

Again, in this case, one can find the Laplace stretch using Eqn. (1.5). The six attributes of Laplace stretch now have three elongations of

$$\bar{a} = \left\|\bar{\boldsymbol{f}}_1\right\| \tag{2.10a}$$

$$\bar{b} = \sqrt{\left\|\bar{\boldsymbol{f}}_2\right\|^2 - (\bar{\boldsymbol{f}}_1 \cdot \bar{\boldsymbol{f}}_2)^2 \,/\, \left\|\bar{\boldsymbol{f}}_1\right\|^2} \tag{2.10b}$$

$$\bar{c} = \sqrt{\left\|\bar{\boldsymbol{f}}_3\right\|^2 - \frac{(\bar{\boldsymbol{f}}_1 \cdot \bar{\boldsymbol{f}}_3)^2}{\left\|\bar{\boldsymbol{f}}_1\right\|^2} - \frac{\left((\bar{\boldsymbol{f}}_2 \cdot \bar{\boldsymbol{f}}_3) - (\bar{\boldsymbol{f}}_1 \cdot \bar{\boldsymbol{f}}_2)(\bar{\boldsymbol{f}}_1 \cdot \bar{\boldsymbol{f}}_3) \,/\, \left\|\bar{\boldsymbol{f}}_1\right\|^2\right)^2}{\left\|\bar{\boldsymbol{f}}_2\right\|^2 - (\bar{\boldsymbol{f}}_1 \cdot \bar{\boldsymbol{f}}_2)^2 \,/\, \left\|\bar{\boldsymbol{f}}_1\right\|^2}} \tag{2.10c}$$

and three shears of

$$\bar{\alpha} = \frac{(\bar{\boldsymbol{f}}_2 \cdot \bar{\boldsymbol{f}}_3) - (\bar{\boldsymbol{f}}_1 \cdot \bar{\boldsymbol{f}}_2)(\bar{\boldsymbol{f}}_1 \cdot \bar{\boldsymbol{f}}_3) \;/\; \|\bar{\boldsymbol{f}}_1\|^2}{\|\bar{\boldsymbol{f}}_2\|^2 - (\bar{\boldsymbol{f}}_1 \cdot \bar{\boldsymbol{f}}_2)^2 \;/\; \|\bar{\boldsymbol{f}}_1\|^2} \tag{2.10d}$$

$$\bar{\beta} = \frac{\bar{\boldsymbol{f}}_1 \cdot \bar{\boldsymbol{f}}_3}{\|\bar{\boldsymbol{f}}_1\|^2} \tag{2.10e}$$

$$\bar{\gamma} = \frac{\bar{\boldsymbol{f}}_1 \cdot \bar{\boldsymbol{f}}_2}{\|\bar{\boldsymbol{f}}_1\|^2}. \tag{2.10f}$$

In both these cases, attributes γ and $\bar{\gamma}$ of the Laplace stretch represent the magnitude of an in-plane shear in the corresponding 12 coordinate plane. Therefore, the 12 coordinate plane is to be selected according to whether γ or $\bar{\gamma}$ is minimal.

Now, from Eqns. (2.6 and 2.9), one can easily notice that

$$\|\boldsymbol{f}_1\| = \|\bar{\boldsymbol{f}}_1\| = \sqrt{1 + \xi_3^2 + \xi_5^2}\; x \tag{2.11a}$$

$$\|\boldsymbol{f}_2\| = \|\bar{\boldsymbol{f}}_3\| = \sqrt{1 + \xi_1^2 + \xi_6^2}\; y \tag{2.11b}$$

$$\|\boldsymbol{f}_3\| = \|\bar{\boldsymbol{f}}_2\| = \sqrt{1 + \xi_2^2 + \xi_4^2}\; z \tag{2.11c}$$

$$\boldsymbol{f}_1 \cdot \boldsymbol{f}_2 = \bar{\boldsymbol{f}}_1 \cdot \bar{\boldsymbol{f}}_3 = (\xi_1 + \xi_3 + \xi_5\xi_6)\; xy \tag{2.11d}$$

$$\boldsymbol{f}_1 \cdot \boldsymbol{f}_3 = \bar{\boldsymbol{f}}_1 \cdot \bar{\boldsymbol{f}}_2 = (\xi_2 + \xi_5 + \xi_3\xi_4)\; xz \tag{2.11e}$$

$$\boldsymbol{f}_2 \cdot \boldsymbol{f}_3 = \bar{\boldsymbol{f}}_2 \cdot \bar{\boldsymbol{f}}_3 = (\xi_4 + \xi_6 + \xi_1\xi_2)\; yz. \tag{2.11f}$$

Therefore, if $\gamma < \bar{\gamma}$, then plane π_3 is to be chosen as the 12 coordinate plane. Otherwise, if $\gamma > \bar{\gamma}$, then plane π_2 is to be chosen as the 12 coordinate plane. To compare γ and $\bar{\gamma}$, one needs to apply the Gram-Schmidt procedure twice to find the Laplace stretches corresponding to the two planes under consideration. However, in view of Eqn. (2.11), once the 1 coordinate axis is assigned, one can equivalently select the 12-coordinate plane by comparing the magnitudes of two inner products without applying a Gram-Schmidt procedure. The procedure of selecting a 12-coordinate plane is outlined below.

- Select a plane between the potential coordinate planes arbitrarily and obtain the corresponding matrix representation for the deformation gradient[1].

- Compare the magnitudes of two inner products, viz., $(\boldsymbol{f}_1 \cdot \boldsymbol{f}_2)$ vs. $(\boldsymbol{f}_1 \cdot \boldsymbol{f}_3)$.
- If $(\boldsymbol{f}_1 \cdot \boldsymbol{f}_2)$ is less than $(\boldsymbol{f}_1 \cdot \boldsymbol{f}_3)$, then the selected plane will be the 12 coordinate plane, otherwise the other plane is chosen to become the 12 coordinate plane.

Moreover, if the in-plane shear γ (or the quantity $(\boldsymbol{f}_1 \cdot \boldsymbol{f}_2)$) is chosen as the parameter to be minimized, then it follows that the out-of-plane shear α is minimal, too. The other out-of-plane shear, i.e., β, does not involve $(\boldsymbol{f}_1 \cdot \boldsymbol{f}_2)$, and hence, cannot be minimized in that sense.

It is important to note that whenever $\gamma = \bar{\gamma}$, then $\boldsymbol{f}_1 \cdot \boldsymbol{f}_2 = \bar{\boldsymbol{f}}_1 \cdot \bar{\boldsymbol{f}}_2 = \boldsymbol{f}_1 \cdot \boldsymbol{f}_3 = \bar{\boldsymbol{f}}_1 \cdot \bar{\boldsymbol{f}}_3$. Hence, the attributes of Laplace stretch become equal for these two cases, i.e.,

$$a = \bar{a}, \quad b = \bar{b}, \quad c = \bar{c}, \quad \alpha = \bar{\alpha}, \quad \beta = \bar{\beta}, \quad \text{if} \quad \gamma = \bar{\gamma}$$

and either of the two associated planes can be chosen as the 12 coordinate plane for our physical frame of reference without any inconsistency arising in the Laplace stretch. Said differently, there is continuity among the physical attributes for Laplace stretch across a switch in coordinate re-indexing. Consequently, the scheme presented here results in a Laplace stretch suitable for use in constitutive development. In contrast, there will likely be discontinuities in the three angles of rotation residing within the components of $\boldsymbol{\mathcal{R}}$ during a switch in coordinate re-indexing, but such discontinuities will not effect constitutive construction.

Now, we generalize this procedure to construct a unique coordinate system $\{\tilde{e}_i\}$ for any arbitrary deformation of the body. As mentioned earlier, in order to find an appropriate 12 coordinate plane for our physical frame of reference, we first need to re-index the associated deformation gradient through an appropriate orthogonal tensor $\mathbf{P}$ selected from a set of six $\mathbf{P}_m, m = 1, \ldots, 6$, such that $\boldsymbol{\mathcal{F}} = \mathbf{P}_m^{\mathsf{T}} \mathbf{F} \mathbf{P}_m$, where the subscript m associates with a unique pairing of 1 coordinate direction and 12 coordinate plane. These orthogonal re-indexing tensors, the re-indexed defor-

[1]This indeed is a reindexed matrix representation of the deformation gradient, corresponding to the selected 1-coordinate direction and the potential coordinate plane under consideration

mation gradients, the associated pairs of 1 coordinate direction and 12 coordinate plane, and the coordinate re-indexing maps are all provided in Table A.1 (App. A).

The process of pivoting for a 1 coordinate direction and a 12 coordinate plane is summarized in Alg. 1 (App. A), where the input is a deformation gradient $\mathbf{F}$ and the outputs are the re-indexing matrix $\mathbf{P}$ and the re-indexed deformation gradient $\boldsymbol{\mathcal{F}}$. Given this information, one can determine the physical attributes for Laplace stretch $a, b, c, \alpha, \beta, \gamma$ from Eqn. (1.5) using the **QR** decomposition $\boldsymbol{\mathcal{F}} = \boldsymbol{\mathcal{R}}\boldsymbol{\mathcal{U}}$ with rotation $\boldsymbol{\mathcal{R}}$ being established via Eqn. (1.2). It is in this re-indexed frame of reference that one's constitutive equation is to be solved in. Say the result is some stress $\boldsymbol{\mathcal{S}}$, then this stress would push into the current configuration κ_t as $\mathbf{S} = \mathbf{P}\boldsymbol{\mathcal{R}}\boldsymbol{\mathcal{S}}\boldsymbol{\mathcal{R}}^{\mathsf{T}}\mathbf{P}^{\mathsf{T}}$ in accordance with Fig. 2.3.

2.3 Summary

In this chapter, a pivoting strategy is introduced to address the two invariant properties that arise from a Gram-Schmidt factorization of the deformation gradient, viz., that the 1 direction and the normal to the 12 plane are invariant under transformations of the Laplace stretch. The 1 direction is chosen such that the edge of a representative cube along this coordinate direction undergoes minimum transverse shear. Out of the two coordinate planes containing the 1 coordinate direction, the one that undergoes minimum transverse shear is chosen as the 12 coordinate plane. Adopting this strategy produces unique components for the Laplace stretch, indifferent to observer. Hence, these measures for stretch can be used to construct constitutive equations.

3. COMPATIBILITY CONDITION FOR LAPLACE STRETCH *

With the issue of representation resolved, now we investigate a compatibility condition for the Laplace stretch whenever a right Cauchy-Green tensor, $\mathbf{C}$ is prescribed. The problem of existence and uniqueness of a finite deformation generating a prescribed right Cauchy-Green tensor has been addressed many times in the past century. The issue is mathematically equivalent to determining a condition such that a prescribed, symmetric, second-order tensor acts as the metric of an Eucledian space. This condition is given by a popular theorem, asserted by Riemann which states that vanishing of the Riemann curvature tensor ensures that the right Cauchy-Green tensor $\mathbf{C}$ is the metric tensor for a Lagrangian frame of reference and, hence, it is possible to obtain a deformation map (or displacement vector) by integrating a system of partial differential equations involving $\mathbf{C}$ and the deformation map (or displacement vector) [86, 91, 8, 2].

Many forms of the Riemann curvature tensor have been derived. A list of other works on this topic is given in Truesdell and Toupin (1960) [91]. However, this compatibility condition does not involve any decomposition of the deformation gradient. Shield (1973) [83] employed a polar decomposition of the deformation gradient in order to obtain an integrability condition for the rotation tensor. He showed that the fourth-order tensor corresponding to his integrability condition and to Riemann's curvature tensor are related through the inverse of a symmetric, stretch tensor arising from a polar decomposition of $\mathbf{F}$. Positive-definiteness of the stretch tensor (hence, it is always invertible) ensures uniqueness in his relation. Thus, the integrability condition for a rotation tensor is equivalent to a vanishing of the Riemann curvature tensor. Blume (1989) [8] and Acharya (1999) [2] determined compatibility conditions in terms of the left Cauchy-Green tensor, i.e., $\mathbf{B} = \mathbf{F}\mathbf{F}^T$, for plane and three-dimensional deformations, respectively. In all these works, the body undergoing deformation is considered to be simply-connected. Yavari (2013) [95] studied the compatibility condition for a non-simply connected body from a geometric point of

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view. Derivation of a compatibility condition for Laplace stretch has been previously attempted by Lembo (2017) [53]. In this work, he considered the rotation field as the primary kinematic variable and followed the procedure introduced by Shield [83]. However, it can be easily shown that Lembo's compatibility condition for Laplace stretch is a direct consequence of the symmetry of the right Cauchy-Green tensor and does not utilize the physical meanings of the components of Laplace stretch. Therefore, in this chapter, we consider the right Cauchy-Green tensor as our primary kinematic variable and use the physical meanings of the components of Laplace stretch to derive our compatibility condition that restricts the dependence of these components on certain spatial variables.

Recall that the base vectors $\{\tilde{\boldsymbol{e}}_I\}$ form a Lagrangian triad in which the Gram-Schmidt factorization of $\mathbf{F}$ is to be performed. Therefore, $\mathbf{C}$ serves as the metric of this coordinate system. For a deformation of the body to be compatible, its current configuration $\kappa_t(\mathcal{B})$ must be a Euclidean space whenever the undeformed configuration $\kappa_r(\mathcal{B})$ is Euclidean. A material manifold is considered to be Euclidean or flat when it is equipped with a metric-compatible, torsionless connection and the associated Riemann curvature tensor vanishes.

Since the torsion of the space $\kappa_t(\mathcal{B})$ vanishes, the connection coefficient, commonly known as the Christoffel symbol, ought to be symmetric. Therefore, the Christoffel symbol pertaining to this coordinate system takes on the form:

$$\mathtt{G}_{ijk} = \frac{1}{2}\left(C_{jk,i} + C_{ik,j} - C_{ij,k}\right) \tag{3.1}$$

where $C_{ij,k} = \partial C_{ij}/\partial X_k$, etc. The Riemann curvature tensor for this coordinate system is the same as the one wherein a polar decomposition is performed, because its definition does not involve any decomposition of $\mathbf{F}$. Hence, the Riemann curvature tensor is defined as:

$$\mathbb{R}_{ijkl} = \mathtt{G}_{jli,k} - \mathtt{G}_{jki,l} + C^{-1}_{pq}\left(\mathtt{G}_{jkp}\mathtt{G}_{ilq} - \mathtt{G}_{jlp}\mathtt{G}_{ikq}\right) \tag{3.2}$$

where $i, j, k, l = 1, 2, 3$ and where repeated subscripts are summed according to Einstein's sum-mation convention.

3.1 Derivation of compatibility condition

We now derive a compatibility condition for $\boldsymbol{\mathcal{U}}$ starting from Riemann's theorem. Note that a vanishing Riemann curvature tensor serves as the compatibility condition irrespective of which decomposition of the deformation gradient is used, since $\mathbf{C}$ serves as the metric for any Lagrangian frame of reference. Cholesky factorization of $\mathbf{C}$ ensures the existence of a *unique* $\boldsymbol{\mathcal{U}}$ for a given $\mathbf{C}$ (Eqn. 1.7). Therefore, we are interested in finding the restriction imposed on $\boldsymbol{\mathcal{U}}$ caused by a vanishing of the Riemann curvature tensor.

Differentiation of Eqn. (1.6) immediately leads to

$$C_{ij,k} = \mathcal{U}_{mi,k}\mathcal{U}_{mj} + \mathcal{U}_{mi}\mathcal{U}_{mj,k} \tag{3.3}$$

Writing $\mathtt{G}$ in terms of $\boldsymbol{\mathcal{U}}$ using Eqn. (3.3) and substituting in Eqn. (3.2), we get

$$\begin{aligned}
\mathbb{R}_{ijkl} = {} & \frac{1}{2}[-\mathtt{W}_{mkl,j}\mathcal{U}_{mi} + \mathtt{W}_{mkl,i}\mathcal{U}_{mj} - \mathtt{W}_{mij,l}\mathcal{U}_{mk} + \mathtt{W}_{mij,k}\mathcal{U}_{ml} - \mathtt{W}_{mij}\mathtt{W}_{mkl}] + \frac{1}{4}[\mathtt{W}_{mlj}\mathtt{W}_{mik} \\
& + \mathtt{W}_{mil}\mathtt{W}_{mjk} + (\mathtt{W}_{nql}\mathtt{D}_{rkj} + \mathtt{W}_{nkq}\mathtt{D}_{rlj})\mathcal{U}^{-1}_{qr}\mathcal{U}_{ni} + \mathtt{W}_{nqi}\mathtt{D}_{rkj}\mathcal{U}_{nl}\mathcal{U}^{-1}_{qr} + \mathtt{W}_{mpj}\mathtt{D}_{ril}\mathcal{U}_{mk}\mathcal{U}^{-1}_{pr} \\
& + (\mathtt{D}_{ril}\mathtt{W}_{mpk} + \mathtt{D}_{rik}\mathtt{W}_{mlp})\mathcal{U}_{mj}\mathcal{U}^{-1}_{pr} + \mathtt{D}_{rlj}\mathtt{W}_{niq}\mathcal{U}_{nk}\mathcal{U}^{-1}_{qr} + \mathtt{D}_{rik}\mathtt{W}_{mjp}\mathcal{U}_{ml}\mathcal{U}^{-1}_{pr} \\
& + \mathtt{W}_{nql}\mathtt{W}_{mpj}\mathcal{U}_{mk}\mathcal{U}_{ni}\mathcal{U}^{-1}_{pr}\mathcal{U}^{-1}_{qr} + \mathtt{W}_{nqi}\mathtt{W}_{mpj}\mathcal{U}_{mk}\mathcal{U}_{nl}\mathcal{U}^{-1}_{pr}\mathcal{U}^{-1}_{qr} \\
& + (\mathtt{W}_{nql}\mathtt{W}_{mpk} + \mathtt{W}_{nqk}\mathtt{W}_{mlp})\mathcal{U}_{mj}\mathcal{U}_{ni}\mathcal{U}^{-1}_{pr}\mathcal{U}^{-1}_{qr} + \mathtt{W}_{niq}\mathtt{W}_{mkp}\mathcal{U}_{mj}\mathcal{U}_{nl}\mathcal{U}^{-1}_{pr}\mathcal{U}^{-1}_{qr} \\
& + \mathtt{W}_{nkq}\mathtt{W}_{mpj}\mathcal{U}_{ml}\mathcal{U}_{ni}\mathcal{U}^{-1}_{pr}\mathcal{U}^{-1}_{qr} + \mathtt{W}_{niq}\mathtt{W}_{mpj}\mathcal{U}_{ml}\mathcal{U}_{nk}\mathcal{U}^{-1}_{pr}\mathcal{U}^{-1}_{qr} + \mathtt{W}_{niq}\mathtt{W}_{mpl}\mathcal{U}_{mj}\mathcal{U}_{nk}\mathcal{U}^{-1}_{pr}\mathcal{U}^{-1}_{qr}]
\end{aligned} \tag{3.4}$$

where $\mathtt{D}_{abc} = \mathcal{U}_{ab,c} + \mathcal{U}_{ac,b}$ and $\mathtt{W}_{abc} = \mathcal{U}_{ab,c} - \mathcal{U}_{ac,b}$ are third-order tensors, symmetric and skew-symmetric in b and c, respectively.

It is convenient to write Eqn. (3.2) in tensor notation for algebraic manipulation. Transpositions of fourth-order tensors used in Kintzel and Başar (2006) [46] are particularly helpful in this case. However, transpositions for third-order tensors were not provided. Therefore, we define these transpositions in a way that they are consistent with Kintzel and Başar's transpositions for fourth-order tensors. A list of transpositions for second-, third- and fourth-order tensors are provided in App. B. Next, we write Eqn. (3.2) in tensor notation

$$
\begin{aligned}
\mathbb{R} = & \frac{1}{2}[-\mathbb{R}_1 + \mathbb{R}_1^{dl} + [\mathbb{R}_1^D]^{dr} - \mathbb{R}_1^D] + \frac{1}{4}[\,-2\mathbb{R}_2 + [\mathbb{R}_2^{dr}]^{ti} + [\mathbb{R}_2^{ti}]^{dr}] \\
& + \frac{1}{4}[[\mathbb{R}_3^{dr}]^{ti} + [\mathbb{R}_3^{dr}]^{to} + [\mathbb{R}_3^{ti}]^T + [\mathbb{R}_3^{to}]^T - [\mathbb{R}_3^{to}]^{dl} - [\mathbb{R}_3^{ti}]^{dl} - [[\mathbb{R}_3^{dr}]^{ti}]^{dr} - [[\mathbb{R}_3^{dr}]^{to}]^{dr}] \\
& + \frac{1}{4}[[\mathbb{R}_4^{ti}]^{dr} + [[\mathbb{R}_4^{dl}]^{ti}]^{dr} + [[\mathbb{R}_4^{dr}]^{ti}]^{dr} + [\mathbb{R}_4^{to}]^{dl} - [\mathbb{R}_4^{dr}]^{ti} - \mathbb{R}_4^{ti} - [\mathbb{R}_4^{dl}]^{ti} - [\mathbb{R}_4^{to}]^T]
\end{aligned} \tag{3.5}
$$

where $\mathbb{T}_{mjkl} = \mathtt{W}_{mkl,j}$ and

$$
\mathbb{R}_1 = \boldsymbol{\mathcal{U}}^T\mathbb{T}; \quad \mathbb{R}_2 = \mathtt{W}^D\mathtt{W}; \quad \mathbb{R}_3 = \boldsymbol{\mathcal{U}}^T\mathtt{W}\boldsymbol{\mathcal{U}}^{-1}\mathtt{D}; \quad \mathbb{R}_4 = (\boldsymbol{\mathcal{U}}^T\mathtt{W}\boldsymbol{\mathcal{U}}^{-1})(\boldsymbol{\mathcal{U}}^T\mathtt{W}\boldsymbol{\mathcal{U}}^{-1})^t. \tag{3.6}
$$

From the definitions for $\mathtt{W}$ and $\mathtt{D}$, it is easily understood that $\mathtt{W}^T = -\mathtt{W}$ and $\mathtt{D}^T = \mathtt{D}$. Now, it is important to investigate similar symmetries of the fourth-order tensors $\mathbb{T}$ and $\mathbb{R}_m, m = 1, 2, 3, 4$. From the definition of $\mathbb{T}$, it follows that $\mathbb{T}^{dr} = -\mathbb{T}$ because $\mathtt{W}^T = -\mathtt{W}$. Using the symmetries mentioned above, we obtain $\mathbb{R}_1^{dr} = -\mathbb{R}_1$, $\mathbb{R}_2^{dr} = -\mathbb{R}_2$ and $\mathbb{R}_3^{dr} = \mathbb{R}_3$. Symmetry of $\mathbb{R}_4$ is obtained from its definition and it is $\mathbb{R}_4^t = \mathbb{R}_4$. Using these symmetries, we attain

$$
\begin{aligned}
\mathbb{R} = & \frac{1}{2}[(\mathbb{R}_1^{dl} - \mathbb{R}_1) + (\mathbb{R}_1^{dl} - \mathbb{R}_1)^D] + \frac{1}{4}[\,-2\mathbb{R}_2 + [\mathbb{R}_2^{dr}]^{ti} + [\mathbb{R}_2^{ti}]^{dr}] \\
& + \frac{1}{4}[(\mathbb{R}_3^{ti} + \mathbb{R}_3^{to}) + [(\mathbb{R}_3^{ti} + \mathbb{R}_3^{to})]^T - [(\mathbb{R}_3^{ti} + \mathbb{R}_3^{to})]^{dl} - [(\mathbb{R}_3^{ti} + \mathbb{R}_3^{to})]^{dr}] \\
& + \frac{1}{4}[(-\mathbb{R}_4^{ti} - [\mathbb{R}_4^{dr}]^{ti} + [\mathbb{R}_4^{ti}]^{dr} + [[\mathbb{R}_4^{dr}]^{ti}]^{dr}) + (-[\mathbb{R}_4^{ti}]^T - [\mathbb{R}_4^{dl}]^{ti} + [\mathbb{R}_4^{ti}]^{dl} + [[\mathbb{R}_4^{dl}]^{ti}]^{dr})].
\end{aligned} \tag{3.7}
$$

Other important symmetries come from the definition for the Riemann curvature tensor, viz., $\mathbb{R}^{dr} = -\mathbb{R}$ and $\mathbb{R}^D = \mathbb{R}$. These are ensured by the symmetries of $\mathbb{R}_1, \mathbb{R}_2$ and $\mathbb{R}_3$ and the interrelations of the transpositions (mentioned in App. B) when $\mathbb{R}$ is written in tensor notation.

We write Eqn. (3.7) in matrix form in the Cartesian basis $\{\tilde{e}_I\}$ in order to use the upper-triangular property of $\boldsymbol{\mathcal{U}}$, which is essential in our derivation. We define the following functions to simplify our calculation.

$$\begin{aligned} f_1(\mathbb{R}_1) &= f_1(\boldsymbol{\mathcal{U}}, \mathbb{T}) = (\mathbb{R}_1^{dl} - \mathbb{R}_1) + (\mathbb{R}_1^{dl} - \mathbb{R}_1)^D \\ f_2(\mathbb{R}_2) &= f_2(\mathtt{W}) = -2\mathbb{R}_2 + [\mathbb{R}_2^{dr}]^{ti} + [\mathbb{R}_2^{ti}]^{dr} \\ f_3(\mathbb{R}_3) &= f_3(\boldsymbol{\mathcal{U}}, \mathtt{W}, \mathtt{D}) = (\mathbb{R}_3^{ti} + \mathbb{R}_3^{to}) + [(\mathbb{R}_3^{ti} + \mathbb{R}_3^{to})]^T - [(\mathbb{R}_3^{ti} + \mathbb{R}_3^{to})]^{dl} - [(\mathbb{R}_3^{ti} + \mathbb{R}_3^{to})]^{dr} \\ f_4(\mathbb{R}_4) &= f_4(\boldsymbol{\mathcal{U}}, \mathtt{D}, \mathtt{W}) = (-\mathbb{R}_4^{ti} - [\mathbb{R}_4^{dr}]^{ti} + [\mathbb{R}_4^{ti}]^{dr} + [[\mathbb{R}_4^{dr}]^{ti}]^{dr}) + (-[\mathbb{R}_4^{ti}]^T - [\mathbb{R}_4^{dl}]^{ti} \\ &\qquad + [\mathbb{R}_4^{ti}]^{dl} + [[\mathbb{R}_4^{dl}]^{ti}]^{dr}) \end{aligned} \tag{3.8}$$

The third-order tensors $\mathtt{W}$ and $\mathtt{D}$ take the following forms in $\tilde{e}_I$:

$$[\mathtt{W}_{ijk}] = \begin{bmatrix} 0 & W_1 & W_3 & -W_1 & 0 & W_6 & -W_3 & -W_6 & 0 \\ 0 & W_2 & W_4 & -W_2 & 0 & W_7 & -W_4 & -W_7 & 0 \\ 0 & 0 & W_5 & 0 & 0 & W_8 & -W_5 & -W_8 & 0 \end{bmatrix} \tag{3.9}$$

where $W_1 = (a\gamma)_{,1} - a_{,2}$; $W_2 = b_{,1}$; $W_3 = (a\beta)_{,1} - a_{,3}$; $W_4 = (b\alpha)_{,1}$; $W_5 = c_{,1}$; $W_6 = (a\beta)_{,2} - (a\gamma)_{,3}$; $W_7 = (b\alpha)_{,2} - b_{,3}$ and $W_8 = c_{,2}$, with

$$[\mathtt{D}_{ijk}] = \begin{bmatrix} 2a_{,1} & (a\gamma)_{,1} + a_{,2} & (a\beta)_{,1} + a_{,3} & a_{,2} + (a\gamma)_{,1} & 2(a\gamma)_{,2} & (a\beta)_{,2} + (a\gamma)_{,3} & (a\gamma)_{,3} + (a\beta)_{,1} & (a\gamma)_{,3} + (a\beta)_{,2} & 2(a\beta)_{,3} \\ 0 & b_{,1} & (b\alpha)_{,1} & b_{,1} & 2b_{,2} & (b\alpha)_{,2} + b_{,3} & (b\alpha)_{,1} & b_{,3} + (b\alpha)_{,2} & 2b\alpha_{,3} \\ 0 & 0 & c_{,1} & 0 & 0 & c_{,2} & c_{,1} & c_{,2} & 2c_{,3} \end{bmatrix}. \tag{3.10}$$

Next, we write the functions in Eqn. (3.8) in the basis $\{\tilde{e}_I\}$. When written in matrix form, each of these functions forms a 9×9 square matrix consisting of nine 3×3 block matrices. Some important features of these matrices are listed below.

- The diagonal elements of the matrix $f_1(\mathbb{R}_1)$ are zero.
- $f_m(\mathbb{R}_m)^D = f_m(\mathbb{R}_m)$, i.e., $[f_m(\mathbb{R}_m)]_{klij} = [f_m(\mathbb{R}_m)]_{ijkl}$.
- The diagonal blocks of matrices $f_n(\mathbb{R}_n), n = 2, 3, 4$, are zero.
- The sub-matrices forming the off-diagonal blocks of $f_n(\mathbb{R}_n)$ are skew-symmetric, i.e., $[f_n(\mathbb{R}_n)]_{ijkl} = -[f_n(\mathbb{R}_n)]_{jikl}$.

- The diagonal elements of each off-diagonal block of $f_n(\mathbb{R}_n)$ are zero.

- The off-diagonal blocks of $f_n(\mathbb{R}_n)$ are skew-symmetric, i.e., $[f_n(\mathbb{R}_n)]_{ijkl} = -[f_n(\mathbb{R}_n)]_{ijlk}$.

Note that even if the symmetries of $\mathbb{R}$ ($\mathbb{R}^{dr} = -\mathbb{R}$ and $\mathbb{R}^D = \mathbb{R}$) are easily realized in tensor notation, they are not obvious from the structure of $\mathbb{R}_m$. Two important observations are made based upon the structure of $f_m(\mathbb{R}_m)$ and their associated symmetry properties.

- Since the diagonal blocks of $f_n(\mathbb{R}_n)$ are zero and $\mathbb{R}_{ijkl} = \sum_{m=1}^{4} f_m(\mathbb{R}_m)$, the only remaining nonzero elements in the diagonal blocks of $\mathbb{R}$ arise from $f_1(\mathbb{R}_1)$. Consequently, elements in the diagonal blocks of $f_1(\mathbb{R}_1)$ must be equal to zero.

- The off-diagonal blocks of $f_n(\mathbb{R}_n)$ are skew-symmetric, whereas this is not the case for $f_1(\mathbb{R}_1)$. The off-diagonal blocks of $f_1(\mathbb{R}_1)$ must be either skew-symmetric or zero because the $f_m(\mathbb{R}_m)$ add up to the Riemann curvature tensor whose off-diagonal blocks are skew-symmetric, i.e., $\mathbb{R}^{dr} = -\mathbb{R}$. For generality, the off-diagonal blocks of $f_1(\mathbb{R}_1)$ are taken to be skew-symmetric.

These two restrictions on $f_1(\mathbb{R}_1)$ give rise to 18 equations, out of which only 15 are independent. These equations are made up of products between the fourth-order tensor $\mathbb{T}$, the Laplace stretch $\boldsymbol{\mathcal{U}}$ and its transpose. The symmetry $\mathbb{R}^D = \mathbb{R}$ is automatically preserved by the structure of $f_m(\mathbb{R}_m)$. The equations are provided in App. B.3.1.

Next we focus on the off-diagonal elements in the off-diagonal blocks of the Riemann curvature tensor. Other entries in $\mathbb{R}$ are identically zero. Note that most of these elements are either equal to or the negative of some other elements due to the symmetry $\mathbb{R}^D = \mathbb{R}$. In fact, only six of these elements are independent. These elements are $\mathbb{R}_{1212}$, $\mathbb{R}_{1312}$, $\mathbb{R}_{2312}$, $\mathbb{R}_{1313}$, $\mathbb{R}_{2313}$ and $\mathbb{R}_{2323}$. Thus, equating these elements to zero, we find six independent equations. These equations constitute multiple terms from $\mathbb{R}_m$.

The set of six equations holds for all possible deformations because the Riemann curvature tensor must be zero for any prescribed Cauchy-Green tensor to ensure a valid finite deformation.

Since the system of equations is homogeneous, $\mathtt{W} = 0$ is a trivial solution. *One can show that the trivial solution is the only solution to the system of equations if all the components of Laplace stretch* $\boldsymbol{\mathcal{U}}$ *in Eqn.* (1.3) *are deemed to be independent.* However, the trivial solution is too restrictive, because it holds only when the rotation tensor $\boldsymbol{\mathcal{R}}$ is homogeneous. This is due to an interdependence between some of the components of $\boldsymbol{\mathcal{U}}$.

It is worth noting that all elements of Laplace stretch in Eqn. (1.3) are not independent. Specifically, the extent of shears $\tilde{\alpha}$, $\tilde{\beta}$ and $\tilde{\gamma}$ explicitly depend upon elongation a or b through

$$\tilde{\alpha} = b\alpha, \quad \tilde{\beta} = a\beta, \quad \tilde{\gamma} = a\gamma. \tag{3.11}$$

Apart from couplings between a, γ, β and b, α, there is no reason for other shears or elongations to be coupled, e.g., a variation in the extent of shear γ is not expected to depend on a variation in elongation c. This is a consequence of the fact that the $\tilde{e}_1$ and $\tilde{e}_1 \times \tilde{e}_2$ coordinate directions remain invariant under transformation $\boldsymbol{\mathcal{U}}$ [63, 64]. Note that, instead of the magnitudes of shear, Srinivasa (2012) [88] uses the *extents* of shear in the expression of Laplace stretch.

To determine restrictions on components of $\mathtt{W}$ (or on those of Laplace stretch $\boldsymbol{\mathcal{U}}$) imposed by compatibility, we pick specific conditions that make some of the components of $\mathtt{W}$ or their coefficients zero. One has to be careful in choosing these conditions to make sure that these conditions have no effect on the component of interest, and that the couplings between shear and elongation in Eqn. (3.11) are taken into account. For example, one should not pick b to vary in a certain way to determine conditions on the variation of α and vice versa. Since the cases are chosen in a way that restrictions on other components of $\mathtt{W}$ do not have any effect on the component of interest, it is evident that the condition on the component of interest emerging from a vanishing of Riemann curvature tensor is valid for all feasible deformations.

It is important to note that some elements of $f_1(\mathbb{R}_1)$ become zero in order to preserve the restrictions on it as stated earlier. Because couplings between shears and elongations, apart from the ones between a, β, γ and b, α are not expected, one can show that the terms involving derivatives of

$W_p, p = 1, ..., 8$, do not appear in the system of six equations arising from a vanishing of Riemann curvature tensor. See App. B.3.1 for details.

$\mathbb{R}_{1212} = 0$ leads to:[1]

$$
\begin{aligned}
&2a\cancel{W_{1,2}} + \left(-\frac{\tilde{\beta}^2}{c^2} + \frac{4\tilde{\alpha}\tilde{\gamma}\tilde{\beta}}{bc^2} - \frac{4\tilde{\alpha}^2\tilde{\gamma}^2}{b^2c^2}\right)W_1^2 - \frac{\tilde{\alpha}^2}{c^2}W_2^2 - \frac{\tilde{\gamma}^2}{c^2}W_3^2 - \frac{b^2}{c^2}W_4^2 - \frac{a^2}{c^2}W_6^2 + \frac{4ab_{,2}}{b}W_1 \\
&- \frac{4a_{,1}b}{a}W_2 + \left(\frac{2\tilde{\alpha}\tilde{\beta}}{c^2} - \frac{4\tilde{\gamma}}{b} - \frac{4a\tilde{\alpha}^2}{bc^2}\right)W_1W_2 + \left(\frac{4\tilde{\gamma}^2\tilde{\alpha}}{bc^2} - \frac{2\tilde{\gamma}\tilde{\beta}}{c^2}\right)W_1W_3 + \frac{2b\tilde{\beta}}{c^2}W_1W_4 \\
&+ \left(\frac{2a\tilde{\beta}}{c^2} - \frac{4a\tilde{\alpha}\tilde{\gamma}}{bc^2}\right)W_1W_6 - \frac{4a\tilde{\alpha}}{c^2}W_1W_7 + \left(\frac{6\tilde{\alpha}\tilde{\gamma}}{c^2} - \frac{4b\tilde{\beta}}{c^2}\right)W_2W_3 + \frac{2a\tilde{\alpha}}{c^2}W_2W_6 + \frac{2b\tilde{\alpha}}{c^2}W_2W_4 \\
&- \frac{2\tilde{\gamma}b}{c^2}W_3W_4 + \frac{2a\tilde{\gamma}}{c^2}W_3W_6 + \frac{4ab}{c^2}W_3W_7 - \frac{2ab}{c^2}W_4W_6 = 0
\end{aligned}
\tag{3.12}
$$

Now, we pick specific cases and determine the conditions that must be met to satisfy Eqn. (3.12). First, we consider a deformation where a, γ and $\tilde{\beta}$ are arbitrary constants, i.e., W_1, W_3 and W_6 are zero. Equation (3.12) reduces to

$$\tilde{\alpha}W_2 - bW_4 = 0. \tag{3.13}$$

Note that W_2 and W_4 involve derivatives of b and α respectively. Because variations of b and α are not expected to depend upon variations of any other components of Laplace stretch, we conclude that the condition in Eqn. (3.13) is valid irrespective of chosen conditions on a, $\tilde{\beta}$ and $\tilde{\gamma}$, and thus, for all feasible deformations. Equation (3.13) further implies that

$$\alpha_{,1} = 0. \tag{3.14}$$

It is evident from Eqn. (3.13) that if b is a function of X_1, then α too must be a function of X_1, and vice versa. This is corroborated by the relation $\tilde{\alpha}_{,1} = \alpha b_{,1}$ obtained by differentiating $\tilde{\alpha} = \alpha b$ and using Eqn. (3.14).

Next, we allow $a, \tilde{\beta}$ and $\tilde{\gamma}$ to vary arbitrarily and choose b and $\tilde{\alpha}$ to be arbitrary constants. In

[1] The term $W_{1,2}$ becomes zero according to Eqn. (B.3.1.19).

this case, Eqn. (3.12) reduces to:

$$\tilde{\beta}W_1 + \tilde{\gamma}W_3 - aW_6 = 0. \tag{3.15}$$

By a similar argument, we conclude that this condition has to be satisfied for all possible deformations because, apart from their interdependence $a, \tilde{\beta}$ and $\tilde{\gamma}$, they do not depend on the other components of $\boldsymbol{\mathcal{U}}$. Expanding in terms of α, β Eqn. (3.15) yields:

$$(a^2\beta\gamma)_{,1} - (a^2\beta)_{,2} - a\gamma a_{,3} + a^2\gamma_{,3} = 0. \tag{3.16}$$

Nothing else can be concluded about the other components of $\mathtt{W}$ from this equation, because the components W_5, W_7, W_8 either appear in Eqn. (3.12) as a product with another component of $\mathtt{W}$, e.g., terms like $-\dfrac{4a\alpha}{c^2}W_1W_7$, or they do not appear at all. To find conditions on a component of $\mathtt{W}$, we need at least one stand-alone term associated with the component of interest that does not appear as a product with other components.

For conditions on W_5, we appeal to the equation arising from equating $\mathbb{R}_{1313}$ to zero. Similar conditions on W_7 and W_8 are derived from the equation $\mathbb{R}_{2323} = 0$. These two equations are provided in App. B.3.2. By choosing suitable conditions on components of $\boldsymbol{\mathcal{U}}$, one can show that W_5 must be zero in order to satisfy equations (B.3.2.1), because all other terms are identically zero whenever Eqs. (3.13) and (3.15) are employed. Thus,

$$W_5 = 0 \implies c_{,1} = 0. \tag{3.17}$$

We use Eqn. (B.3.2.2) to find conditions on W_7 and W_8. Choosing a to be an arbitrary constant and $\beta = \gamma = 0$ (or b, α to be arbitrary constants) and using the conditions derived above and independence of $b, \tilde{\alpha}$ (or $a, \tilde{\beta}, \tilde{\gamma}$) and c, one can conclude that

$$W_7 = 0 \implies (b\alpha)_{,2} = b_{,3} \tag{3.18}$$

and finally,

$$W_8 = 0 \implies c_{,2} = 0. \tag{3.19}$$

All other relevant elements of the Riemann curvature tensor, viz., $\mathbb{R}_{1312}, \mathbb{R}_{2312}$ and $\mathbb{R}_{2313}$, become identically zero whenever the conditions derived above are employed. Therefore, a vanishing Riemann curvature tensor implies that Eqs. (3.13)– (3.19) must be satisfied. On the other hand, for any feasible deformation that satisfies these equations, the Riemann curvature tensor vanishes. Furthermore, in view of the coupling between certain shears and elongations mentioned earlier, it is not possible to find a deformation for which these equations are not satisfied, yet the Riemann curvature tensor goes to zero. Therefore, these equations serve as the necessary and sufficient conditions for vanishing of a Riemann curvature tensor and, hence, for a deformation to be compatible.

3.2 Discussion

3.2.1 Compatibility condition of Laplace stretch for prescribed F

Whenever a deformation gradient is prescribed, the necessary and sufficient integrability condition for the existence of a unique deformation map is $\mathrm{curl}(\mathbf{F}) = \mathbf{0}$, which implies

$$F_{ij,k} = F_{ik,j}. \tag{3.20}$$

Adopting a **QR** decomposition of the deformation gradient, one can obtain a partial differential equation for the rotation $\boldsymbol{\mathcal{R}}$ as

$$\frac{\partial \boldsymbol{\mathcal{R}}}{\partial \boldsymbol{X}} = \boldsymbol{\mathcal{R}}\mathtt{Z} \tag{3.21}$$

where

$$\mathtt{Z}_{pnk} = \left[\mathtt{G}_{ikr}\mathcal{U}_{rp}^{-1} - \mathcal{U}_{pi,k}\right]\mathcal{U}_{in}^{-1}. \tag{3.22}$$

Using the definition for the Christoffel symbol in Eqn. (3.1), a relationship between $\mathbf{C}$, $\mathbf{F}$ and Eqn. (3.20) leads to

$$F_{pi}F_{pj,k} = \mathtt{G}_{jki} \implies F_{ij,k} = F_{ip}C_{pq}^{-1}\mathtt{G}_{jkq}. \tag{3.23}$$

Differentiating Eqn. (3.23) with respect to $\boldsymbol{X}$ and eliminating the first derivative of $\mathbf{F}$ by using the later part of Eqn. (3.23), we get

$$F_{pi}F_{pj,kl} = \mathtt{G}_{jki,l} - C^{-1}_{pq}\mathtt{G}_{jkp}\mathtt{G}_{ilq}. \tag{3.24}$$

Since $F_{pi}F_{pj,kl} = F_{pi}F_{pj,lk}$, one finally gets $\mathbb{R}_{ijkl} = 0$. Therefore, the equations (3.13)–(3.19) must be satisfied. Thus, the only restriction of $\boldsymbol{\mathcal{U}}$ provided by the integrability condition of a prescribed deformation gradient is the same as the restriction pertaining to a given Cauchy-Green tensor (or Laplace stretch). In fact, $\mathrm{curl}(\mathbf{F}) = \mathbf{0}$ does not have any direct effect on $\boldsymbol{\mathcal{U}}$. This can be shown from a decomposition of deformation gradient into an orthogonal rotation and the Laplace stretch.

$$\mathrm{curl}(\mathbf{F}) = \mathbf{0} \implies (\mathcal{R}\mathcal{U})_{ij,k} = (\mathcal{R}\mathcal{U})_{ik,j}. \tag{3.25}$$

Expansion of this expression, and use of Eqn. (3.21) yield

$$\mathtt{Z}_{pnk}\mathcal{U}_{nj} - \mathtt{Z}_{pnj}\mathcal{U}_{nk} = \mathcal{U}_{pk,j} - \mathcal{U}_{pj,k} \tag{3.26}$$

Substitution of Eqn. (3.22) into Eqn. (3.26) implies $\mathtt{G}_{ijk} = \mathtt{G}_{ikj}$, which immediately follows from the definition of the Christoffel symbol. Note that Lembo's compatibility condition is an alternative statement for Eqn. (3.26).

3.2.2 Implication of compatibility condition for Laplace stretch and utility of QR factorization

The derived compatibility conditions for Laplace stretch restrict the dependence of its components on spatial variables X_I. In view of physical interpretations of these components, one can easily understand the dependence of elongation and shear, i.e., deformations in all six degrees of freedom on the spatial variables of a reference configuration and their interdependence to generate a valid finite deformation field.

As discussed before, coupling between certain shears and elongations plays a crucial role in deriving these conditions. If all the components of Laplace stretch are assumed to be independent, then one can show that the trivial solution $\mathrm{curl}(\boldsymbol{\mathcal{U}}) = \mathbf{0}$ is the only solution for the system of equations, which further implies that the rotation tensor has to be homogeneous. When all the components of Laplace stretch are considered to be dependent on each other, the necessary and sufficient compatibility condition is a vanishing of Riemann curvature tensor $\mathbb{R}$. Note that these conditions are the same as the ones obtained by equating the six independent elements of $\mathbb{R}$, expressed in terms of elements of $\mathbf{C}$, to zero. Although these conditions ensure that the reference configuration is a Euclidean space for which the right Cauchy-Green tensor acts as a metric, they lack any direct physical interpretation. Clearly, an inability to determine physical meaning for the components of $\mathbf{C}$ is responsible for this shortcoming. In fact, it is not possible to understand the interdependence between the components of $\mathbf{C}$ whenever a traditional polar decomposition of the deformation gradient is used and, hence, all the components are deemed to be coupled.

However, with the use of a $\mathbf{QR}$ decomposition, it is easy to understand that not all components of the Laplace stretch are coupled. Specifically, the only existing couplings are (i) a, $\tilde{\gamma}$ and $\tilde{\beta}$; (ii) b and $\tilde{\alpha}$. The elongation c does not depend on any of the components of Laplace stretch. The decoupling of certain components of Laplace stretch demands that five constituents from the Riemann curvature tensor, expressed in terms of elements of Laplace stretch and their derivatives, must be individually zero to ensure compatibility. Thus, the derived compatibility conditions are vastly different from the set of six equations arising from a vanishing of Riemann curvature tensor. Obviously, if these constituents are zero, the Riemann curvature tensor vanishes. *When these constituents are not individually zero, one can pick a suitable condition on some components of Laplace stretch such that the other terms are not coupled with the former ones and show that Riemann curvature tensor does not identically go to zero.* For example, one can pick $a, \tilde{\beta}, \tilde{\gamma}, c$ to be arbitrary constants and show that the equations arising from a vanishing of Riemann curvature tensor leave residues of the form $p(\tilde{\alpha} b_{,1} - b\tilde{\alpha}_{,1})^m + q(\tilde{\alpha}_{,2} - b_{,3})^n$ where p, q are arbitrary constants and m, n are integers. Thus the equations are not identically satisfied. Therefore, when some of the elements of Laplace stretch are not coupled, the derived equations (3.13)– (3.19) must be satisfied in order for the Riemann curvature tensor to vanish. Thus, they serve as the necessary and sufficient conditions for existence and uniqueness of a valid finite deformation field for a prescribed Cauchy-Green tensor or for a prescribed Laplace stretch.

3.3 Summary

In this chapter, the compatibility conditions for Laplace stretch arising from a Gram-Schmidt factorization of the deformation gradient has been obtained. We show that these conditions must be satisfied to ensure existence and uniqueness of a deformation map for prescribed $\mathbf{C}$ or $\boldsymbol{\mathcal{U}}$ when coupling between certain shears and elongations is in action. When off-diagonal terms of Laplace stretch $\boldsymbol{\mathcal{U}}$ are expressed in terms of magnitudes of shear α, β, γ, the compatibility conditions can be expressed as

$$\begin{aligned}
&\alpha_{,1} = 0 \\
&(a^2\beta\gamma)_{,1} - (a^2\beta)_{,2} - a\gamma a_{,3} + a^2\gamma_{,3} = 0 \\
&c_{,1} = 0 \\
&(b\alpha)_{,2} - b_{,3} = 0 \\
&c_{,2} = 0
\end{aligned} \tag{3.27}$$

Restriction on $\boldsymbol{\mathcal{U}}$ imposed by the integrability condition of a given deformation gradient has also been explored and shown to be the same as that for a prescribed Cauchy-Green tensor or a prescribed Laplace stretch. Coupling between certain components of Laplace stretch representing shear and elongation plays a crucial role in deriving these conditions. Finally, the implication of these compatibility conditions and the utility of Gram-Schmidt factorization of deformation gradient in this context is discussed.

4. CHARACTERIZATION OF GEOMETRICALLY NECESSARY DISLOCATIONS *

With the compatibility conditions for Laplace stretch derived, now we turn our focus to study the incompatibility of an intermediate configuration, pertinent to the plastic Laplace stretch $\boldsymbol{\mathcal{U}}^p$, and thereby, determine a measure for the geometrically necessary dislocations (GND) density. Characterization of the dislocations based on a Kröner–Lee decomposition of the deformation gradient has been the central aspect of many researchers' work in the past starting with Nye (1953) [71] when he established a relation between the local rotation of a triad located at each point of an unstrained lattice with local dislocations. It is important to note that unlike the total deformation gradient, its elastic and plastic parts are not, in general, compatible and hence the intermediate configuration cannot be considered as an Euclidean space, i.e., a material manifold with a metric-compatible connection and a vanishing torsion and curvature. This incompatibility of deformation is often associated with geometrically necessary dislocations—a lattice imperfection that causes plastic flow. Kondo (1955) [47] was the first among many researchers to identify this correspondence. Since then, many expressions for the dislocation density has been proposed in the literature (cf. Bilby *et al.* [7, 11], Eshelby (1956) [28], Fox (1966) [31], Davini and Parry [24, 25], Naghdi and Srinivasa (1994) [66], Le and Stumpf (1996) [51], Acharya and Bassani (2000) [1], Cermelli and Gurtin (2001) [15] and Gurtin (2006) [43], Gupta *et al.* (2007) [42], Clayton [18, 19] and Yavari and Goriely (2012) [96]). A detailed historical account of this field can be found in Acharya and Bassani (2000) [1] and Cermelli and Gurtin (2001) [15]. The dislocation theory is particularly useful when invoked to develop a strain-gradient and size-dependent theory of plasticity [30, 70, 38, 1, 50].

Like many other fundamental aspects of plasticity, a 'correct' definition of a dislocation density tensor has been a point of contention in the mechanics community for a long time. In fact, Acharya (2008) [3] pointed out that it is possible to have different physically-valid measures of dis-

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location density based on different physically reasonable criteria. Keeping this in mind, we make another attempt to obtain a measure for geometrically necessary dislocation (GND) density using a **QR** framework and gain some more physical insights in the process. As mentioned earlier, a significant advantage of using a **QR** decomposition over the traditional Kröner–Lee decomposition is that one can directly measure the components of the plastic Laplace stretch $\boldsymbol{\mathcal{U}}^p$ from experiments (see § 1.2.3) in an appropriate configuration $\tilde{\kappa}_p$. The primary motivation behind this work is to exploit this property of the plastic Laplace stretch to define a more physically intuitive GND density measure. Since Laplace stretch is capable of *completely* capturing the deformation of a representative cube in all six degrees of freedom, it is certainly reasonable to measure the GND density in an intermediate configuration $\tilde{\kappa}_p$ associated with $\boldsymbol{\mathcal{U}}^p$. Thus, the GND density measured in this configuration can be termed as the GND density due to plastic straining. Note that in the traditional measures of GND density using a Kröner–Lee decomposition, a different intermediate configuration κ_p has been used. The configurations κ_p and $\tilde{\kappa}_p$ are related through the plastic rotation field $\boldsymbol{\mathcal{R}}^p$, which need not be homogeneous. Therefore, when the GND density is measured in the configuration κ_p, the incompatibility of the plastic rotation field must be taken into account. Therefore, the total GND density measured in the configuration κ_p [1] can be additively decomposed into GND density due to plastic straining (measured in the configuration $\tilde{\kappa}_p$) and a term representing the incompatibility of plastic rotation field. The former is a more physically intuitive measure of GND density owing to the physical interpretations of the components of Laplace stretch.

4.1 Configurations relevant to plastic deformation

Before characterizing the Burgers vector and dislocation density tensor, we shall determine an appropriate configuration of the body where these two quantities will be measured. Note that unlike the total deformation, each of its components is incompatible. This leads to the fact that if the reference configuration κ_r is an Euclidean space, *only* the space κ_t is Euclidean. Therefore, it is possible to define different geometric dislocation tensors based on the incompatibility (torsion) of any of these non-Euclidean, intermediate configurations. Cermelli and Gurtin (2001) [15] noted

[1] This measure is same as the one derived in Cermelli and Gurtin (2001) [15].

that the abundance of geometric dislocation tensors in the literature is a problem. They proposed a criteria to rule out most of these definitions and then proposed a 'correct' definition of geometric dislocation tensor. However, Acharya (2008) [3] noted that it is not reasonable to stipulate such a criteria to rule out other definitions of geometric dislocation tensors. Indeed, all these definitions are valid and some of them have advantages over the others. Keeping this in mind, we choose a configuration where the body is subjected to a deformation only due to the movement of dislocations.

As mentioned earlier, in our framework, the rotation tensor $\boldsymbol{\mathcal{R}}$ plays an important role in coordinate transformation. Specifically, the inverse to this rotation tensor, i.e., $\boldsymbol{\mathcal{R}}^T$, rotates an Eulerian triad into the experimenter's frame of reference. If $\boldsymbol{e}_i$ and $\tilde{\boldsymbol{e}}_I$ denote Cartesian bases for the Eulerian and experimenter's frames of reference, respectively, then $\boldsymbol{e}_i = \boldsymbol{\mathcal{R}}\tilde{\boldsymbol{e}}_I$ [34]. In view of the physical meaning of the components of Laplace stretch, it is clearly understood that deformation of a body in all six degrees of freedom is completely described by the six components of $\boldsymbol{\mathcal{U}}$, as shown in §1.2.1. However, the components of $\boldsymbol{\mathcal{U}}$ are not all independent, and their dependence has an important consequence in strain compatibility.

Therefore, plastic deformation of the body is completely described by the inelastic part of Laplace stretch $\boldsymbol{\mathcal{U}}^p$ in an experimenter's frame of reference, per Eqn. (1.21). The configuration $\tilde{\kappa}_p$ of the body is particularly important because it is in this configuration where the deformation of the body is purely due to the plastic component of Laplace stretch $\boldsymbol{\mathcal{U}}^p$. Due to the "deformation gradient-like" nature of the Laplace stretch, the plastic deformation caused by a movement of dislocations is *fully* characterized in this configuration.

Therefore, we shall compute a Burgers vector and a dislocation density tensor in our physical (experimenter's) frame of reference. Once computed, these quantities can easily be pushed forward or pulled back into the intermediate configuration κ_p or any other configuration by suitable field transfer formulæ.

4.2 Geometric features of intermediate configuration and measure of incompatibility

Keeping with our communities' tradition of adopting a differential geometric approach to solve mechanics problems, we now explore some of the geometric features of space $\tilde{\kappa}_p$. This space is not compatible in the sense that the coefficient of a suitably defined metric-compatible connection in this space is not symmetric. It is instructive to discuss the different types of material manifolds that frequently appear in the literature. This classification of material manifolds is based on two geometric features, viz., curvature and torsion (the skew-symmetric part of the connection coefficient). A material manifold with a metric-compatible connection and a non-vanishing torsion and curvature is called a Riemann-Cartan manifold. If the torsion vanishes while maintaining a nonzero curvature tensor, then the manifold becomes Riemannian. On the other hand, a manifold with nonzero torsion and a vanishing curvature is known as a Weitzenböck manifold. The most commonly used manifold is an Euclidean (or flat) manifold where both the curvature tensor and torsion vanish [96].

Torsion of the connection coefficient is generally considered to be a measure of incompatibility in a deformation. In this section, we show that space $\tilde{\kappa}_p$ has a non-vanishing torsion expressed in terms of a spatial gradient of the plastic part of Laplace stretch $\boldsymbol{\mathcal{U}}^p$ with respect to referential coordinates. The dislocation density tensor that results in closure failure of a Burgers circuit involves a torsion of the space $\tilde{\kappa}_p$ in its definition, and it becomes zero when the torsion vanishes. This derivation closely follows Clayton's (2012) [18] approach for anholonomic deformation.

Let us choose a set of Cartesian basis vectors $\tilde{\boldsymbol{e}}_a$ in the configuration $\tilde{\kappa}_p$, i.e., the bases of an experimenter's frame. In view of Eqn. (1.29), the plastic part of Laplace stretch can be written in this coordinate frame as

$$\boldsymbol{\mathcal{U}}^p = \mathcal{U}^{pa}_{\ A}(\boldsymbol{X}, t)\ \tilde{\boldsymbol{e}}_a \otimes \boldsymbol{E}^A(\boldsymbol{X}) \tag{4.1}$$

where $\boldsymbol{E}^A$ denotes a Cartesian basis for the reference configuration κ_r. Convected basis vectors and their reciprocals in $\tilde{\kappa}_p$ are defined as

$$\boldsymbol{E}'^{A}(\tilde{\boldsymbol{x}}^p, t) = \mathcal{U}^{p-1A}_{\ \ a}(\tilde{\boldsymbol{x}}^p, t)\, \tilde{\boldsymbol{e}}^a \quad \text{and} \quad \boldsymbol{E}'_A(\boldsymbol{X}, t) = \mathcal{U}^{pa}_{A}(\boldsymbol{X}, t)\, \tilde{\boldsymbol{e}}_a. \tag{4.2}$$

We are now able to compute the metric of space $\tilde{\kappa}_p$ by using the convected basis vectors defined above, specifically

$$\boldsymbol{E}'_A \cdot \boldsymbol{E}'_B = \mathcal{U}^{pa}_{A}\, \mathcal{U}^{pa}_{B} := C^p_{AB}. \tag{4.3}$$

Equation (4.3) uses the fact that $\tilde{\boldsymbol{e}}_a \cdot \tilde{\boldsymbol{e}}_b = \delta_{ab}$ for Cartesian basis $\tilde{\boldsymbol{e}}_a$. Note that the Cauchy-Green tensor $\mathbf{C}$ can be written as

$$\mathbf{C} = \boldsymbol{\mathcal{U}}^{pT}\mathbf{C}^e\boldsymbol{\mathcal{U}}^p \tag{4.4}$$

where an elastic Cauchy-Green tensor is given as $\mathbf{C}^e = \boldsymbol{\mathcal{U}}^{eT}\boldsymbol{\mathcal{U}}^e$. During an elastic unloading, $\boldsymbol{\mathcal{U}}^e \rightarrow \mathbf{I}$, thus, $\mathbf{C} \rightarrow \mathbf{C}^p = \boldsymbol{\mathcal{U}}^{pT}\boldsymbol{\mathcal{U}}^p$.

We now define a suitable linear connection associated with the metric $\mathbf{C}^p$ and its associated covariant derivative. For a general space, the covariant derivative ∇ is defined in terms of its action on a vector field $\boldsymbol{W}$ with respect to another vector field $\boldsymbol{V}$. In reference coordinates, i.e., in the configuration κ_r, the covariant derivative of $\boldsymbol{W}$ with respect to $\boldsymbol{V}$ is given as

$$\nabla_{\boldsymbol{V}}\boldsymbol{W} = \left(V^B\, \partial_B W^A + \Gamma^A_{BC} W^C V^B\right) \boldsymbol{E_A} \tag{4.5}$$

where $\boldsymbol{\Gamma}$ is the connection coefficient of the space κ_r and $\boldsymbol{E}_A = \partial_A \boldsymbol{X}$ is the basis vector of that space. It can be shown that the connection coefficient follows the identity

$$\Gamma^A_{BC}\partial_A = \nabla_{\partial_B}\partial_C. \tag{4.6}$$

Therefore, to determine the connection coefficient, we need to find a gradient of the convected basis vector with respect to the referential coordinates, in particular

$$\partial_B \boldsymbol{E'}_A = \partial_B \mathcal{U}^{pa}_{\ A} \, \tilde{\boldsymbol{e}}_a = \mathcal{U}^{p-1}{}^D_{\ a} \partial_B \mathcal{U}^{pa}_{\ A} \, \boldsymbol{E'}_D. \tag{4.7}$$

Let $\overset{\mathbf{C}^p}{\boldsymbol{\Gamma}}$ represent the connection coefficient associated with metric $\mathbf{C}^p$. The last part of Eqn. (4.7) is obtained by using the interrelation (4.2) between basis vectors of $\tilde{\kappa}_p$ and its convected basis vectors. Using the property of connection coefficient $\partial_B \boldsymbol{E'}_A = \overset{\mathbf{C}^p}{\Gamma} \boldsymbol{E}'^D$, we define

$$\overset{\mathbf{C}^p}{\Gamma}{}^D_{BA} = \mathcal{U}^{p-1}{}^D_{\ a} \, \partial_B \mathcal{U}^{pa}_{\ A}. \tag{4.8}$$

This connection coefficient is clearly not symmetric because $\boldsymbol{\mathcal{U}}^p$ is an upper-triangular matrix. The torsion of this connection, i.e., the skew-symmetric part of its connection coefficient, is therefore defined as

$$T^D_{AB} = \frac{1}{2}\left(\overset{\mathbf{C}^p}{\Gamma}{}^D_{BA} - \overset{\mathbf{C}^p}{\Gamma}{}^D_{AB}\right) = \frac{1}{2}\mathcal{U}^{p-1}{}^D_{\ a} \left(\partial_B \mathcal{U}^{pa}_{\ A} - \partial_A \mathcal{U}^{pa}_{\ B}\right). \tag{4.9}$$

A non-vanishing torsion of a connection is a natural measure of incompatibility. Clearly, a non-vanishing torsion makes the associated space $\tilde{\kappa}_p$ non-Euclidean and, therefore, the geometry is definitely non-Riemannian. Nevertheless, it is still possible to construct a local Cartesian coordinate system in this space.

In view of Eqn. (4.9), one can conclude that $\mathrm{Curl}(\boldsymbol{\mathcal{U}}^p)$ provides a measure for the local incompatibility of deformation for a body in configuration $\tilde{\kappa}_p$. This is due to the fact that the plastic part of Laplace stretch is always nonzero. Therefore, for a connection to be symmetric, i.e., for the configuration $\tilde{\kappa}_p$ to be compatible, one must have $\mathrm{Curl}(\boldsymbol{\mathcal{U}}^p) = \mathbf{0}$. In §4.3, we show that the dislocation density tensor vanishes only when $\mathbf{T}$ is zero, i.e., the deformation $\boldsymbol{\mathcal{U}}^p$ is compatible.

Herein the incompatibility (torsion) is determined in the context of inelasticity. In the later section, it will be shown that the derived measure of incompatibility is directly related to what is traditionally called the *geometric dislocation tensor*. However, the derived measure of incompatibility is not limited to elasto-plasticity and has a much wider range of application. In fact, one can derive similar measures of incompatibility whenever the deformation gradient is multiplicatively decomposed into two or more kinematic variables. Such decompositions are abundant in the literature [58]. For instance, Vujosevic and Lubarda (2002) [94] decomposed the total deformation gradient into isothermal deformation gradient $\mathbf{F}_e$ and thermal deformation gradient $\mathbf{F}_\theta$ in the context of thermoelasticity; Rodriguez *et. al.* (1994) [81] decomposed $\mathbf{F}$ into an elastic component $\mathbf{F}_e$ and a growth component $\mathbf{F}_g$ while modeling the growth in soft elastic tissues. In all these cases, the intermediate configuration is incompatible and hence, the measure of incompatibility can be computed following the procedure described in § 4.2. Needless to say, the measures of incompatibility in these cases will bear different physical interpretations.

4.3 Burgers vector and dislocation density tensor

4.3.1 Closure failure of a Burgers circuit

Consider a curve ζ in configuration $\tilde{\kappa}_p$ that was initially a closed loop before deformation in the reference configuration κ_r. The path integral of a spatial variable along a curve physically represents the distance between its two ends. Therefore, when calculated in an Euclidean space, say the reference configuration κ_r or the current configuration κ_t, the path integral of a spatial variable along the closed loop ζ will be zero. However, this is not the case when the path integral is calculated in an intermediate configuration. In fact, in this configuration, the path integral represents the closure failure of the initially closed loop ζ. Therefore, if ζ is considered as a Burgers circuit, this path integral, calculated in an intermediate configuration $\tilde{\kappa}_p$, represents the Burgers vector, as understood in the materials science literature. Hence, the cumulative Burgers vector of all dislocations inside the surface enclosed by ζ is given as

$$\tilde{\boldsymbol{b}} = \oint_\zeta \mathrm{d}\tilde{\boldsymbol{x}}^p = \oint_\zeta \boldsymbol{\mathcal{U}}^p \,\mathrm{d}\boldsymbol{X}. \tag{4.10}$$

Let $\tilde{\boldsymbol{n}}$ be the unit normal to surface $\tilde{S}$ whose boundary is curve ζ, and let S be the surface corresponding to $\tilde{S}$ in the undeformed configuration. When transferred into the reference configuration κ_r, $\boldsymbol{n}_R$ denotes the unit normal to the surface S. Now applying Stokes' theorem to Eqn. (4.10), we get

$$\tilde{\boldsymbol{b}} = \int_S (\mathrm{Curl}(\boldsymbol{\mathcal{U}}^p))^T \boldsymbol{n}_R \,\mathrm{d}A_R. \tag{4.11}$$

Here 'Curl' represents the curl operator taken with respect to reference coordinates. Upon transforming the referential vector area $\boldsymbol{n}_R \,\mathrm{d}A_R$ to configuration $\tilde{\kappa}_p$ by $\boldsymbol{n}_R \,\mathrm{d}A_R = J_p \,\boldsymbol{\mathcal{U}}^{p-T}\, \tilde{\boldsymbol{n}} \,\mathrm{d}\tilde{a}$ with $J_p = \det(\boldsymbol{\mathcal{U}}^p) = a^p b^p c^p$, we obtain

$$\tilde{\boldsymbol{b}} = \int_{\tilde{S}} \frac{1}{J_p} (\mathrm{Curl}(\boldsymbol{\mathcal{U}}^p))^T \boldsymbol{\mathcal{U}}^{pT}\, \tilde{\boldsymbol{n}} \,\mathrm{d}\tilde{a}. \tag{4.12}$$

Equation (4.12) represents the cumulative Burgers vector of all dislocations threading an arbitrary surface $\tilde{S}$ in configuration $\tilde{\kappa}_p$. If $\tilde{\mathbf{G}}_p$ denotes the geometric dislocation tensor, then $\tilde{\mathbf{G}}_p^T \tilde{\boldsymbol{n}}$ represents the local Burgers vector, given as $\dfrac{1}{J_p}(\mathrm{Curl}(\boldsymbol{\mathcal{U}}^p))^T \boldsymbol{\mathcal{U}}^{pT}\, \tilde{\boldsymbol{n}} \,\mathrm{d}\tilde{a}$, for a surface $\tilde{S}$ in $\tilde{\kappa}_p$. Thus, a dislocation density tensor in configuration $\tilde{\kappa}_p$ obtains the form

$$\tilde{\mathbf{G}}_p = \frac{1}{J_p} \boldsymbol{\mathcal{U}}^p \,\mathrm{Curl}(\boldsymbol{\mathcal{U}}^p). \tag{4.13}$$

Physically, $\tilde{\mathbf{G}}_p$ provides a measure of the local Burgers vector per unit area of a body in configuration $\tilde{\kappa}_p$. Note that $\tilde{\mathbf{G}}_p^T \tilde{\boldsymbol{n}}$ represents the local Burgers vector measured *per unit area*. It is also common to assign the term *dislocation density* to the total length of dislocation lines *per unit volume* of the material.

In terms of the components of $\boldsymbol{\mathcal{U}}^p$, the components of this dislocation density tensor $\tilde{\mathbf{G}}_p$ can be written as

$$
\begin{aligned}
\tilde{G}_{p11} &= \frac{1}{b^p c^p}\left[\left(a^p\beta^p\right)_{,2} - \left(a^p\gamma^p\right)_{,3}\right] + \frac{\gamma^p}{b^p c^p}\left[a^p_{,3} - \left(a^p\beta^p\right)_{,1}\right] + \frac{\beta^p}{b^p c^p}\left[\left(a^p\gamma^p\right)_{,1} - a^p_{,2}\right]\\
\tilde{G}_{p12} &= \frac{1}{b^p c^p}\left[\left(b^p\alpha^p\right)_{,2} - b^p_{,3}\right] - \frac{\gamma^p}{b^p c^p}\left(b^p\alpha^p\right)_{,1} + \frac{\beta^p}{b^p c^p} b^p_{,1}\\
\tilde{G}_{p13} &= \frac{1}{b^p c^p} c^p_{,2} - \frac{\gamma^p}{b^p c^p} c^p_{,1}\\
\tilde{G}_{p21} &= \frac{1}{a^p c^p}\left[a^p_{,3} - \left(a^p\beta^p\right)_{,1}\right] + \frac{\alpha^p}{a^p c^p}\left[\left(a^p\gamma^p\right)_{,1} - a^p_{,2}\right]\\
\tilde{G}_{p22} &= -\frac{1}{a^p c^p}\left(b^p\alpha^p\right)_{,1} + \frac{\alpha^p}{a^p c^p} b^p_{,1}\\
\tilde{G}_{p23} &= -\frac{1}{a^p c^p} c^p_{,1}\\
\tilde{G}_{p31} &= \frac{1}{a^p b^p}\left[\left(a^p\gamma^p\right)_{,1} - a^p_{,2}\right]\\
\tilde{G}_{p32} &= \frac{1}{a^p b^p} b^p_{,1}\\
\tilde{G}^{p33} &= 0
\end{aligned}
\tag{4.14}
$$

Here '$_{,i}$' represents the derivative of a quantity with respect to referential coordinate X_i. This obtained dislocation density tensor clearly remains invariant under a superposed compatible elastic deformation.

One can express the derived dislocation density tensor $\tilde{\mathbf{G}}_p$ in terms of the torsion $\mathbf{T}$ of space $\tilde{\kappa}_p$ and its plastic Laplace stretch $\boldsymbol{\mathcal{U}}^p$. A deformation in $\tilde{\kappa}_p$ is compatible whenever $\mathbf{T}$ is zero. Because $\boldsymbol{\mathcal{U}}^p$ is always nonzero and invertible, a vanishing of $\mathbf{T}$ implies that the Curl($\boldsymbol{\mathcal{U}}^p$) is zero. By similar argument, one can easily realize that the dislocation density tensor vanishes only when the Curl($\boldsymbol{\mathcal{U}}^p$) vanishes. Thus, *the dislocation density tensor becomes zero if and only if the torsion* $\mathbf{T}$ *vanishes and the plastic deformation field* $\boldsymbol{\mathcal{U}}^p$ *is compatible.*

In view of the physical meaning of $\boldsymbol{\mathcal{U}}^p$, one can realize that the geometric dislocation tensor $\tilde{\mathbf{G}}_p$ measures the incompatibility of the plastic deformation field due to the distortion (straining) of the crystal lattice caused by the movement of dislocations. In that sense, $\tilde{\mathbf{G}}_p$ is equivalent to the traditional definition of dislocation tensor, viz., $\mathbf{F}^p\mathrm{Curl}(\mathbf{F}^p)$ [82, 15], derived using a Kröner–Lee decomposition of the deformation gradient.

It is important to note that the scalar quantity $\rho = \boldsymbol{l} \cdot \tilde{\mathrm{G}}\boldsymbol{b}$ is often referred to as dislocation density in the literature [15, 50]. Herein vectors $\boldsymbol{l}$ and $\boldsymbol{b}$ denote the line direction and Burgers vector of a dislocation per unit area. Consequently, ρ is just another measure for $\tilde{\mathrm{G}}$, and one can easily understand which measure is in use from the context.

4.3.2 Burgers vector and dislocation density tensor in terms of $\boldsymbol{\mathcal{U}}^e$

Because the elastic part of Laplace stretch $\boldsymbol{\mathcal{U}}^e$ can be expressed in terms of the total Laplace stretch $\boldsymbol{\mathcal{U}}$ and its plastic part $\boldsymbol{\mathcal{U}}^p$ [36], one can also determine the Burgers vector and dislocation density tensor in terms of $\boldsymbol{\mathcal{U}}^e$, starting from a deformation analysis done in configuration κ_t. Because Laplace stretch is capable of describing deformation in all six degrees of freedom, one can define a deformed configuration $\tilde{\kappa}_t$ for the experimenter's frame of reference such that if $\mathrm{d}\tilde{\boldsymbol{x}}$ denotes an infinitesimal fiber of the body in this configuration, then

$$\mathrm{d}\tilde{\boldsymbol{x}} = \boldsymbol{\mathcal{U}}\,\mathrm{d}\boldsymbol{X} = \boldsymbol{\mathcal{R}}^T\,\mathrm{d}\boldsymbol{x}. \tag{4.15}$$

The inverse elastic Laplace stretch $\boldsymbol{\mathcal{U}}^{e-1}$ maps the infinitesimal fiber $\mathrm{d}\tilde{\boldsymbol{x}}$ in $\tilde{\kappa}_t$ to $\tilde{\kappa}_p$ where the Burgers vector per unit area and dislocation density tensor are measured. These configurations and associated maps are shown in Fig. 4.1.

An infinitesimal fiber $\mathrm{d}\tilde{\boldsymbol{x}}_p$ in configuration $\tilde{\kappa}_p$, where a deformation of the body is caused solely by the movement of dislocations, is related to its corresponding fiber in the current configuration κ_t through

$$\mathrm{d}\tilde{\boldsymbol{x}}_p = \boldsymbol{\mathcal{U}}^{e-1}\mathrm{d}\tilde{\boldsymbol{x}} = \boldsymbol{\mathcal{U}}^{e-1}\boldsymbol{\mathcal{R}}^T\mathrm{d}\boldsymbol{x}. \tag{4.16}$$

Using a similar argument as above, we find that

$$\tilde{\boldsymbol{b}}_e = \oint_\zeta \mathrm{d}\tilde{\boldsymbol{x}}^p = \oint_{\tilde{S}} \frac{1}{\det(\boldsymbol{\mathcal{U}}^{e-1}\boldsymbol{\mathcal{R}}^T)}(\mathrm{curl}(\boldsymbol{\mathcal{U}}^{e-1}\boldsymbol{\mathcal{R}}^T))^T.(\boldsymbol{\mathcal{R}}\boldsymbol{\mathcal{U}}^{e-T})\,\tilde{\boldsymbol{n}}\,\mathrm{d}\tilde{a} \tag{4.17}$$

where 'curl' denotes the curl operator taken with respect to spatial coordinates, and where $\tilde{\boldsymbol{b}}_e$ denotes the cumulative Burgers vector per unit area represented in terms of $\boldsymbol{\mathcal{U}}^e$. If $\tilde{\mathrm{G}}_e$ denotes the

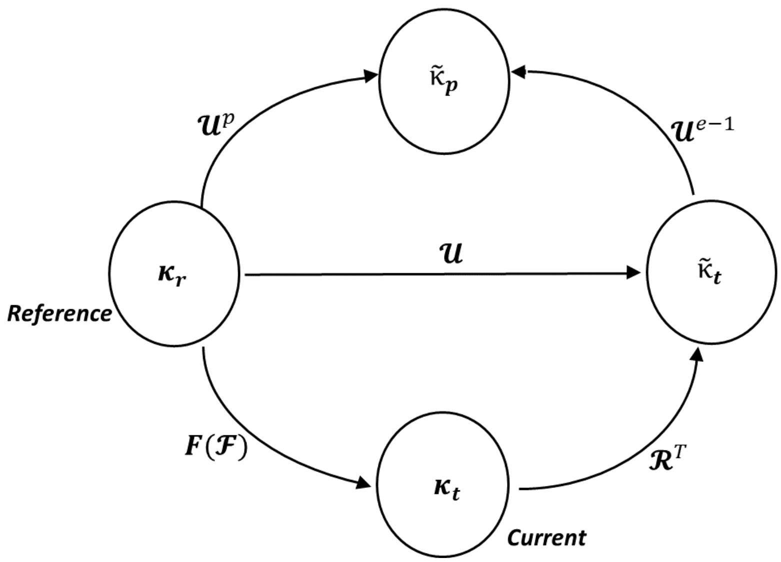

Figure 4.1: Deformation maps showing a transformation of tangent vectors between different configurations of the body.

dislocation density tensor, represented in terms of $\mathcal{U}^e$, then

$$\tilde{\mathrm{G}}_e = \frac{1}{\det(\mathcal{U}^{e-1}\mathcal{R}^T)}\mathcal{U}^{e-1}\mathcal{R}^T\mathrm{curl}(\mathcal{U}^{e-1}\mathcal{R}^T) = \det(\mathcal{U}^e)\mathcal{U}^{e-1}\mathcal{R}^T\mathrm{curl}(\mathcal{U}^{e-1}\mathcal{R}^T). \qquad (4.18)$$

The last part of Eqn. (4.18) is obtained by employing the fact that det($\mathcal{R}$)=1. Therefore, the geometrically necessary dislocation density tensor, expressed in the experimenter's frame of reference, is defined as

$$\tilde{\mathrm{G}} = \frac{1}{J_p}\mathcal{U}^p\ \mathrm{Curl}(\mathcal{U}^p) = \det(\mathcal{U}^e)\ \mathcal{U}^{e-1}\ \mathcal{R}^T\ \mathrm{curl}(\mathcal{U}^{e-1}\mathcal{R}^T) \qquad (4.19)$$

or $\tilde{\mathrm{G}} = \tilde{\mathrm{G}}_e = \tilde{\mathrm{G}}_p$. Note that $\tilde{\mathrm{G}}$ denotes the geometric dislocation tensor *due to 'permanent' distortion or straining of the crystal lattice*.

In the literature, $\tilde{\mathrm{G}}$ is sometimes referred to as Burgers tensor or the geometric dislocation tensor. Although the dislocation density tensors $\tilde{\mathrm{G}}$, $\tilde{\mathrm{G}}_e$ and $\tilde{\mathrm{G}}_p$ obtained herein are defined in terms of upper-triangular stretch tensors, none of them are upper-triangular. Because the dislocation density tensor transforms as a second-order tensor, when pushed forward into the intermediate configuration κ_p, it takes the form:

$$\mathbf{G} = \boldsymbol{\mathcal{R}}^p\, \tilde{\mathbf{G}}\, \boldsymbol{\mathcal{R}}^{pT} \tag{4.20}$$

where $\mathbf{G}$ denotes the dislocation density tensor in the intermediate configuration κ_p, which arises in a traditional Kröner–Lee decomposition. Similarly, the derived dislocation density tensor can be pulled back or pushed forward to any other configurations by suitable field transfer formulæ.

Note that the definition of the dislocation density tensor presented here is significantly different from the ones found in literature; most of which involve $\mathbf{F}^{e-1}$ or $\mathbf{F}^p$ and, in some cases, the rotation tensor $\mathbf{R}$. This is due to the fact that in the literature a polar decomposition is applied to the elastic and plastic parts of the deformation gradient arising from its Kröner-Lee decomposition. However, in our definition, a $\mathbf{QR}$ decomposition is applied first to the deformation gradient with the resulting Laplace stretch being decomposed into elastic and plastic components, which is assured because of the closure property of a group. The derived expression for the dislocation density tensor is also consistent with our definition of a plastic velocity gradient $\boldsymbol{\mathcal{L}}^p$, defined as $\boldsymbol{\mathcal{L}}^p := \dot{\boldsymbol{\mathcal{U}}}^p \boldsymbol{\mathcal{U}}^{p-1}$ instead of $\dot{\mathbf{F}}^p \mathbf{F}^{p-1}$ [36].

4.3.3 Incompatibility of plastic rotation field

Although the geometric dislocation tensor $\tilde{\mathbf{G}}_p$ (or $\tilde{\mathbf{G}}$) measures the incompatibility of the deformation field that causes plastic straining to a crystal lattice, it is unable to capture the incompatibility of a plastic rotation field. This, however, should not be seen as a drawback of the theory. Rather selecting the configuration $\tilde{\kappa}_p$ for measuring the dislocation tensor is intentional in order to gain more insight.

As mentioned earlier the rotation tensor $\boldsymbol{\mathcal{R}}$ acts as a coordinate transformation matrix. Specifically, $\boldsymbol{\mathcal{R}}$ rotates an Eulerian triad into the set of basis of our physical frame of reference, $\tilde{e}_I$. In the absence of an elastic rotation field, the rotation tensor $\boldsymbol{\mathcal{R}}$ becomes $\boldsymbol{\mathcal{R}}^p$. Therefore, physically $\boldsymbol{\mathcal{R}}^p$ denotes the local rotation of the crystal lattice vectors in the absence of elastic deformation. In general, this rotation field is not homogeneous and therefore, the spatial variation of the rotation $\boldsymbol{\mathcal{R}}^p$ measures the incompatibility of the plastic rotation field. Let us define the geometric dislocation tensor due to a plastic rotation field, $\tilde{\mathbf{G}}_r$ in a way that it has the same structure as $\tilde{\mathbf{G}}_p$. Thus, $\tilde{\mathbf{G}}_r$ is defined as

$$\tilde{\mathbf{G}}_r = \boldsymbol{\mathcal{R}}^p \,\mathrm{Curl}(\boldsymbol{\mathcal{R}}^p). \tag{4.21}$$

This definition is consistent with Nye's [71] dislocation tensor. Nye (1953) [71] assumed that the crystal lattice is unstrained, but the local rotation between the director vectors varies in spatial direction. Therefore, this assumption is perfectly in sync in view of the physical meaning of $\boldsymbol{\mathcal{R}}^p$. The spatial variation of $\boldsymbol{\mathcal{R}}^p$ effectively determines the spatial variation of the coordinate frame (lattice director vectors) in which the components of plastic Laplace stretch $\boldsymbol{\mathcal{U}}^p$ is measured. Thus, $\tilde{\mathbf{G}}_r$ is nothing but an analogue of Nye's dislocation tensor in our framework.

In this definition, the space $\tilde{\kappa}_p$ is considered as a reference. The primary issue with defining a physically meaningful dislocation tensor is that it should be measured with respect to the undeformed configuration κ_r or the deformed configuration κ_t. In case of $\tilde{\mathbf{G}}_r$, however, it is impossible to measure it with respect to κ_r without bypassing the plastic Laplace stretch $\boldsymbol{\mathcal{U}}^p$. Nevertheless, one can define a physically meaningful dislocation tensor due to plastic rotation by computing the incompatibility in the space κ_p with κ_r as a reference and show that it is equivalent to $\tilde{\mathbf{G}}_r$.

If one chooses to measure the dislocation tensor in the configuration κ_p with the undeformed configuration κ_r considered as a reference, then following the procedure in § 4.3.1, it can be easily shown that the geometric dislocation tensor in this configuration takes on the form

$$\mathbf{G}_{\kappa_p} = \boldsymbol{\mathcal{R}}^p\boldsymbol{\mathcal{U}}^p \,\mathrm{Curl}(\boldsymbol{\mathcal{R}}^p\boldsymbol{\mathcal{U}}^p). \tag{4.22}$$

Writing the equation in indicial notation with respect to a Cartesian coordinate system E_i and doing some algebraic manipulation, we obtain

$$G_{\kappa_p}{}^{ij} = \epsilon^{ABM}\, \mathcal{R}^{pi}_{s}\, \mathcal{U}^{ps}_{M}\, \mathcal{R}^{pj}_{q,A}\, \mathcal{U}^{pq}_{B} \;+\; \mathcal{R}^{pi}_{r}\, \tilde{G}_p{}^{rq}\, \mathcal{R}^{pj}_{q}. \tag{4.23}$$

Here 'p' is not a dummy index; it represents plastic component. Let us define the geometric dislocation tensor $\mathbf{G}_r$ measured in the configuration κ_p such that ${\mathbf{G}_r}^{ij} := \epsilon^{ABM}\, \mathcal{R}^{pi}_{s}\, \mathcal{U}^{ps}_{M}\, \mathcal{R}^{pj}_{q,A}\, \mathcal{U}^{pq}_{B}$. Therefore, substituting in Eqn. (4.23), we obtain

$$\mathbf{G}_{\kappa_p} = \mathbf{G}_r \;+\; \boldsymbol{\mathcal{R}}^p\, \tilde{\mathbf{G}}_p\, \boldsymbol{\mathcal{R}}^{pT}. \tag{4.24}$$

When *only* a rotation field is applied to the body, i.e., $\boldsymbol{\mathcal{U}}^p \;\to\; \mathbf{I}$, then $\mathbf{G}_r$ becomes equal to $\tilde{\mathbf{G}}_r$. This is also evident because in this case, the reference configuration κ_r and the intermediate configuration $\tilde{\kappa}_p$ coincides. Since the dislocation tensor due to straining of the crystal lattice is zero in this case, the total dislocation tensor measured in κ_p, $\mathbf{G}_{\kappa_p}$ also reduces to $\tilde{\mathbf{G}}_r$. Similarly, when the rotation field is homogeneous, then $\mathbf{G}_r \to \mathbf{0}$ and $\mathbf{G}_{\kappa_p} \to \boldsymbol{\mathcal{R}}^p\tilde{\mathbf{G}}_p\boldsymbol{\mathcal{R}}^{pT}$. In view of Eqn. (4.20), it is easy to understand that the reduced dislocation tensor $\mathbf{G}_{\kappa_p}$ under the condition of a homogeneous rotation field is the dislocation tensor $\tilde{\mathbf{G}}_p$ pushed forward to the configuration κ_p. Note that only in the presence of $\tilde{\mathbf{G}}_r$, the coordinate frame in which **QR** decomposition is performed, varies spatially and thus, in that case, the measurement of the components of $\boldsymbol{\mathcal{U}}^p$ becomes ambiguous.

4.4 Summary

In this chapter, the geometrically necessary dislocation density tensor and Burgers vector are studied using an elastic-plastic decomposition of Laplace stretch $\boldsymbol{\mathcal{U}} = \boldsymbol{\mathcal{U}}^e\boldsymbol{\mathcal{U}}^p$ arising from a Gram-Schmidt factorization of the deformation gradient $\boldsymbol{\mathcal{F}} = \boldsymbol{\mathcal{R}}\boldsymbol{\mathcal{U}}$. The derived dislocation density tensor has the form of $\tilde{\mathbf{G}} = J_p^{-1}\, \boldsymbol{\mathcal{U}}^p\, \mathrm{Curl}(\boldsymbol{\mathcal{U}}^p)$. The term $\mathrm{Curl}(\boldsymbol{\mathcal{U}}^p)$ is related the to torsion of configuration $\tilde{\kappa_p}$, where deformation of the body is caused solely by the movement of dislocations. Thus, it provides a measure of incompatibility of plastic deformation in that configuration. This incompatibility prevents space $\tilde{\kappa}_p$ from being Euclidean, and vanishes only when $\tilde{\mathbf{G}}$ becomes zero. The dislocation density tensor has also been derived in terms of the elastic components of Laplace stretch and the associated rotation tensor. When the dislocation tensor is measured in the configuration κ_p, it can be decomposed into two physically meaningful components: dislocation tensor due to incompatibility of plastic rotation, and dislocation tensor due to plastic “straining".

5. CONSTITUTIVE MODELING USING CONJUGATE STRESS/STRAIN BASE PAIRS *

In this chapter, we develop a constitutive model for elastic-plastic materials using the scalar, conjugate, stress/strain, base pairs associated with **QR** kinematics. As mentioned earlier, this model has certain advantages over the traditionally used tensor invariants. Specifically, from an experimenter's standpoint, the issue with parametrization of material models owing to the co-variance of the tensor invariants is resolved. Moreover, this model is computationally simple as one does not have to perform eigenvalue analysis to obtain the tensor invariants. Development of constitutive models for elastic-plastic materials has been the central theme of many researchers' works (see Green and Naghdi (1964, 1971) [40, 41], Rice (1971) [79], Naghdi and Trapp (1975) [68], Nemat-Nasser (1982) [69], Lubliner (1984) [59], Simo and Ortiz (1985) [84], Dafalias(1987) [23], Eve *et al.* (1990) [29], Lubarda(1991) [57] and Miehe (1998) [65] for a partial list of references) as well as a longstanding point of contention [14, 67] in the mechanics community for at least the past century. The property that distinguishes an elastic material from an inelastic one is the ability of the latter to dissipate energy, i.e., convert mechanical work done into heat. Therefore, thermodynamics play a crucial role in the development of constitutive models for inelastic materials. A standard thermodynamical approach based upon the Clausius-Duhem inequality provides rather weak guidance for the development of evolution equations for plastic strain and its rate. Therefore, several additional principles, e.g., maximum plastic work, maximum plastic dissipation, and Drucker's stability postulate have been used in the literature [68, 59, 85].

In this work, we adopt the techniques of Rajagopal and Srinivasa (1998) [74, 75] where it is considered that a body may possess multiple natural configurations. The response of a body is, thus, described as a family of elastic responses from these natural configurations. It is evident from our discussion in § 1.2.3 that the intermediate configuration $\tilde{\kappa}_p$ acts as a natural configuration in this framework. In this theory, two constitutive assumptions are made: one for the Helmholtz potential

*"A constitutive model for elastic-plastic material using scalar conjugate stress/strain base pairs" by Paul, S., Freed, A. D., 2021. (under review)

function ψ, and another for the dissipation function ξ. The evolution equation for the plastic strain rate is obtained by applying the principle of maximum rate of entropy production [78]. Rajagopal and Srinivasa (2004) showed that although this principle is not followed by all materials, because it is not as fundamental as the second law of thermodynamics, it can be useful for a wide class of materials. This principle is also in sync with Onsager's principle of minimum rate of entropy production (1931) [73] and is a generalized version of Ziegler's normality rule (1963) [97]. Here we assume that the material exhibits an isotropic response throughout the deformation process.

5.1 Constitutive modeling

In order to specify an elastic response measured from a current natural configuration and its evolution equation, we need to consider three thermodynamical quantities: (*i*) the stored energy characterized by a Helmholtz potential, (*ii*) the work done on an internal mass element, and (*iii*) a rate of dissipation function that measures the amount of mechanical work being converted into heat. The balance of energy equation stipulates that the rate of dissipation is obtained as the difference between a rate of change in the external work done and a rate of change in the Helmholtz potential. The rate of work done (or power) can easily be computed from the corresponding stress and strain attributes as

$$\dot{W} = \pi\dot{\delta} + \sum_{i=1}^{3}\sigma_i\dot{\varepsilon}_i + \sum_{i=1}^{3}\tau_i\dot{\gamma}_i \tag{5.1}$$

where δ, ε_i and γ_i are the dilatational, squeeze and shear strain attributes whereas π, σ_i and τ_i represent their corresponding thermodynamic conjugates (stress attributes) respectively. The list of variables $l_{\mathcal{U}}$, $l_{\dot{\mathcal{U}}}$, $l_{\mathcal{U}^p}$, $l_{\dot{\mathcal{U}}^p}$ defined in § 1.2.3 will play a vital role in the subsequent analysis.

5.1.1 Elastic domain and the Helmholtz potential function

We assume that for each natural configuration $\tilde{\kappa}_p$ there also exists a non-empty elastic domain. If the Green strain $\mathbf{E} = 1/2(\mathbf{C} - \mathbf{I})$ lies within the elastic domain, the plastic velocity gradient must be zero, because $\boldsymbol{\mathcal{U}}^p$ essentially represents a microstructural change, i.e., evolution of the natural configuration $\tilde{\kappa}_p$. Therefore, for a fixed natural configuration $\tilde{\kappa}_p$, the elastic domain can be represented by

$$\boldsymbol{\mathcal{L}}^p = \mathbf{0}. \tag{5.2}$$

In view of the bijective map in Eqn. (1.40), the elastic domain for a fixed natural configuration can also be characterized as

$$l_{\dot{\mathcal{U}}^p} = \mathbf{0} \implies \dot{\delta}^p = \dot{\varepsilon}_1^p = \dot{\varepsilon}_2^p = \dot{\varepsilon}_3 = \dot{\gamma}_1^p = \dot{\gamma}_2^p = \dot{\gamma}_3^p = 0. \tag{5.3}$$

Note that the tensor equation (5.2) reduces to a set of six scalar equations when represented in terms of these plastic strain rates.

Now, for each fixed natural configuration $\tilde{\kappa}_p$, we assume that the elastic response is characterized by a Helmholtz potential function ψ, which depends upon the deformation of a body measured from its reference configuration κ_r and its natural configuration $\tilde{\kappa}_p$, i.e., the Laplace stretch $\boldsymbol{\mathcal{U}}$ and its plastic component $\boldsymbol{\mathcal{U}}^p$. Therefore, the Helmholtz potential has the form

$$\psi = \overline{\psi}\,(\boldsymbol{\mathcal{U}}, \boldsymbol{\mathcal{U}}^p). \tag{5.4}$$

In view of § 1.2.2, the tensor arguments of ψ in Eqn. (5.4) can be replaced by the lists of scalar strain bases $l_{\mathcal{U}}$ and $l_{\mathcal{U}^p}$. Thus, the Helmholtz potential takes on a functional form of

$$\psi = \hat{\psi}\,(l_{\mathcal{U}}, l_{\mathcal{U}^p}) = \hat{\psi}\,(\delta, \varepsilon_1, \varepsilon_2, \varepsilon_3, \gamma_1, \gamma_2, \gamma_3, \delta^p, \varepsilon_1^p, \varepsilon_2^p, \varepsilon_3^p, \gamma_1^p, \gamma_2^p, \gamma_3^p). \tag{5.5}$$

5.1.2 The rate of dissipation function

The isothermal energy balance equation stipulates that the rate of dissipation, ξ, is equal to a difference between the mechanical power and a rate of change in the Helmholtz potential function. Therefore, the rate of dissipation can be written as

$$\xi := \dot{W} - \rho_0 \dot{\psi} \geq 0. \tag{5.6}$$

The non-negativity of ξ is to ensure that some form of the rate of dissipation inequality (e.g., Clausius-Duhem inequality) is identically satisfied. Because the dissipation of mechanical energy into heat is associated with changes in microstructure, (i.e., evolution of the natural configuration $\tilde{\kappa}_p$) and therefore, the plastic deformation of a body, it is reasonable to assume that the rate of dissipation function is dependent upon the plastic components of Laplace stretch and their rates, or in other words, on the strain measures $l_{\mathcal{U}^p}$ and their rates $l_{\dot{\mathcal{U}}^p}$, as described in § 5.1.1. For now, we further assume that the dissipation function is a closed, bounded and continuously differentiable function. The differentiability of the rate of dissipation function has an important significance, which will be discussed shortly. Therefore, the rate of dissipation function ξ is considered to have functional form of

$$\xi = \hat{\xi}(l_{\mathcal{U}^p}, l_{\dot{\mathcal{U}}^p}) = \hat{\xi}\left(\delta^p, \varepsilon_1^p, \varepsilon_2^p, \varepsilon_3^p, \gamma_1^p, \gamma_2^p, \gamma_3^p, \dot{\delta}^p, \dot{\varepsilon}_1^p, \dot{\varepsilon}_2^p, \dot{\varepsilon}_3^p, \dot{\gamma}_1^p, \dot{\gamma}_2^p, \dot{\gamma}_3^p\right). \tag{5.7}$$

For the sake of simplicity, here we have assumed that the material is perfectly plastic, i.e., it does not exhibit any hardening or softening behavior. Such material behavior can easily be incorporated into the model by considering additional variables in the arguments of the rate of dissipation, ξ and specifying their evolution equation. The elastic response of a body for a fixed natural configuration $\tilde{\kappa}_p$ is completely non-dissipative. Therefore, in view of § 5.1.1, we conclude that

$$\hat{\xi}\left(l_{\mathcal{U}^p}, \{0,0,0,0,0,0,0\}\right) = 0. \tag{5.8}$$

Now, substituting Eqns. (5.1 and 5.5) into Eqn. (5.7), we obtain

$$\begin{aligned}
&\left(\pi - \rho_0 \frac{\partial \hat{\psi}}{\partial \delta}\right)\dot{\delta} + \left(\sigma_1 - \rho_0 \frac{\partial \hat{\psi}}{\partial \varepsilon_1}\right)\dot{\varepsilon_1} + \left(\sigma_2 - \rho_0 \frac{\partial \hat{\psi}}{\partial \varepsilon_2}\right)\dot{\varepsilon_2} + \left(\sigma_3 - \rho_0 \frac{\partial \hat{\psi}}{\partial \varepsilon_3}\right)\dot{\varepsilon_3} \\
&+ \left(\tau_1 - \rho_0 \frac{\partial \hat{\psi}}{\partial \gamma_1}\right)\dot{\gamma_1} + \left(\tau_2 - \rho_0 \frac{\partial \hat{\psi}}{\partial \gamma_2}\right)\dot{\gamma_2} + \left(\tau_3 - \rho_0 \frac{\partial \hat{\psi}}{\partial \gamma_3}\right)\dot{\gamma_3} = \hat{\xi} \\
&+ \rho_0 \left(\frac{\partial \hat{\psi}}{\partial \delta^p}\dot{\delta}^p + \frac{\partial \hat{\psi}}{\partial \varepsilon_1^p}\dot{\varepsilon}_1^p + \frac{\partial \hat{\psi}}{\partial \varepsilon_2^p}\dot{\varepsilon}_2^p + \frac{\partial \hat{\psi}}{\partial \varepsilon_3^p}\dot{\varepsilon}_3^p + \rho_0 \frac{\partial \hat{\psi}}{\partial \gamma_1}\dot{\gamma}_1 + \rho_0 \frac{\partial \hat{\psi}}{\partial \gamma_2}\dot{\gamma}_2 + \rho_0 \frac{\partial \hat{\psi}}{\partial \gamma_3}\dot{\gamma}_3\right)
\end{aligned} \tag{5.9}$$

where the hats on top of ψ and ξ imply that they are expressed in terms of their respective conjugate strain measures according to Eqns. (5.5 and 5.7).

We notice that the left-hand side of Eqn. (5.9) is a function of the list of variables $l_{\mathcal{U}}$ and $l_{\dot{\mathcal{U}}}$ for a given natural configuration $\tilde{\kappa}_p$, whereas the right-hand side is independent of those variables. If the elastic response of the material is assumed to be that of a Green elastic solid, then the stress attributes can be written as

$$\pi = \rho_0 \, \frac{\partial \hat{\psi}}{\partial \delta}, \qquad \sigma_i = \rho_0 \, \frac{\partial \hat{\psi}}{\partial \varepsilon_i}, \qquad \tau_i = \rho_0 \, \frac{\partial \hat{\psi}}{\partial \gamma_i} \tag{5.10}$$

where $i = 1, 2, 3$. Using the interdependence of the squeeze stress/strain pairs (specifically, $\sigma_3 = -(\sigma_1 + \sigma_2)$ and $\varepsilon_3 = -(\varepsilon_1 + \varepsilon_2)$), Eqn. (5.10) can be alternatively written as

$$\pi = \rho_0 \, \frac{\partial \hat{\psi}}{\partial \delta}, \tag{5.11a}$$

$$2\sigma_1 + \sigma_2 = \rho_0 \, \frac{\partial \hat{\psi}}{\partial \varepsilon_1}, \tag{5.11b}$$

$$\sigma_1 + 2\sigma_2 = \rho_0 \, \frac{\partial \hat{\psi}}{\partial \varepsilon_2}, \tag{5.11c}$$

$$\tau_i = \rho_0 \, \frac{\partial \hat{\psi}}{\partial \gamma_i}, \quad i = 1, 2, 3. \tag{5.11d}$$

The assumption of an elastic response stipulates that the rate of dissipation function satisfies the constraint

$$\hat{\xi} = -\rho_0 \left[\frac{\partial \hat{\psi}}{\partial \delta^p} \, \dot{\delta}^p + \sum_{i=1}^{3} \left(\frac{\partial \hat{\psi}}{\partial \varepsilon_i^p} \, \dot{\varepsilon}_i^p + \frac{\partial \hat{\psi}}{\partial \gamma_i} \, \dot{\gamma}_i \right) \right]. \tag{5.12}$$

Equations (5.11a–5.11d) imply that the stresses are derivable from the Helmholtz potential ψ. A similar result was obtained by Freed (2017) [32] for the elastic case. However, the main deviation from Freed's result is that in the elastoplastic case the Helmholtz potential is also a function of the variables listed in $l_{\mathcal{U}^p}$, and thus, is dependent upon the natural configuration $\tilde{\kappa}_p$ and its evolution.

5.1.3 Maximization of the rate of dissipation

It is well-known that although a satisfaction of the second law of thermodynamics is a necessary condition for any valid constitutive model, it is not sufficient for determining an evolution equation for the natural configurations. In our theory, the second law of thermodynamics is identically satisfied though an assumption of the non-negativity of ξ. However, we need to make a more stringent assumption to determine the list of variables $l_{\dot{\mathcal{U}}^p}$, which in turn serves as an evolution equation for $\tilde{\kappa}_p$. Here we adopt the criterion for a maximum rate of dissipation that states that *out of all admissible values in the list of variables $l_{\dot{\mathcal{U}}^p}$ (alternatively, the plastic velocity gradient $\boldsymbol{\mathcal{L}}^p$), the one that maximizes the rate of dissipation, while satisfying the reduced rate of dissipation equation* (5.12)*, is the one that governs evolution of the natural configuration $\tilde{\kappa}_p$.* This criterion was proposed by Rajagopal and Srinivasa (1998) [75, 78] and can be viewed as an extension of Onsager's minimum rate of entropy production criterion and Ziegler's normality rule. Therefore, mathematically, the determination of $l_{\dot{\mathcal{U}}^p}$ becomes a constrained optimization problem with respect to the list of variables $l_{\dot{\mathcal{U}}^p}$, with the rate of dissipation ξ as its objective function and the reduced rate of dissipation equation (5.12) as a constraint. If ξ is assumed to be a sufficiently smooth function in the plastic strain-rate domain, then the problem can be carried out by using a traditional Lagrange multiplier approach. The solution yields a set of seven scalar equations, each corresponding to a mode of deformation, given by

$$\frac{\partial \hat{\xi}}{\partial \dot{\delta}^p} = -\lambda\,\rho_0\,\frac{\partial \hat{\psi}}{\partial \delta^p}; \quad \frac{\partial \hat{\xi}}{\partial \dot{\varepsilon}_i^p} = -\lambda\,\rho_0\,\frac{\partial \hat{\psi}}{\partial \varepsilon_i^p}; \quad \frac{\partial \hat{\xi}}{\partial \dot{\gamma}_i^p} = -\lambda\,\rho_0\,\frac{\partial \hat{\psi}}{\partial \gamma_i^p} \tag{5.13}$$

where $i = 1, 2, 3$, with $\lambda = -\overline{\lambda}/(1+\overline{\lambda})$, and where $\overline{\lambda}$ is a Lagrange multiplier. It is possible to evaluate λ through a satisfaction of the constraint equation (5.12).

5.1.4 Special form for ψ and rate independent plasticity

Notice that Eqn. (5.13) is a set of seven implicit equations for the plastic strain rates listed in $l_{\dot{\mathcal{U}}^p}$. Such implicit equations are difficult to solve and do not provide much physical interpretations. Therefore, it is instructive to choose a specific form for the Helmholtz potential function at this juncture. As mentioned earlier, the Helmholtz potential ψ characterizes the elastic response of a material for a fixed natural configuration, and hence, it is common practice to consider the Helmholtz potential as a function of the elastic strain attributes (e.g., Srinivasa (2010) [89]), i.e.,

$$\psi = \hat{\psi}(\delta^e, \varepsilon_1^e, \varepsilon_2^e, \varepsilon_3^e, \gamma_1^e, \gamma_2^e, \gamma_3^e). \tag{5.14}$$

However, in view of Eqn. (1.39), one can write the elastic strain attributes in terms of the total strain attributes and their plastic components. In other words, the difference between the total strain attributes and their corresponding plastic components always represent the elastic strain attributes, or linear combinations thereof. Therefore, because the Helmholtz potential function is to be specified for a fixed natural configuration, it is reasonable to assume that is a homogeneous, quadratic function of the difference between the total strain attributes and their corresponding plastic components. Specifically, one can write

$$\begin{aligned}\psi = \hat{\psi}(l_{\mathcal{U}}, l_{\mathcal{U}^p}) = \frac{1}{2} \Big[& N_{00} \left(\delta - \delta^p\right)^2 + \sum_{i=1}^{3} N_{0i} \left(\delta - \delta^p\right) \left(\varepsilon_i - \varepsilon_i^p\right) + \sum_{i=1}^{3} N_{0(i+3)} \left(\delta - \delta^p\right) \left(\gamma_i - \gamma_i^p\right) \\ & + \sum_{\substack{i,j=1 \\ i \le j}}^{3} N_{ij} \left(\varepsilon_i - \varepsilon_i^p\right) \left(\varepsilon_j - \varepsilon_j^p\right) + \sum_{i,j=1}^{3} N_{i(j+3)} \left(\varepsilon_i - \varepsilon_i^p\right) \left(\gamma_j - \gamma_j^p\right) \\ & + \sum_{\substack{i,j=1 \\ i \le j}}^{3} N_{(i+3)(j+3)} \left(\gamma_i - \gamma_i^p\right) \left(\gamma_j - \gamma_j^p\right) \Big].\end{aligned} \tag{5.15}$$

where N's are material parameters. These material parameters are not all independent. In fact, for an isotropic material, these material parameters can be expressed in terms of two, independent Lamé constants. The Helmholtz potential is chosen in this way to avoid any complication in analysis that may arise due to couplings between the normal and shear plastic-strain attributes whenever their elastic counterparts are expressed in terms of the sets of variables $l_{\mathcal{U}}$ and $l_{\mathcal{U}^p}$. Moreover, the form for ψ in Eqn. (5.15) essentially leads to a Green elastic solid response[1] measured from a fixed natural configuration $\tilde{\kappa}_p$.

[1] I.e., the response of a hyperelastic solid.

The choice of this special form has a deeper consequence when developing the rest of our constitutive model. From this assumed form for ψ, by simple calculations, one can easily obtain

$$
\begin{aligned}
\pi &= \rho_0 \frac{\partial \hat{\psi}}{\partial \delta} = -\rho_0 \frac{\partial \hat{\psi}}{\partial \delta^p}, \\
\sigma_i &= \rho_0 \frac{\partial \hat{\psi}}{\partial \varepsilon_i} = -\rho_0 \frac{\partial \hat{\psi}}{\partial \varepsilon_i^p}, \\
\tau_i &= \rho_0 \frac{\partial \hat{\psi}}{\partial \gamma_i} = -\rho_0 \frac{\partial \hat{\psi}}{\partial \gamma_i^p}.
\end{aligned}
\tag{5.16}
$$

Now, substituting these relations into the reduced rate of dissipation equation (5.13), we obtain

$$
\pi \, \dot{\delta}^p + \sum_{i=1}^{3} (\sigma_i \, \dot{\varepsilon}_i^p + \tau_i \, \dot{\gamma}_i^p) = \xi. \tag{5.17}
$$

This is the reduced rate of equation for our chosen form for the Helmholtz potential function, and should be used as a constraint for the subsequent development of our constitutive model. For future reference, we note that because Eqn. (5.16) is invertible, the rate of dissipation function ξ can be expressed in terms of the stress attributes and the list of variables $l_{\dot{\mathcal{U}}^p}$, i.e., $\xi = \overline{\xi}(l_\sigma, l_{\dot{\mathcal{U}}^p})$. Therefore, it is now possible to carry out a maximization of the rate of dissipation function subject to the constraint (5.17) and taken with respect to either stress or plastic strain-rate attributes, thereby making an inversion of the relations (5.13) possible.

Yield condition

Before obtaining an evolution equation for the natural configurations $\tilde{\kappa}_p$, we need to determine under what conditions the natural configurations change (or the material yields). Note that our theory does not presuppose the existence of a yield surface, as is the case in classical plasticity theory. In fact, whether the material under consideration shows yielding behavior or a creep-like behavior is determined by the nature of the rate of dissipation function. As we mentioned earlier, whenever the variables listed in $l_{\dot{\mathcal{U}}^p}$ are all zero, the dissipation function vanishes and the material exhibits an elastic response. However, if the dissipation function is considered to be a positively homogeneous function of order 1, then it is non-differentiable whenever $l_{\dot{\mathcal{U}}^p}$ is zero. In fact, a dissipation function that is non-differentiable at $l_{\dot{\mathcal{U}}^p} = \mathbf{0}$ corresponds to a material with a definite yield surface, whereas a sufficiently smooth dissipation function (even at $l_{\dot{\mathcal{U}}^p} = \mathbf{0}$) leads to creep-like material behavior. Clearly, for materials showing yielding behavior, one cannot use a Lagrange multiplier technique to maximize the rate of dissipation function ξ. Nevertheless, it is possible to define a suitable yield function for both these cases.

It is to note that the maximum rate of dissipation criterion stipulates that whenever a dissipative process is possible, it will occur. In other words, a body undergoes a non-dissipative process *only when* there is no possibility of a dissipative process. In general, the elastic domain of a material can be characterized by those values of l_σ for which all the plastic strain-rate attributes are zero. Notice that a satisfaction of Eqn. (5.17) is crucial to the occurrence of a dissipative process. Specifically, the only admissible nonzero values of $l_{\dot{\mathcal{U}}^p}$ are those that satisfy the reduced rate of dissipation equation (5.17). Among these admissible values, the ones that maximize the rate of dissipation function $\xi = \overline{\xi}(l_\sigma, l_{\dot{\mathcal{U}}^p})$ are chosen as the 'correct' plastic strain-rate attributes. Therefore, we can alternatively[2] characterize the elastic domain based upon whether Eqn. (5.17) is satisfied. Clearly, from Eqn. (5.17), we can conclude that $l_\sigma = \mathbf{0}$ belongs to this set of values. Because the dissipation function ξ is bounded, closed and continuous on the plastic strain-rate attributes $l_{\dot{\mathcal{U}}^p}$ for a prescribed set of values for l_σ, it is always possible to find values for the plastic strain-rate attributes such that

$$\pi\,\dot{\delta}^p + \sigma_1\,\dot{\varepsilon}_1^p + \sigma_2\,\dot{\varepsilon}_2^p + \sigma_3\,\dot{\varepsilon}_3^p + \tau_1\,\dot{\gamma}_1^p + \tau_2\,\dot{\gamma}_2^p + \tau_3\,\dot{\gamma}_3^p < \overline{\xi}(l_\sigma, l_{\dot{\mathcal{U}}^p}). \tag{5.18}$$

For these values of $l_{\dot{\mathcal{U}}^p}$, because the reduced rate of dissipation equation (5.17) is violated, we can conclude that for these values of $l_{\dot{\mathcal{U}}^p}$, the material exhibits an elastic (i.e., non-dissipative) response. We can now formally introduce a yield function for the material. For a given l_σ, let us define a function $Y(l_{\dot{\mathcal{U}}^p})$ as

$$Y(l_{\dot{\mathcal{U}}^p}) := \max_{l_{\dot{\mathcal{U}}^p} \neq \mathbf{0}} \frac{\pi\,\dot{\delta}^p + \sigma_1\,\dot{\varepsilon}_1^p + \sigma_2\,\dot{\varepsilon}_2^p + \sigma_3\,\dot{\varepsilon}_3^p + \tau_1\,\dot{\gamma}_1^p + \tau_2\,\dot{\gamma}_2^p + \tau_3\,\dot{\gamma}_3^p}{\overline{\xi}(l_\sigma, l_{\dot{\mathcal{U}}^p})}. \tag{5.19}$$

[2]Note that here the stress attributes l_σ are held fixed and $l_{\dot{\mathcal{U}}^p}$ are allowed to vary.

When $Y(l_{\dot{\mathcal{U}}^p}) = 1$, it is possible to find a combination for the sets of values of l_σ and $l_{\dot{\mathcal{U}}^p}$ that satisfies the reduced rate of dissipation equation (5.17), and thus, this condition provides a set of admissible, nonzero values for the plastic strain-rate attributes $l_{\dot{\mathcal{U}}^p}$. Therefore, the yield condition is defined as $Y(l_{\dot{\mathcal{U}}^p}) = 1$ with function $Y(l_{\dot{\mathcal{U}}^p})$ being referred to as the yield function. Clearly, if $Y(l_{\dot{\mathcal{U}}^p}) < 1$, then equation (5.18) is satisfied, and as such, the material response is elastic. It has been shown that this yield function is convex in strain-rate space (see App. C).

Normality rule

We now derive a key result pertinent to our constitutive theory. If the rate of dissipation function ξ is assumed to be a continuously differentiable function, i.e., the material exhibits a creep-like behavior, then substitution of the relations (5.16) into Eqn. (5.13) produces

$$\pi = \frac{1}{\lambda}\,\frac{\partial\hat{\xi}}{\partial\dot{\delta}^p}, \qquad \sigma_i = \frac{1}{\lambda}\,\frac{\partial\hat{\xi}}{\partial\dot{\varepsilon}_i^p}, \qquad \tau_i = \frac{1}{\lambda}\,\frac{\partial\hat{\xi}}{\partial\dot{\gamma}_i^p} \tag{5.20}$$

where $i = 1, 2, 3$. Therefore, from the above equations, one can conclude that *the stress attributes are directed along the gradient of the rate of dissipation function with respect to their corresponding plastic strain-rate attributes*. Clearly, Eqn. (5.20) is equivalent to the normality rule used in classical plasticity theory whenever $l_{\dot{\mathcal{U}}^p} \neq \mathbf{0}$.

Note that the set of equations (5.20) is valid only when $l_{\dot{\mathcal{U}}^p} \neq \mathbf{0}$, i.e., whenever the material is undergoing plastic deformation. In this case, the reduced rate of dissipation equation (5.17) must be satisfied. Now, the Lagrange multiplier λ can be evaluated by substituting the relations (5.20) into the reduced rate of dissipation equation (5.17) and is given as

$$\lambda = \frac{1}{\xi}\left[\dot{\delta}^p\,\frac{\partial\xi}{\partial\dot{\delta}^p} + \sum_{i=1}^{3}\left(\dot{\varepsilon}_i^p\,\frac{\partial\xi}{\partial\dot{\varepsilon}_i^p} + \dot{\gamma}_i^p\,\frac{\partial\xi}{\partial\dot{\gamma}_i^p}\right)\right]. \tag{5.21}$$

For the materials that exhibit yielding behavior, the rate of dissipation function is no longer differentiable with respect to the plastic strain-rate attributes at the yield surface. Therefore, we must adopt a standard method from convex analysis, instead of employing the Lagrange multiplier technique, to derive similar results for this case. Let us consider a list of prescribed stress attributes l_σ and two plastic strain-rate attributes: (*i*) $\bar{l}_{\dot{\mathcal{U}}^{\surd}}$ that satisfy the yield condition $Y(\bar{l}_{\dot{\mathcal{U}}^p}) = 1$ and (*ii*) $l_{\dot{\mathcal{U}}^{\surd}}$ for which $Y(l_{\dot{\mathcal{U}}^p}) < 1$. Now, since the rate of dissipation function is assumed to be a bounded, closed, homogeneous function of order 1 in the plastic strain-rate attribute space, and among the two processes only the former is dissipative, it can easily be concluded that for given stress attributes $\xi(l_\sigma, l_{\dot{\mathcal{U}}^p}) \leq \xi(l_\sigma, \bar{l}_{\dot{\mathcal{U}}^p})$.

Now, in view of the expression for the yield condition, it is easily understood that

$$\frac{\pi\,\dot{\delta}^p + \sum_{i=1}^{3}(\sigma_i\,\dot{\varepsilon}_i^p + \tau_i\,\dot{\gamma}_i^p)}{\xi(l_\sigma, l_{\dot{\mathcal{U}}^p})} \leq \frac{\pi\,\dot{\bar{\delta}}^p + \sum_{i=1}^{3}\left(\sigma_i\,\dot{\bar{\varepsilon}}_i^p + \tau_i\,\dot{\bar{\gamma}}_i^p\right)}{\xi(l_\sigma, \bar{l}_{\dot{\mathcal{U}}^p})} = 1. \tag{5.22}$$

Using the fact that $\xi(l_\sigma, l_{\dot{\mathcal{U}}^p}) \leq \xi(l_\sigma, \bar{l}_{\dot{\mathcal{U}}^p})$, we arrive at

$$\begin{aligned} &\pi\,(\dot{\bar{\delta}}^p - \dot{\delta}^p) + \sum_{i=1}^{3}\left[\sigma_i\,(\dot{\bar{\varepsilon}}_i^p - \dot{\varepsilon}_i^p) + \tau_i\,(\dot{\bar{\gamma}}_i^p - \dot{\gamma}_i^p)\right] \geq 0 \\ \implies\; &\pi\,(\dot{\delta}^p - \dot{\bar{\delta}}^p) + \sum_{i=1}^{3}\left[\sigma_i\,(\dot{\varepsilon}_i^p - \dot{\bar{\varepsilon}}_i^p) + \tau_i\,(\dot{\gamma}_i^p - \dot{\bar{\gamma}}_i^p)\right] \leq 0. \end{aligned} \tag{5.23}$$

Now the convex hull $\mathbb{C}_{\dot{\mathcal{U}}^p}$ of the set $l_{\dot{\mathcal{U}}^p}$ is given as

$$\mathbb{C}_{\dot{\mathcal{U}}^p} = \lambda_0\,\dot{\delta}^p + \sum_{i=1}^{3}(\lambda_i\,\dot{\varepsilon}_i^p + \lambda_{i+3}\,\dot{\gamma}_i^p) \;\text{ with }\; \lambda_0, \lambda_1, ..., \lambda_6 \geq 0 \;\text{ and }\; \sum_{i=0}^{6}\lambda_i = 1.$$

Clearly, the second formula in Eqn. (5.23) implies that *the stress attributes l_σ are along the normal cone to the convex hull $\mathbb{C}_{\dot{\mathcal{U}}^p}$ at $\bar{l}_{\dot{\mathcal{U}}^p}$ in the plastic strain-rate space.* Recall that the plastic strain rates $\bar{l}_{\dot{\mathcal{U}}^p}$ correspond to the condition $Y(\bar{l}_{\dot{\mathcal{U}}^p}) = 1$. Geometrically, the convex hull $\mathbb{C}_{\dot{\mathcal{U}}^p}$ represents the set of all straight lines whose ends compose the set $l_{\dot{\mathcal{U}}^p}$. Equation (5.23) implies that the stress attributes l_σ do not make an acute angle with any line segment $\mathbb{C}_{\dot{\mathcal{U}}^p}$ with $\bar{l}_{\dot{\mathcal{U}}^p}$ as endpoints for any set of values for $l_{\dot{\mathcal{U}}^p}$. Thus, l_σ is along the normal cone to the convex hull $\mathbb{C}_{\dot{\mathcal{U}}^p}$ at $\bar{l}_{\dot{\mathcal{U}}^p}$ (cf. Rockafellar(1970) [80, §2]). Therefore, Eqn. (5.23) acts as a normality rule for the materials that exhibit yielding behavior.

It is important to note that for materials that exhibit a creep-like behavior (and hence, has a smooth rate of dissipation function over any set of values for $l_{\dot{\mathcal{U}}^p}$), it is possible to derive a normality condition for each individual stress/plastic strain-rate pair (i.e., Eqn. (5.20)). Such conditions, however, cannot be obtained for an individual stress/plastic strain-rate pair for materials that exhibit a yielding behavior. Much like the yield condition (5.19), for the latter case, the normality rule (5.23) involves all the stress/plastic strain-rate pairs.

Causality

In the above derivation, the stress attributes are held fixed, whereas the plastic strain-rate attributes are allowed to vary in order to maximize the rate of dissipation. Although the derived plastic flow rules are useful [97], the causality in Eqn. (5.20) is reversed. Physically, the stress and plastic strain-rate attributes act as “determinants" and “resultants", respectively, in the terminology of Rajagopal and Srinivasa (2019) [77]. Note that with the assumed form of the Helmholtz potential function in Eqn. (5.15), it is now possible to express the rate of dissipation function ξ and the reduced rate of dissipation constraint (5.17) in terms of the stress attributes l_σ.

For a given set of plastic strain-rate attributes $l_{\dot{\mathcal{U}}^p}$, the yield function can now be written as

$$Y(l_\sigma) = \max_{l_\sigma \neq \mathbf{0}} \frac{\pi\, \dot{\delta}^p + \sum_{i=1}^{3} \left(\sigma_i\, \dot{\varepsilon}_i^p + \tau_i\, \dot{\gamma}_i^p\right)}{\bar{\xi}(l_\sigma, l_{\dot{\mathcal{U}}^p})}. \tag{5.24}$$

It can easily be shown that the yield function is convex in the stress attributes space. (See App. C.1 for a detailed derivation.)

Now, maximization of the rate of dissipation function ξ with respect to l_σ yields

$$\dot{\delta}^p = \mu\, \frac{\partial \xi}{\partial \pi}, \qquad \dot{\varepsilon}_i^p = \mu\, \frac{\partial \xi}{\partial \sigma_i}, \qquad \dot{\gamma}_i^p = \mu\, \frac{\partial \xi}{\partial \tau_i} \tag{5.25}$$

where μ is the consistency parameter that satisfies the condition that $\mu = 0$ whenever $Y(l_\sigma) < 1$. The consistency parameter μ can be determined by substituting the plastic strain-rate attributes $l_{\dot{\mathcal{U}}^p}$ into the reduced rate of dissipation equation (5.17). Whenever μ is nonzero (implying, $\xi > 0$), it is possible to find nonzero values for the plastic strain-rate attributes. Thus, these conditions can be written as

$$\begin{aligned} \mu &= 0 \quad \text{when } Y(l_\sigma) < 1 \\ &> 0 \quad \text{when } Y(l_\sigma) = 1. \end{aligned} \tag{5.26}$$

Equation (5.26) is equivalent to the well-known consistency (KKT) condition used in classical plasticity theory.

From the above discussion, it can easily be understood that the set of equations (5.20) acts as a dual of the flow rules (5.25). Note that in the derivations of both of these equations, the assumed form for the Helmholtz potential function plays a key role. In fact, even though it is possible to derive the flow rules (5.20) for some other form (Eqn. 5.13) without an assumption for the form of ψ, the same cannot be said about the flow rule (5.25). The assumed form for ψ is instrumental in the derivation of the latter. It is worth noting that the rate of dissipation function acts as a *plastic potential* in the flow rule (5.25). Following the arguments of Srinivasa (2010) [89], one can easily show that whenever the rate of dissipation function ξ is a function of the plastic strain-rate attributes alone, then the yield function acts as a plastic potential, resulting in an associative flow rule. On the other hand, a non-associative flow rule emerges whenever the rate of dissipation is separable in terms of the functions of l_σ and $l_{\dot{\mathcal{U}}^p}$ (i.e., $\xi = \overline{\xi}(l_\sigma, l_{\dot{\mathcal{U}}^p}) = g(l_\sigma)\, h(l_{\dot{\mathcal{U}}^p})$) respectively. A demonstration of these properties has been provided in § C.2.

5.2 Volume-preserving plastic deformation

For metals and polymers, it is often assumed that the plastic deformation process is volume-preserving [60], i.e., det$(\boldsymbol{\mathcal{U}}^p) = 1$, which further implies that the plastic dilatational strain δ^p and its rate are zero. However, materials like certain soils, rocks and foams exhibit a dilatant pressure-dependent elastoplastic behavior [89] in which the volume of the natural configuration $\tilde{\kappa}_p$ does not remain a constant anymore. In this case, no other constraint in addition to the reduced rate of dissipation equation (5.17) is required. Therefore, the constitutive model developed so far is suitable for the latter class of materials. In this section, we show that the developed constitutive model can accommodate volume-preserving plastic deformation with slight modifications in the constrained optimization problem.

In the current theory, the assumption of a volume-preserving plastic deformation is manifested by considering the condition of a zero, plastic, dilatational, strain rate, $\dot{\delta}^p$, as an additional constraint, instead of using it as a kinematic variable.[3] In this case, the plastic dilatation term δ^p and its rate must be dropped from the argument of $\hat{\xi}$ in Eqn. (5.7). Therefore, when the plastic deformation is assumed to be volume-preserving, the rate of dissipation function reduces to the form

$$\xi_{cv} = \hat{\xi}_{cv}\left(\varepsilon_i^p, \gamma_i^p, \dot{\varepsilon}_i^p, \dot{\gamma}_i^p\right) \tag{5.27}$$

where $i = 1, 2, 3$. Similarly, the Helmholtz potential function reduces to the form

$$\psi_{cv} = \hat{\psi}_{cv}(\delta, \varepsilon_i, \gamma_i, \dot{\varepsilon}_i^p, \dot{\gamma}_i^p). \tag{5.28}$$

Like before, we assume that the elastic response of the material is that of a Green elastic solid. Since the stress attributes depend only on the *total* strain attributes, they can be obtained from the Helmholtz potential function according to Eqn. (5.10). Now using the definition for the rate of dissipation function (Eqn. 5.6), one can obtain a reduced rate of dissipation equation that, in this case, is

$$\hat{\xi}_{cv} = -\rho_0 \sum_{i=1}^{3} \left(\frac{\partial \psi}{\partial \varepsilon_i^p}\, \dot{\varepsilon}_i^p + \frac{\partial \psi}{\partial \gamma_i^p}\, \dot{\gamma}_i^p \right). \tag{5.29}$$

Note that the rate of dissipation function is no longer a function of the plastic dilatational strain rate $\dot{\delta}^p (= 0)$. Now, maximizing the rate of dissipation function $\hat{\xi}_{cv}$ with respect to the set of kinematic variables $\{\dot{\varepsilon}_i^p, \dot{\gamma}_i^p\}$, with Eqn. (5.29) and $\dot{\delta}^p = 0$ as constraints, we finally obtain

$$\frac{\partial \hat{\xi}}{\partial \dot{\varepsilon}_i^p} = -\lambda\, \rho_0\, \frac{\partial \hat{\psi}}{\partial \varepsilon_i^p}; \qquad \frac{\partial \hat{\xi}}{\partial \dot{\gamma}_i^p} = -\lambda\, \rho_0\, \frac{\partial \hat{\psi}}{\partial \gamma_i^p} \tag{5.30}$$

where λ is a Lagrange multiplier. Equation (5.30) has been derived by using the fact that the deformation modes, dilatation and squeeze, are independent of each other. This can also be corroborated

[3]We do not use the condition δ^p as a constraint, because the optimization is carried out only with respect to the plastic strain-rate attributes.

by computing the partial derivative of the plastic strain-rate term with respect to any of the plastic squeeze strain rate (i.e., $\partial\dot{\delta}^p/\partial\dot{\varepsilon}^p_i = 0$). Now, following the procedure described in § 5.1.4, one can derive the yield and normality condition whenever a special form for the Helmholtz potential function is assumed. If the Helmholtz function, in this case, is assumed as

$$\begin{aligned}\psi = \hat{\psi}(l_{\mathcal{U}}, l_{\mathcal{U}^p}) = \frac{1}{2}\Big[&N_{00}\,\delta^2 + \sum_{i=1}^{3} N_{0i}\,(\delta-\delta^p)\,(\varepsilon_i-\varepsilon_i^p) + \sum_{i=1}^{3} N_{0(i+3)}\,(\delta-\delta^p)\,(\gamma_i-\gamma_i^p)\\ &+ \sum_{\substack{i,j=1\\ i\le j}}^{3} N_{ij}\,(\varepsilon_i-\varepsilon_i^p)\,(\varepsilon_j-\varepsilon_j^p) + \sum_{i,j=1}^{3} N_{i(j+3)}\,(\varepsilon_i-\varepsilon_i^p)\,(\gamma_j-\gamma_j^p)\\ &+ \sum_{\substack{i,j=1\\ i\le j}}^{3} N_{(i+3)(j+3)}\,(\gamma_i-\gamma_i^p)\,(\gamma_j-\gamma_j^p)\Big],\end{aligned} \tag{5.31}$$

then the yield function can be written as

$$Y_{cv}(l_{\dot{\mathcal{U}}^p}) := \max_{l_{\dot{\mathcal{U}}^p}\neq \mathbf{0}} \frac{\sum_{i=1}^{3}(\sigma_i\,\dot{\varepsilon}_i^p + \tau_i\,\dot{\gamma}_i^p)}{\bar{\xi}(l_\sigma, l_{\dot{\mathcal{U}}^p})}. \tag{5.32}$$

It can be easily shown that in this case the yield surface is convex in the plastic strain-rate (or stress) space. Finally, maximization of the rate of dissipation function yields

$$\sigma_i = \lambda\,\frac{\partial\xi}{\partial\dot{\varepsilon}_i^p}, \qquad \tau_i = \lambda\,\frac{\partial\xi}{\partial\dot{\gamma}_i^p}. \tag{5.33}$$

Equation (5.33) provides an implicit equation for the plastic strain-rate attributes. Now, one can carry out the maximization by varying the stress attributes instead. In this case, the plastic strain-rate attributes can be obtained through the flow rule as

$$\dot{\varepsilon}_i^p = \mu\,\frac{\partial\xi}{\partial\sigma_i}, \qquad \dot{\gamma}_i^p = \mu\,\frac{\partial\xi}{\partial\tau_i} \tag{5.34}$$

where μ denotes the consistency parameter.

5.3 Summary

A novel constitutive model for elastic-plastic materials is developed using scalar, conjugate, stress/strain, base pairs arising from a **QR** decomposition of the deformation gradient. It has been shown that the multiplicative elastic-plastic decomposition of the Laplace stretch leads to an additive strain decomposition, which is commonly used in a small strain theory. This decomposition plays a key role in developing our constitutive model. In addition to the laws of thermodynamics, a maximum rate of dissipation criterion has been used to derive an evolution equation for the plastic strain rates.

6. THE CONCEPT OF PLASTIC SPIN BASED ON A **QR** KINEMATICS *

In the previous chapter, we developed a constitutive model for an isotropic, elastic-plastic material. Although this model resolves the issue of co-variance between traditionally used tensor invariants, it is unable to capture the material response induced by evolving microstructure during the plastic deformation process. Typically, the kinematics of a material substructure enters into a macroscopic model through the use of internal variables. These internal variables can be scalars, vectors or second-order tensors and physically represent a gamut of quantities such as back stress, orientation of the lattice director vectors in case of polycrystalline materials etc. The concept of plastic spin is a crucial aspect of the theory of plasticity and often closely associated with these internal variables as it enters into the constitutive model implicitly through an appropriate definition of a co-rotational rate of the internal state variables. This concept has been developed and incorporated into constitutive models starting with the works by Mandel (1971) [61, 62] and Kratochvil (1971) [48] and later developed by Loret (1983) [56], Dafalias [22, 23, 21], Onat (1984) [72], Aifantis [4, 6] and others.

A plastic spin can be defined as an anti-symmetric spin tensor representing the rotation between the material substructure and its macroscopic counterpart during a plastic deformation. Like many other fundamental features of the plasticity theory, the necessity of incorporating a plastic spin into the constitutive model has been a longstanding point of contention. This debate, however, has partly taken place due to the fact that the concept of plastic spin has often been misconstrued in the literature as the anti-symmetric part of the plastic velocity gradient. Thereby, some researchers have debunked its necessity in constitutive modeling as the work conjugate of the plastic velocity gradient is a symmetric stress tensor. This misinterpretation seriously undermines the importance of the concept of plastic spin, as noted by Dafalias (1998) [21]. On the other hand, Steigmann and Gupta (2011) [90] argued that the plastic spin arises due to the non-uniqueness of the intermediate

* "Investigation of the concept of plastic spin using a **QR** decomposition of the deformation gradient" by Paul, S., Freed, A. D., 2021. (under review)

configuration, commonly used in the multiplicative decomposition of the deformation gradient, $\mathbf{F} = \mathbf{F}^e\,\mathbf{F}^p$. It is well-known that this intermediate configuration can be determined accurately only up to a rigid body rotation. They showed that the kinematic quantities in two intermediate configurations, separated by a rigid body rotation are mechanically equivalent and therefore, it is possible to bypass the need for incorporating plastic spin into constitutive model whenever a multiplicative decomposition of the deformation gradient is used. In this paper, we explore the concept of plastic spin in the context of a **QR** decomposition of the deformation gradient. A particular significance of this decomposition is that in this framework, the intermediate configuration is unique, even at the kinematic level owing to the group property of the upper-triangular elastic and plastic stretches. We show that even in this case, the plastic spin plays a crucial role in constitutive modeling, especially for materials that exhibit an evolving anisotropy during plastic deformation process.

6.1 The plastic spin

While constructing constitutive models for elastic-plastic materials, it is a common practice to consider only the quantities representing the macroscopic deformation of a body, e.g., the Laplace stretch $\boldsymbol{\mathcal{U}}$ and its plastic part $\boldsymbol{\mathcal{U}}^p$ as kinematic variables and their corresponding work conjugates. However, in these models, it is not possible to keep track of the evolution of the underlying microstructural properties of the materials with these kinematic variables. Therefore, although these models work well for isotropic materials, they are unable to capture materials exhibiting evolving microstructural properties such as plastically-induced anisotropy. In order to resolve this issue, internal state variables are typically used that act as a macroscopic manifestation of these microstructural properties. Let $\mathbf{a}_i$ denote a set of internal variables in the current configuration κ_t. Upon elastic unloading, these set of variables are pulled back into the configuration κ_p and are denoted by $\mathbf{A}_i$. $\mathbf{a}_i$ and $\mathbf{A}_i$ are related through the inverse of the elastic deformation gradient and its transpose. However, the specific relation depends on the nature of a particular internal variable. For instance, if $\mathbf{a}_i$ is a tensor-valued internal variable, then $\mathbf{A}_i$ can be obtained as $\mathbf{A}_i = \det(\mathbf{F}^e)\,\mathbf{F}^{e^{-1}}\,\mathbf{a}_i\,\mathbf{F}^{e^{-T}}$. Since $\mathbf{A}_i$ represents a macroscopic manifestation of the microstructural changes, the material response must also depend on these internal variables.

In the previous chapter, we have developed a material model for isotropic, elastic-perfectly plastic materials by employing a maximum rate of dissipation criterion. In this framework, one needs to specify constitutive assumptions for two quantities– *(i)* the Helmholtz potential function, ψ and, *(ii)* the rate of dissipation function ξ. In order to incorporate material behavior induced by the microstructural changes, one needs to consider the internal state variables as arguments of the Helmholtz potential ψ and the rate of dissipation function ξ. One particular material behavior caused by microstructural changes is the plastically-induced anisotropy. This anisotropy is exhibited at a microstructural level and is different from the macroscopic behavior exhibited by initially anisotropic material; the latter of which enters into our constitutive model through a particular mapping between the kinematic (e.g., components of Laplace stretch) and kinetic (e.g., components of the Kirchhoff stress tensor, pulled back into our physical frame of reference) quantities and their corresponding strain and stress attributes [27]. A plastically-induced (and thus, evolving) anisotropy can be incorporated by considering certain parameters of these maps as variables.

Since the internal state variables are used in constitutive modeling of the material, an evolution equation must be specified for each $\mathbf{A}_i$ in order to keep track of its evolution and change in orientation during plastic deformation. Moreover, an appropriate rate of the internal state variable must be specified. Motivated by single crystal plasticity, Mandel (1971) [61] introduced the idea of a triad of orthogonal director vectors attached to the material substructure. When the material undergoes a plastic deformation, the orientation of this triad with respect to a global reference configuration represents the orientation of the material substructure. In other words, the change in orientation of this orthogonal triad denotes the change in orientation of the kinematic internal variables during a plastic deformation. Thus, an appropriate rate of the internal state variable must be defined in such a way that it co-rotates with this orthogonal triad during the plastic deformation process. Clearly, the rotation of this orthogonal triad is associated with a substructural spin that denotes the spin of the macroscopic manifestation of the material microstructure. The unstressed intermediate configuration whose orientation is determined by the orientation of the director vectors after plastic deformation is termed as an isoclinic configuration. Dafalias (1987) [23] adopted a different approach to this problem. In his work, he defined a plastic spin as the difference between a material spin associated with the (macroscopic) continuum and a substructural spin. The material spin can be directly related to the kinematic quantity describing the macroscopic plastic deformation, e.g., the anti-symmetric part of the plastic velocity gradient $\mathbf{L}^p := \dot{\mathbf{F}}^p \mathbf{F}^{p^{-1}}$. Thus, once a constitutive equation for the plastic spin is specified, one can easily obtain the substructural spin at a particular time step. A time integration of the substructural spin further provides the rotation of Mandel's director vectors. Therefore, the concept of director vectors is not inherent to this approach; rather this concept appears as a consequence of the assumption of existence of a plastic spin. The reason behind adopting this approach is that sometimes the concept of director vectors is thought to be restricted to those internal variables that are orientational in nature. However, in the latter approach, the director vectors are used for easy understanding, rather than taking the center stage of the theory. Nevertheless, in our framework, the concept of director vectors inherently appears in the kinematics of the plastic deformation (even, the total deformation) and hence, can be easily adopted to explore the concept of plastic spin.

Recall that for the total deformation, the inverse to the rotation tensor $\boldsymbol{\mathcal{R}}^T$ rotates an Eulerian set of bases into a new set of bases $\tilde{\boldsymbol{e}}_I$ whereas the deformation of a cube whose sides are along the base vectors $\tilde{\boldsymbol{e}}_I$ is *completely* described by the components of the Laplace stretch. Since the decomposition $\mathbf{F}^p = \boldsymbol{\mathcal{R}}^p \boldsymbol{\mathcal{U}}^p$ can be considered as a Gram-Schmidt process applied on the matrix of the plastic deformation gradient, this decomposition also has the same physical interpretation as the **QR** decomposition of the total deformation gradient $\mathbf{F}$. Specifically, the inverse to the plastic rotation tensor $\boldsymbol{\mathcal{R}}^{p^T}$ rotates the base vectors of the intermediate configuration κ_p into a new set of bases $\tilde{\boldsymbol{e}}_I^p$ in the configuration $\tilde{\kappa}_p$ where the plastic deformation of a representative cube whose edges are placed along $\tilde{\boldsymbol{e}}_I^p$ is *completely* described by the plastic Laplace stretch, $\boldsymbol{\mathcal{U}}^p$. Clearly, the configuration $\tilde{\kappa}_p$ can be considered as an isoclinic configuration in the terminology of Mandel (1971) [61] and $\boldsymbol{\mathcal{R}}^p$ (or its inverse) represents the rotation of the director vectors, or in other words, the substructure. Therefore, the spin associated with this rotation can be termed as substructural spin and can be defined as [1]

$$\boldsymbol{\omega}_s^p := \dot{\boldsymbol{\mathcal{R}}}^{\boldsymbol{p}} \, \boldsymbol{\mathcal{R}}^{p^T}. \tag{6.1}$$

It is important to note that the plastic velocity gradients, $\mathbf{L}^p$ and $\boldsymbol{\mathcal{L}}^p$, associated with Lee's multiplicative decomposition and an elastic-plastic decomposition of Laplace stretch respectively, are related via the substructural spin as

$$\mathbf{L}^p = \boldsymbol{\omega}_s^p + \boldsymbol{\mathcal{R}}^{\boldsymbol{p}} \, \boldsymbol{\mathcal{L}}^p \, \boldsymbol{\mathcal{R}}^{\boldsymbol{p}^{\boldsymbol{T}}}. \tag{6.2}$$

The material spin associated with the configuration κ_p is given by the anti-symmetric part of the plastic velocity gradient, $\mathbf{L}^p$. Now let us consider an internal state variable, $\mathbf{A}_i$ in the configuration κ_p. In our framework, we *only* consider internal state variables of kinematic nature. To incorporate internal, kinetic state variables in our theory, one first needs to consider their kinematic conjugates such that the product of these two provide a stored or dissipated energy or work done on a material element. Once the evolution equations for these kinematic variables are specified, the kinetic state variables are then determined through an appropriate constitutive formulation. Here we restrict ourselves to work with only kinematic, internal variables owing to the fact that the concept of plastic spin was introduced in order to determine a proper objective rate of the kinematic variables which will be used in their respective evolution equations.

Recall that the configuration $\tilde{\kappa}_p$ physically represents the substructure of the material and hence, all the constitutive relations are formulated in this configuration. Therefore, the internal state variable is first pushed back into this configuration through the relation $\boldsymbol{\mathcal{A}}_i = \boldsymbol{\mathcal{R}}^{p^T} \, \mathrm{A}_i \, \boldsymbol{\mathcal{R}}^{\boldsymbol{p}}$ [2]. When expressed in the set of bases $\{\tilde{\boldsymbol{e}}_I\}$, it is reasonable to assume that the matrix of $\boldsymbol{\mathcal{A}}_i$ will be a full matrix. We further assume that this matrix has a non-zero determinant, i.e., $\det(\boldsymbol{\mathcal{A}}_i) \neq 0$. One can

[1]One can also defined the substructural spin as $\dot{\boldsymbol{\mathcal{R}}}^{p^T} \, \boldsymbol{\mathcal{R}}^p$ which upon integration provides the rotation tensor $\boldsymbol{\mathcal{R}}^{p^T}$. Note that $\boldsymbol{\mathcal{R}}^{p^T}$ is directly responsible for rotating the director vectors. Since $\boldsymbol{\mathcal{R}}^{\boldsymbol{p}^{\boldsymbol{T}}} \, \boldsymbol{\mathcal{R}}^{\boldsymbol{p}} = \boldsymbol{I}$, one can show that $\dot{\boldsymbol{\mathcal{R}}}^p \, \boldsymbol{\mathcal{R}}^{\boldsymbol{p}^{\boldsymbol{T}}} = -\dot{\boldsymbol{\mathcal{R}}}^{p^T} \, \boldsymbol{\mathcal{R}}^{\boldsymbol{p}}$. Therefore, both of these definitions are equivalent.

[2]Here, the internal state variables are considered to be second-order tensors.

now perform a Gram-Schmidt procedure on the matrix of $\boldsymbol{\mathcal{A}}_i$ resulting in

$$\boldsymbol{\mathcal{A}}_i = \boldsymbol{\mathcal{R}}^{\mathcal{A}_i} \boldsymbol{\mathcal{U}}^{\mathcal{A}_i} \tag{6.3}$$

where $\boldsymbol{\mathcal{R}}^{\mathcal{A}_i}$ is an orthogonal and $\boldsymbol{\mathcal{U}}^{\mathcal{A}_i}$ is an upper-triangular matrix. Clearly, the upper-triangular matrix $\boldsymbol{\mathcal{U}}^{\mathcal{A}_i}$ represents the "rotation-free" part of the internal state variable $\boldsymbol{\mathcal{A}}_i$ and its components are given in a new set of bases obtained through a rotation of the set of bases $\{\tilde{e}_I\}$ by $\boldsymbol{\mathcal{R}}^{\mathcal{A}_i}$. The assumption of a non-zero determinant for the matrix of $\boldsymbol{\mathcal{A}}_i$ ensures that its decomposition in Eqn. (6.3) is unique. For the time being, we focus on the rotation part of the internal variable. Nevertheless its counterpart $\boldsymbol{\mathcal{U}}^{\mathcal{A}_i}$ plays an essential role in constitutive formulation and will be discussed later.

From the physical significance of a Gram-Schmidt decomposition as discussed in § 1.2.1, it is apparent that the orthogonal tensor $\boldsymbol{\mathcal{R}}^{\mathcal{A}_i}$ represents the change in orientation of the internal state variable $\boldsymbol{\mathcal{A}}_i$ with respect to the bases of the space $\tilde{\kappa}_p$ and hence, the substructure of the material. Therefore, a spin tensor $\boldsymbol{\Omega}^p$ defined as $\boldsymbol{\Omega}^p := \dot{\boldsymbol{\mathcal{R}}}^{\mathcal{A}_i} \boldsymbol{\mathcal{R}}^{\mathcal{A}_i T}$ represents the spin of the structural internal variable $\boldsymbol{\mathcal{A}}_i$ with respect to the substructure. This spin tensor can now be defined as the plastic spin corresponding to the internal structure variable $\boldsymbol{\mathcal{A}}_i$ in accordance with the terminology of Dafalias (1998) [21]. One can possibly assume that the material spin can be related to the substructural spin and the plastic spin via

$$\mathrm{skw}(\mathbf{L}^p) = \boldsymbol{\omega}_s^p + \boldsymbol{\Omega}^p. \tag{6.4}$$

Notice that a stark difference exists between Dafalias' [21] findings and the substructural spin defined in Eqn. (6.1). In his work, Dafalias argued that all the internal state variables need not co-rotate with the same spin tensor with respect to the substructure of the material. Therefore, relying on Eqn. (6.4), the material spin is decomposed into substructural spin and plastic spin, corresponding to each internal state variable. Clearly, this decomposition will vary from one internal state variable to another. In our framework, the substructural spin arises from a more physical argument and is much in sync with Mandel's idea of director vectors. Although it is possible to consider different plastic spins (i.e., spins of internal variables with respect to the substructure), Eqn. (6.4) puts a restriction on the values of these plastic spins. In fact, Eqn. (6.4) restricts all the plastic spins to be the same. It is also worth noting that since the rotation tensor $\boldsymbol{\mathcal{R}}^{\mathcal{A}_i}$ is obtained from a Gram-Schmidt factorization of the matrix of $\boldsymbol{\mathcal{A}}_i$, the elements of this rotation tensor solely depends on the column vectors of the matrix of $\boldsymbol{\mathcal{A}}_i$. Thus, in general, Eqn. (6.4) is too restrictive and may not hold for all possible internal state variables.

If the relation between material, substructual and plastic spin holds, then, in view of Eqn. (6.4), the plastic spin can be written as

$$\boldsymbol{\Omega}^p = \boldsymbol{\mathcal{R}}^{\boldsymbol{p}} \, \mathrm{skw}(\boldsymbol{\mathcal{L}}^p) \, \boldsymbol{\mathcal{R}}^{\boldsymbol{p}^T} \tag{6.5}$$

where skw() denotes the anti-symmetric part of a second-order tensor. Therefore, the plastic spin can be expressed as the anti-symmetric part of the plastic velocity gradient $\boldsymbol{\mathcal{L}}^p$ associated with the plastic Laplace stretch $\boldsymbol{\mathcal{U}}^p$, pushed forward into the configuration κ_p. Thus, Eqn. (6.4) acts as a constitutive assumption for the plastic spin. Moreover, now it is possible to establish distinctive connections between the three spin tensors with the three pertinent kinematic variables. While the anti-symmetric part of L^p and $\boldsymbol{\mathcal{L}}^p$ in the configuration κ_p are associated with the material and plastic spin respectively, the substructural spin can be obtained from the plastic rotation tensor $\boldsymbol{\mathcal{R}}^{\boldsymbol{p}}$.

6.1.1 Single crystal plasticity

The above result has a particular significance in single crystal plasticity. Let us first consider that only one slip system is activated in the crystal. For a single crystal lattice, a slip system α is completely characterized by a slip direction $\boldsymbol{s}^\alpha$ and normal to the slip plane $\boldsymbol{m}^\alpha$. Vectors $\boldsymbol{s}^\alpha$ and $\boldsymbol{m}^\alpha$ are constants for a slip system with $\|\boldsymbol{s}^\alpha\| = \|\boldsymbol{m}^\alpha\| = 1$ and orthogonal to each other, i.e., $\boldsymbol{s}^\alpha \cdot \boldsymbol{m}^\alpha = 0$. Note that these slip direction and slip plane-normal are measured in an Eulerian frame of reference, i.e., configuration κ_p of the body, in our notation. Now, the Schmidt tensor for this slip system is defined as

$$\mathbb{S}^\alpha = \boldsymbol{s}^\alpha \otimes \boldsymbol{m}^\alpha. \tag{6.6}$$

Because plastic flow in a single crystal is caused by slipping on a particular slip system, whose slip strain rate is denoted by γ^α, then the evolution of the plastic deformation gradient must be governed by

$$\mathbf{L}^p = \gamma^\alpha \, \mathbb{S}^\alpha = \gamma^\alpha \, \boldsymbol{s}^\alpha \otimes \boldsymbol{m}^\alpha. \tag{6.7}$$

Now pulling back these fields into configuration $\tilde{\kappa}^p$, the plastic velocity gradient of our physical frame of reference $\boldsymbol{\mathcal{L}}^p$, can be written as

$$\boldsymbol{\mathcal{L}}^p + \boldsymbol{\mathcal{R}}^{\boldsymbol{p}^T} \, \boldsymbol{\omega}_s^p \, \boldsymbol{\mathcal{R}}^{\boldsymbol{p}} = \gamma^\alpha \, \boldsymbol{\mathcal{R}}^{\boldsymbol{p}^T} \, \mathbb{S}^\alpha \, \boldsymbol{\mathcal{R}}^{\boldsymbol{p}} = \gamma^\alpha \, \tilde{\boldsymbol{s}}^\alpha \otimes \tilde{\boldsymbol{m}}^\alpha. \tag{6.8}$$

where the substructural spin has been pulled back into the current configuration $\tilde{\kappa}_p$. The slip direction and the slip plane normal are also pulled back into this configuration through the relation

$$\tilde{\boldsymbol{s}}^\alpha = \boldsymbol{\mathcal{R}}^{\boldsymbol{p}^T} \boldsymbol{s}^\alpha; \qquad \tilde{\boldsymbol{m}}^\alpha = \boldsymbol{\mathcal{R}}^{\boldsymbol{p}^T} \boldsymbol{m}^\alpha. \tag{6.9}$$

Now from Eqn. (6.8), the anti-symmetric part of the plastic velocity gradient, $\boldsymbol{\mathcal{L}}^p$ can be written as

$$\operatorname{skw}(\boldsymbol{\mathcal{L}}^p) = \boldsymbol{\Omega} + \gamma^\alpha \operatorname{skw}(\tilde{\boldsymbol{s}}^\alpha \otimes \tilde{\boldsymbol{m}}^\alpha) \tag{6.10}$$

where $\boldsymbol{\Omega} = -\boldsymbol{\mathcal{R}}^{\boldsymbol{p}^T} \, \boldsymbol{\omega}_s^p \, \boldsymbol{\mathcal{R}}^{\boldsymbol{p}}$. Dafalias (1998) [21] noted that in traditional single crystal plasticity theory, the spin tensor $\boldsymbol{\Omega}$ is often neglected. In fact, the concept of plastic spin enters into the theory through this spin tensor. From the above derivation, it can be clearly understood that this spin tensor appears in Eqn. (6.8) as a direct consequence of using a **QR** decomposition and no further assumption of the existence of a plastic spin is required. Physically, this is possible owing to the physical interpretation of the rotation tensor $\boldsymbol{\mathcal{R}}^{\boldsymbol{p}}$ and its close association with the concept of director vectors as discussed earlier. Eqn. (6.8) can be easily extended to a single crystal system in which multiple slip systems are activated. In this case, this equation takes on the form

$$\mathrm{skw}(\boldsymbol{\mathcal{L}}^p) = \boldsymbol{\Omega} + \sum_{\alpha=1}^{A} \gamma^\alpha \, \mathrm{skw}(\tilde{\boldsymbol{s}}^\alpha \otimes \tilde{\boldsymbol{m}}^\alpha) \tag{6.11}$$

where A is the number of active slip systems.

6.2 Incorporation into constitutive model

The primary objective of introducing the concept of plastic spin is to define an appropriate objective rate of the kinematic variables including the internal state variables in their respective evolution equations. As mentioned earlier, the internal state variables may represent different physical quantities. One such quantity that is typically represented by an internal state variable is plastically-induced anisotropy that evolves during the plastic deformation. However, in our theory, plastically-induced anisotropy is incorporated into the constitutive model in a different way. Therefore, in this section, we focus on developing a constitutive model for elastic-plastic materials that captures plastically-induced anisotropy as well as a general, tensor-valued, kinematic internal variable. Here we develop constitutive models using scalar, conjugate stress/strain base pairs for isotropic and anisotropic elastic materials. As mentioned earlier, this constitutive formulation is derived by deconstructing the stress power at a material point into different modes of deformation.

In terms of the strain attributes and their thermodynamic conjugates defined in Eqns. (1.11a)–(1.11g), the stress power can be expressed as

$$\dot{W} = \pi\dot{\delta} + \sum_{i=1}^{3} \left(\sigma_i \dot{\varepsilon}_i + \tau_i \dot{\gamma}_i\right) \tag{6.12}$$

where π, σ_i and τ_i are the volumetric, squeeze and shear strain attributes and thermodynamic conjugates to δ, ε_i and γ_i respectively. The stress and strain attributes are related to the components of velocity gradient and Kirchhoff stress through bijective maps that depend on the type of materials under consideration. It is interesting to note that in this framework, an anisotropic material response does not enter into the constitutive model directly through the material parameters. Instead, the anisotropy is enfolded in the encoding/decoding map that relates the components of the velocity gradient $\boldsymbol{\mathcal{L}}$ and the strain rate attributes, and the components of the Kirchhoff stress $\boldsymbol{\mathcal{S}}$ and the stress attributes. For an anisotropic, elastic materials the components of the Kirchhoff stress $\boldsymbol{\mathcal{S}}$ and $\boldsymbol{\mathcal{L}}$ are related to the stress and the strain rate attributes through Eqns. (1.19) and (1.18) respectively.

Now the question of which kinematic variables (plastic strain rate attributes or objective rate of internal state variable) are to be used depends on the configuration in which the constitutive relations are formulated. From the discussion in § 1.2.1 and 6.1, it is quite evident that the configuration $\tilde{\kappa}_p$ is of utmost importance in our framework, mainly for two reasons– *(i)* the components of the plastic Laplace stretch are measured in this configuration and, *(ii)* physically it represents a macroscopic manifestation of the material substructure. Recall that unlike the plastic deformation gradient, $\mathbf{F}^p$, arising from a multiplicative decomposition of the deformation gradient, the plastic Laplace stretch stems from a decomposition of the "rotation-free" Laplace stretch, $\boldsymbol{\mathcal{U}}$. Moreover, the plastic Laplace stretch is measured in the configuration $\tilde{\kappa}_p$ which implies that the measured plastic strain rate attributes identically co-rotate with the substructure of the material. Therefore, it is reasonable to define the plastic strain rate attributes through an appropriate encoding/decoding map in a similar fashion as in Eqn. (1.18). The plastic strain rate attributes are defined as

$$\begin{Bmatrix} \dot{\delta}^p \\ \dot{\varepsilon}_1^p \\ \dot{\varepsilon}_2^p \\ \dot{\gamma}_1^p \\ \dot{\gamma}_2^p \\ \dot{\gamma}_3^p \end{Bmatrix} = \begin{bmatrix} vw/3u & uw/3v & uv/3w & 0 & 0 & 0 \\ vw/3u & -uw/3v & 0 & 0 & 0 & 0 \\ 0 & uw/3v & -uv/3w & 0 & 0 & 0 \\ 0 & 0 & 0 & c^p/b^p & 0 & 0 \\ 0 & 0 & 0 & 0 & c^p/a^p & b^p\gamma_1^p/a^p \\ 0 & 0 & 0 & 0 & 0 & b^p/a^p \end{bmatrix} \begin{Bmatrix} \mathcal{L}_{11}^p \\ \mathcal{L}_{22}^p \\ \mathcal{L}_{33}^p \\ \mathcal{L}_{23}^p \\ \mathcal{L}_{13}^p \\ \mathcal{L}_{12}^p \end{Bmatrix} \tag{6.13}$$

with

$$l_{\dot{\mathcal{U}}^p} := \{\ \dot{\delta}^p \quad \dot{\varepsilon}_1^p \quad \dot{\varepsilon}_2^p \quad \dot{\varepsilon}_3^p \quad \dot{\gamma}_1^p \quad \dot{\gamma}_2^p \quad \dot{\gamma}_3^p\ \} \tag{6.14}$$

where $\boldsymbol{\mathcal{L}}^{\boldsymbol{p}} := \dot{\boldsymbol{\mathcal{U}}}^{\boldsymbol{p}}\boldsymbol{\mathcal{U}}^{\boldsymbol{p}-1}$ and $\dot{\varepsilon}_3^p = -(\dot{\varepsilon}_1^p + \dot{\varepsilon}_2^p)$. For convenience, let us replace the parameters u,

v and w with $n_j, j = 1, 2, 3$, defined as $n_1 := u/vw, n_2 := v/uw$ and $n_3 := w/uv$. Note that although Eqns. (1.13), (1.14), (1.15) and, (1.32), (1.39) are still valid in case of plastically-induced (and hence, evolving) anisotropic materials, the definitions of the total strain attributes and their plastic counterparts need to be revised. While determining the total and plastic strain attributes by integrating the strain rates, one must keep in mind that the parameters u, v and w (or alternatively, $n_j, j = 1, 2, 3$) must be considered as variables here in order to capture the development of induced anisotropy.

This definition of plastic strain rate attributes is in contrast with Dafalias (1985,1998) [22, 21] where it was necessary to work with a co-rotational rate of the kinematic variables (e.g., the plastic velocity gradient and the associated rate of deformation tensor) especially when development of plastically-induced anisotropy is considered. In our framework, the plastically-induced anisotropy is incorporated by means of considering the anisotropy parameters u, v and w (or, n_j) as variables evolving with the plastic deformation. In connection to this approach, it is also instructive that Van der Giessen (1989,1991) [92, 93] addressed the issue of plastically-induced anisotropy by considering the deformation of an additional set of director vectors embedded in the material substructure. This additional set of director vectors is not the same as the one introduced by Mandel [61, 62] and is designated to solely represent the evolving material anisotropy throughout the deformation process. Although our approach mathematically resembles the idea of Van der Giessen to some extent, the underlying physics behind these two approaches are vastly different. In our method, the parameters u, v and w simply represent the strength of anisotropy along one of the base vectors $\tilde{\boldsymbol{e}}_I, I = 1, 2, 3$ over the others. As noted earlier, the base vectors $\tilde{\boldsymbol{e}}_I$, obtained from a Gram-Schmidt factorization of the deformation gradient, are physically similar to the idea of director vectors introduced by Mandel. Thus, no additional set of director vectors are required to capture the plastically-induced anisotropy in this case.

Although for plastic strain rate attributes it is sufficient to use only a simple time derivative of the pertinent kinematic variable in their definitions, the same is not true for internal state variables. In general, the internal state variables need not co-rotate with the material substructure resulting in a full matrix structure for the pulled back internal variable $\boldsymbol{\mathcal{A}}_i$ when represented in the set of base vectors $\tilde{\boldsymbol{e}}_I$. In fact, a Gram-Schmidt factorization of this matrix reveals that the internal state variable rotates with a spin Ω^p with respect to the material substructure. The time integration of this spin tensor produces the orthogonal rotation $\boldsymbol{\mathcal{R}}^{\mathcal{A}_i}$. It is evident from the discussion on **QR** decomposition in § 1.2.1 that the matrix of $\boldsymbol{\mathcal{A}}_i$ takes on the form of an upper-triangular matrix $\boldsymbol{\mathcal{U}}^{\mathcal{A}_i}$ in a new set of base vectors rotated from the substructure (i.e., the configuration $\tilde{\kappa}_p$) by $\boldsymbol{\mathcal{R}}^{\mathcal{A}_i}$. Therefore, to incorporate the internal state variables in our constitutive formulation, we must work with a co-rotational rate of its “rotation-free" part $\boldsymbol{\mathcal{U}}^{\mathcal{A}_i}$ with respect to the plastic spin $\boldsymbol{\Omega}^p$, defined as

$$\overset{\circ}{\boldsymbol{\mathcal{U}}}^{\mathcal{A}_i} := \dot{\boldsymbol{\mathcal{U}}}^{\mathcal{A}_i} - \boldsymbol{\Omega}^p \boldsymbol{\mathcal{U}}^{\mathcal{A}_i} + \boldsymbol{\mathcal{U}}^{\mathcal{A}_i} \boldsymbol{\Omega}^p \tag{6.15}$$

where $\overset{\circ}{\square}$ represents a co-rotational rate with respect to a spin tensor (in this case, $\boldsymbol{\Omega}^p$). The upper-triangular matrix $\boldsymbol{\mathcal{U}}^{\mathcal{A}_i}$ physically represents the current state of the internal variable at a particular time instant. Moreover, due to its upper-triangular nature, it is possible to decompose this matrix similar to the decomposition of Laplace stretch in Eqns. (1.8) and (1.9) and define a list of variables containing seven scalar variables, each corresponding to a separate mode of deformation of the material substructure, that collectively represent an internal state variable in a rotated coordinate frame with respect to the substructure. This list of variables consisting of these scalar variables is given as

$$l_{\mathcal{A}_i} = \{ \; \delta^{\mathcal{A}_i} \quad \varepsilon_1^{\mathcal{A}_i} \quad \varepsilon_2^{\mathcal{A}_i} \quad \varepsilon_3^{\mathcal{A}_i} \quad \gamma_1^{\mathcal{A}_i} \quad \gamma_2^{\mathcal{A}_i} \quad \gamma_3^{\mathcal{A}_i} \; \} \tag{6.16}$$

where $\delta^{\mathcal{A}_i}, \varepsilon_j^{\mathcal{A}_i}, \gamma_j^{\mathcal{A}_i}, j = 1, 2, 3$ represent the internal state variable $\boldsymbol{\mathcal{A}}_i$ corresponding to dilatation, squeeze and shear of the substructure respectively. Despite of the physical meaning of the components of $l_{\mathcal{A}_i}$ and its congruence with the current theory, these scalar variables cannot be used in the constitutive formulation. Since there is no reason for the co-rotational rate of the internal state variable $\overset{\circ}{\boldsymbol{\mathcal{U}}}^{\mathcal{A}_i}$ to be upper-triangular, it cannot be decomposed into different modes of deformation and thus, cannot be expressed by a collection of scalar variables. Therefore, one must deal with tensorial variables when it comes to the internal state variable $\boldsymbol{\mathcal{A}}_i$. This is a major consequence of using the co-rotational rate, or in other words, using the concept of plastic spin in our theory.

Now we proceed to derive the evolution equations for the plastic strain rate attributes $l_{\dot{\mathcal{U}}^p}$, the anisotropy parameters n_j and, the internal state variables $\boldsymbol{\mathcal{A}}_i$. Here in addition to the laws of thermodynamics, we use a maximum rate of dissipation criterion. In our framework, the configuration $\tilde{\kappa}_p$ acts as a natural configuration from which the elastic response of the body is measured. The natural configuration itself evolves with plastic deformation process. Therefore, the response of a body can be described as a family of elastic responses measured from a set of evolving natural configurations. We assume that for each natural configuration there exists a non-null elastic domain. Therefore, we admit two functions prior to applying a maximum rate of dissipation criterion: *(i)* a Helmholtz potential function ψ from which the elastic response of a body for a fixed natural configuration is derived and, *(ii)* a dissipation function ξ representing the energy dissipated during a plastic deformation process, i.e., the evolution of the natural configuration $\tilde{\kappa}_p$. For the sake of generality, throughout the constitutive formulation, we will assume that the material response is anisotropic.

Since the elastic response of the body depends upon the deformation of the body measured from the undeformed configuration κ_r and the fixed natural configuration $\tilde{\kappa}_p$, it is reasonable to assume that the Helmholtz potential function has the form

$$\psi = \overline{\psi}(\boldsymbol{\mathcal{U}}, \boldsymbol{\mathcal{U}^p}, \overline{n}_j) = \hat{\psi}(l_{\mathcal{U}}, l_{\mathcal{U}^p}, \overline{n}_j) \tag{6.17}$$

where $\dot{\overline{n}}_j = n_j, j = 1, 2, 3$. Note that we have not considered the internal state variables $\boldsymbol{\mathcal{A}}_i$ in the arguments of ψ since the internal state variables are associated only with the plastic deformation of the body. Now the elastic domain of the material for a fixed natural configuration is characterized by

$$\boldsymbol{\mathcal{L}^p} = \mathbf{0} \implies \dot{\delta}^p = \dot{\varepsilon}^p_j = \dot{\gamma}^p_j = 0. \tag{6.18}$$

The rate of dissipation function can be determined from an isothermal energy balance equation. If

$\boldsymbol{\mathcal{P}}_i$ denotes the kinetic conjugate [3] of the internal state variable, then the rate of dissipation can be defined as

$$\xi := \dot{W} - \rho_0 \dot{\psi} - \boldsymbol{\mathcal{P}}_i : \overset{\circ}{\boldsymbol{\mathcal{U}}}^{\mathcal{A}_i} \geq 0 \tag{6.19}$$

where for any two tensors $\mathbf{A}$ and $\mathbf{B}$, $\mathbf{A} : \mathbf{B}$ denotes the scalar dot product such that $\mathbf{A} : \mathbf{B} = A_{ij}\, B_{ij}$. The assumption of non-negativity of ξ ensures that the Clausius-Duhem inequality is identically satisfied. From Eqn. (6.19), it is evident that the dissipation function has the functional form of

$$\xi = \bar{\xi}(\boldsymbol{\mathcal{U}}^{\boldsymbol{p}}, \dot{\boldsymbol{\mathcal{U}}}^{\boldsymbol{p}}, n_j, \overset{\circ}{\boldsymbol{\mathcal{U}}}^{\mathcal{A}_i}) = \hat{\xi}(\delta^p, \varepsilon^p_j, \gamma^p_j, \dot{\delta}^p, \dot{\varepsilon}^p_j, \dot{\gamma}^p_j, n_j, \overset{\circ}{\boldsymbol{\mathcal{U}}}^{\mathcal{A}_i}). \tag{6.20}$$

Note that unlike the Helmholtz potential function ψ, the argument of the dissipation rate $\hat{\xi}$ contains both scalar as well as tensorial kinematic variables owing to the nature of the co-rotation rate of the internal state variables. Moreover, the Helmholtz potential function and the rate of dissipation function both explicitly and implicitly depend on the anisotropy parameters n_j as they are directly related only to the dilatational and squeeze strain rate attributes. Now invoking Eqn. (6.17) into Eqn. (6.19), we obtain

$$\begin{aligned}\left(\pi - \rho_0 \frac{\partial \hat{\psi}}{\partial \delta}\right) \dot{\delta} + \sum_{j=1}^{3} \left[\left(\sigma_j - \rho_0 \frac{\partial \hat{\psi}}{\partial \varepsilon_j}\right) \dot{\varepsilon}_j + \left(\tau_j - \rho_0 \frac{\partial \hat{\psi}}{\partial \gamma_j}\right) \dot{\gamma}_j \right] &= \xi + \rho_0 \frac{\partial \hat{\psi}}{\partial \delta^p} \dot{\delta}^p \\ + \rho_0 \sum_{j=1}^{3} \left[\frac{\partial \hat{\psi}}{\partial \varepsilon^p_j} \dot{\varepsilon}^p_j + \rho_0 \frac{\partial \hat{\psi}}{\partial \gamma_j} \dot{\gamma}_j + \frac{\partial \hat{\psi}}{\partial \overline{n}_j}\, n_j \right] &+ \boldsymbol{\mathcal{P}}_i : \overset{\circ}{\boldsymbol{\mathcal{U}}}^{\mathcal{A}_i}.\end{aligned} \tag{6.21}$$

Let us assume that the elastic response of the body is that of a Green elastic solid. Therefore, the total stress attributes can be written in terms of the derivatives of the Helmholtz potential function

[3] often termed as a microstress

with respect to the total strain attributes as

$$\pi = \rho_0 \, \frac{\partial \hat{\psi}}{\partial \delta}, \tag{6.22a}$$

$$2\sigma_1 + \sigma_2 = \rho_0 \, \frac{\partial \hat{\psi}}{\partial \varepsilon_1}, \tag{6.22b}$$

$$\sigma_1 + 2\sigma_2 = \rho_0 \, \frac{\partial \hat{\psi}}{\partial \varepsilon_2}, \tag{6.22c}$$

$$\tau_j = \rho_0 \, \frac{\partial \hat{\psi}}{\partial \gamma_j}, \quad j = 1, 2, 3. \tag{6.22d}$$

with $\sigma_3 = -(\sigma_1 + \sigma_2)$ and $\varepsilon_3 = -(\varepsilon_1 + \varepsilon_2)$. With this assumption on the elastic response of the body, Eqn. (6.21) reduces to

$$\hat{\xi} + \rho_0 \frac{\partial \hat{\psi}}{\partial \delta^p} \dot{\delta}^p + \rho_0 \sum_{j=1}^{3} \left[\frac{\partial \hat{\psi}}{\partial \varepsilon_j^p} \dot{\varepsilon}_j^p + \rho_0 \frac{\partial \hat{\psi}}{\partial \gamma_j} \dot{\gamma}_j + \frac{\partial \hat{\psi}}{\partial \overline{n}_j} \, n_j \right] + \boldsymbol{\mathcal{P}}_i : \overset{\circ}{\boldsymbol{\mathcal{U}}}^{\mathcal{A}_i} = 0. \tag{6.23}$$

Now to determine evolution equations for the plastic strain rates and the internal state variables, we apply a principle of maximum rate of dissipation. According to this criterion, of all the admissible values for the plastic velocity gradient $\boldsymbol{\mathcal{L}}^{\boldsymbol{p}}$, anisotropy parameters n_j and the co-rotational rate of internal state variable $\overset{\circ}{\boldsymbol{\mathcal{U}}}^{\mathcal{A}_i}$ satisfying the reduced rate of dissipation constraint (6.23), the ones that maximize the rate of dissipation ξ govern the evolution of the natural configuration $\tilde{\kappa}_p$. Note that if the anisotropy parameters u, v and w were considered to be constants, i.e., evolution of anisotropy with the plastic deformation process were not to be considered, one could carry out the maximization of ξ with respect to the variables listed in $l_{\dot{\mathcal{U}}^p}$ individually, instead of the plastic velocity gradient $\boldsymbol{\mathcal{L}}^{\boldsymbol{p}}$ or its components. However, in this case, the components of the plastic velocity gradient need to be expressed in terms of the plastic strain rate attributes and the anisotropy parameters before carrying out the optimization process. This is achieved by inverting the relation (1.18) which yields

$$\begin{Bmatrix} \mathcal{L}_{11} \\ \mathcal{L}_{22} \\ \mathcal{L}_{33} \\ \mathcal{L}_{23} \\ \mathcal{L}_{13} \\ \mathcal{L}_{12} \end{Bmatrix} = \begin{bmatrix} n_1 & 2n_1 & n_1 & 0 & 0 & 0 \\ n_2 & -n_2 & n_2 & 0 & 0 & 0 \\ n_3 & -n_3 & -2n_3 & 0 & 0 & 0 \\ 0 & 0 & 0 & b^p/c^p & 0 & 0 \\ 0 & 0 & 0 & 0 & a^p/c^p & -a^p\gamma_1^p/c^p \\ 0 & 0 & 0 & 0 & 0 & a^p/b^p \end{bmatrix} \begin{Bmatrix} \dot{\delta}^p \\ \dot{\varepsilon}_1^p \\ \dot{\varepsilon}_2^p \\ \dot{\gamma}_1^p \\ \dot{\gamma}_2^p \\ \dot{\gamma}_3^p \end{Bmatrix}. \tag{6.24}$$

Note that the relationships between the components of $\boldsymbol{\mathcal{L}^p}$ and the shear strain rates $\dot{\gamma}_i^p$ do not involve the anisotropy parameters. Therefore, for the shear modes of deformation, it is reasonable to carry out the maximization of ξ with respect to the strain rate attributes $\dot{\gamma}_i^p$. However, this cannot be done for the dilatation and squeeze modes of deformation. In these cases, an optimization process must be carried out explicitly with respect to the components of $\boldsymbol{\mathcal{L}^p}$, specifically $\boldsymbol{\mathcal{L}^p}_{11}$, $\boldsymbol{\mathcal{L}^p}_{22}$ and $\boldsymbol{\mathcal{L}^p}_{33}$. Here we have considered that the volume of the body changes during plastic deformation. Therefore, the optimization process is executed with only the reduced rate of dissipation constraint (6.23). In case of metal plasticity, it is often considered that the plastic deformation process is volume-preserving, i.e., $\dot{\delta}^p = 0$. This condition enters into the constitutive model as an additional constraint when a volume-preserving motion is considered.

The maximization process can be worked out using two different methods depending on the nature of the rate of dissipation function. If ξ is assumed to be a smooth function, then the optimization process can be carried out using a standard Lagrange multiplier technique with respect to the components of $\boldsymbol{\mathcal{L}}^p$, the anisotropy parameters n_j and, the co-rotational rate of internal state variables $\overset{\circ}{\boldsymbol{\mathcal{U}}}^{\mathcal{A}_i}$ with ξ being the objective function and Eqn. (6.23) as a constraint. A smooth rate of dissipation function is typically exhibited by materials that do not have a definite yield surface and possess a creep behavior. Details of this maximization process are provided in App. D. Using a Lagrange multiplier technique to maximize ξ, we obtain

$$\frac{\partial \hat{\xi}}{\partial \dot{\delta}^p} = -\lambda\, \rho_0\, \frac{\partial \hat{\psi}}{\partial \delta^p}; \qquad \frac{\partial \hat{\xi}}{\partial \dot{\varepsilon}_j^p} = -\lambda\, \rho_0\, \frac{\partial \hat{\psi}}{\partial \varepsilon_j^p}; \qquad \frac{\partial \hat{\xi}}{\partial \dot{\gamma}_j^p} = -\lambda\, \rho_0\, \frac{\partial \hat{\psi}}{\partial \gamma_j^p} \tag{6.25 a}$$

$$\frac{\partial \hat{\xi}}{\partial n_j} = -\lambda\, \rho_0\, \frac{\partial \hat{\psi}}{\partial \overline{n}_j} \tag{6.25 b}$$

$$\frac{\partial \hat{\xi}}{\partial \mathring{\boldsymbol{\mathcal{U}}}^{\mathcal{A}_i}} = -\lambda\, \boldsymbol{\mathcal{P}}_i \tag{6.25 c}$$

where $\lambda = \overline{\lambda}/(1+\overline{\lambda})$ and $\overline{\lambda}$ is the Lagrange multiplier to be determined by substituting Eqns. (6.25 a), (6.25 b) and (6.25 c) into the reduced rate of dissipation constraint (6.23). Thus, λ can be obtained as

$$\lambda = \frac{1}{\xi}\left[\dot{\delta}^p\, \frac{\partial \hat{\xi}}{\partial \dot{\delta}^p} + \sum_{j=1}^{3}\left(\dot{\varepsilon}_j^p \frac{\partial \hat{\xi}}{\partial \dot{\varepsilon}_j^p} + \dot{\gamma}_j^p \frac{\partial \hat{\xi}}{\partial \dot{\gamma}_j^p} + n_j \frac{\partial \hat{\xi}}{\partial n_j}\right) + \frac{\partial \hat{\xi}}{\partial \mathring{\boldsymbol{\mathcal{U}}}^{\mathcal{A}_i}} : \mathring{\boldsymbol{\mathcal{U}}}^{\mathcal{A}_i}\right]. \tag{6.26}$$

Clearly, the evolution equations (Eqns. (6.25 a) – (6.25 c)) for the plastic strain attributes, anisotropy parameters and the internal state variables are a set of implicit equations. In the above derivation, the rate of dissipation is maximized keeping the stress attributes fixed while the strain rate attributes and other kinematic variables are allowed to vary. It is possible to derive explicit evolution equations for the kinematic variables if the condition is reversed, i.e., their conjugate kinetic variables are allowed to vary while the strain attributes and other kinematic variables are held fixed. This inversion is typically difficult for the plastic strain attributes and the associated stress unless a special form for the Helmholtz potential function ψ is assumed. Moreover, the evolution equations obtained thus far helps us to identify the thermodynamic conjugates corresponding to the anisotropy parameters n_j. If m_j denotes the microforce responsible for the change in anisotropy parameter $\overline{n}_j$, then in view of Eqn. (6.25 b), m_j can be defined as $m_j := \rho_0\, \partial\hat{\psi}/\partial\overline{n}_j$.

Since Eqn. (1.39) is valid for the revised definition of strain attributes for anisotropic materials, it can be concluded that the difference between the total strain attributes and their corresponding plastic counterparts represents the elastic strain attributes or their linear combinations. Therefore, it is reasonable to assume that the Helmholtz potential function has the form

$$\psi = \hat{\psi}(l_{\mathcal{U}}, l_{\mathcal{U}^p}, \overline{n}_j) = \frac{1}{2}\Big[N_{00}\,\overline{g}_{00}(\overline{n}_j)\,(\delta-\delta^p)^2 + \sum_{i=1}^{3} N_{0i}\,\overline{g}_{oi}(\overline{n}_j)\,(\delta-\delta^p)\,(\varepsilon_i-\varepsilon_i^p)$$
$$+ \sum_{i=1}^{3} N_{0(i+3)}\,\overline{g}_{0(i+3)}(\overline{n}_j)\,(\delta-\delta^p)\,(\gamma_i-\gamma_i^p) + \sum_{\substack{i,j=1\\ i\le j}}^{3} N_{ij}\,\overline{g}_{ij}(\overline{n}_j)\,(\varepsilon_i-\varepsilon_i^p)\,(\varepsilon_j-\varepsilon_j^p)$$
$$+ \sum_{i,j=1}^{3} N_{i(j+3)}\,\overline{g}_{i(j+3)}(\overline{n}_j)\,(\varepsilon_i-\varepsilon_i^p)\,(\gamma_j-\gamma_j^p) + \sum_{\substack{i,j=1\\ i\le j}}^{3} N_{(i+3)(j+3)}\,(\gamma_i-\gamma_i^p)\,(\gamma_j-\gamma_j^p)\Big]. \tag{6.27}$$

where the N's are material parameters and $\overline{g}$'s are functions of the anisotropy parameters n_j. Here the decoupling of the contributions of the anisotropy parameters and the strain attributes to the Helmholtz potential function is possible because the total and plastic strain attributes are related to the components of velocity gradient $\boldsymbol{\mathcal{L}}$ and the plastic velocity gradient $\boldsymbol{\mathcal{L}^p}$ through the same encoding/decoding maps [4] respectively. The material parameters N are not all independent. This form for ψ leads to a Green elastic solid (i.e., hyperelastic) response. With this assumed form for the Helmholtz potential function, the stress attributes can be written as

$$\begin{aligned} \pi &= \rho_0 \frac{\partial\hat{\psi}}{\partial\delta} = -\rho_0 \frac{\partial\hat{\psi}}{\partial\delta^p}, \\ \sigma_j &= \rho_0 \frac{\partial\hat{\psi}}{\partial\varepsilon_j} = -\rho_0 \frac{\partial\hat{\psi}}{\partial\varepsilon_j^p}, \\ \tau_j &= \rho_0 \frac{\partial\hat{\psi}}{\partial\gamma_j} = -\rho_0 \frac{\partial\hat{\psi}}{\partial\gamma_j^p}. \end{aligned} \tag{6.28}$$

Substituting these relations into the reduced rate of dissipation equation (6.23), we obtain

$$\pi\,\dot{\delta}^p + \sum_{j=1}^{3}\big(\sigma_j\,\dot{\varepsilon}_j^p + \tau_j\,\dot{\gamma}_j^p - m_j\,n_j\big) - \boldsymbol{\mathcal{P}}_i : \overset{\circ}{\boldsymbol{\mathcal{U}}}^{\mathcal{A}_i} = \hat{\xi}. \tag{6.29}$$

[4]The encoding/decoding map that relates the total strain attributes to the velocity gradient $\boldsymbol{\mathcal{L}}$ involves the total stretch components a, b and c whereas their plastic counterparts are used in the map between plastic strain attributes and the components of $\boldsymbol{\mathcal{L}^p}$. However, this difference does not deter us from decoupling the contribution of the anisotropy parameters from that of the strain attributes as the stretch components are used in expressing only the shear strain attributes in terms of relevant components of velocity gradient. These components, in turn, are free from the effects of an evolving anisotropy.

Since the reduced rate of dissipation criterion has now been expressed as a product of the kinematic and their conjugate, kinetic attributes, it is now possible to carry out the maximization process with respect to either the set of kinematic or their conjugate, kinetic variables. Thereby, one can now derive a set of explicit evolution equations for the plastic strain attributes, anisotropy parameters and the internal state variables.

Before deriving explicit evolution equations for the kinematic variables, we need to talk about a yield criterion of the material in this framework. Following the arguments of Srinivasa (2010) [89], in view of the reduced rate of dissipation criterion (6.29), the yield criterion can be written as

$$Y(l_{km}) := \max_{l_{km} \neq \mathbf{0}} \frac{\pi\,\dot{\delta}^p + \sum_{j=1}^{3}\left(\sigma_j\,\dot{\varepsilon}_j^p + \tau_j\,\dot{\gamma}_j^p - m_j\,n_j\right) - \boldsymbol{\mathcal{P}}_i : \overset{\circ}{\boldsymbol{\mathcal{U}}}^{\mathcal{A}_i}}{\bar{\xi}(l_\sigma, l_{\mathcal{U}^p}, l_{\dot{\mathcal{U}}^p})} = 1 \tag{6.30}$$

where l_{km} denotes the list of kinematic variables such that

$$l_{km} = \{\ \dot{\delta}^p \quad \dot{\varepsilon}_1^p \quad \dot{\varepsilon}_2^p \quad \dot{\varepsilon}_3^p \quad \dot{\gamma}_1^p \quad \dot{\gamma}_2^p \quad \dot{\gamma}_3^p \quad n_1 \quad n_2 \quad n_3 \quad \overset{\circ}{\boldsymbol{\mathcal{U}}}^{\mathcal{A}_i}\ \}.$$

If the yield function $Y(l_{km}) < 1$ for some values of l_{km}, then the reduced rate of dissipation equation is violated and therefore, the response of the material is elastic. One can easily show that this yield function $Y(l_{km})$ is convex in the l_{km} space.

Let us now consider the case where the strain attributes, anisotropy parameters and the internal state variables are held fixed while their corresponding kinetic variables are allowed to vary. Let us also define a list of variables l_{kt} that contains all the kinetic variables as

$$l_{kt} = \{\ \pi \quad \sigma_1 \quad \sigma_2 \quad \sigma_3 \quad \tau_1 \quad \tau_2 \quad \tau_3 \quad m_1 \quad m_2 \quad m_3 \quad \boldsymbol{\mathcal{P}}_i\ \}.$$

In this case, the yield function can be defined as

$$Y(l_{kt}) := \max_{l_{kt} \neq \mathbf{0}} \frac{\pi\,\dot{\delta}^p + \sum_{j=1}^{3}\left(\sigma_j\,\dot{\varepsilon}_j^p + \tau_j\,\dot{\gamma}_j^p - m_j\,n_j\right) - \boldsymbol{\mathcal{P}}_i : \overset{\circ}{\boldsymbol{\mathcal{U}}}^{\mathcal{A}_i}}{\bar{\xi}(l_\sigma, l_{\mathcal{U}^p}, l_{\dot{\mathcal{U}}^p})} = 1. \tag{6.31}$$

One can also show that the yield function, defined in this way, is convex in the l_{kt} space. Now, a routine calculation to maximize the rate of dissipation function ξ with the reduced rate of dissipation constraint (6.29) with respect to the kientic variables listed in l_{kt} leads to

$$\begin{gathered} \dot{\delta}^p = \mu\,\frac{\partial \xi}{\partial \pi}, \qquad \dot{\varepsilon}_i^p = \mu\,\frac{\partial \xi}{\partial \sigma_i}, \qquad \dot{\gamma}_i^p = \mu\,\frac{\partial \xi}{\partial \tau_i}, \\ n_j = \mu\,\frac{\partial \xi}{\partial m_j}, \qquad \overset{\circ}{\boldsymbol{\mathcal{U}}}^{\mathcal{A}_i} = \frac{\partial \xi}{\partial \boldsymbol{\mathcal{P}}_i} \end{gathered} \tag{6.32}$$

where μ is the consistency parameter that satisfies the condition that $\mu = 0$ whenever $Y(l_{kt}) < 1$. The consistency parameter μ can be determined by substituting the plastic strain-rate attributes $l_{\dot{\mathcal{U}}^p}$, the anisotropy parameters n_j and the co-rotational rate of internal state variable $\overset{\circ}{\boldsymbol{\mathcal{U}}}^{\mathcal{A}_i}$ into the reduced rate of dissipation equation (6.29). Thus, Eqn. (6.32) provides explicit expressions for the evolution of the kinematic variables. Geometrically, Eqn. (6.32) implicates that the stress attributes are along the normal to the dissipation function at their corresponding strain rate attributes whereas the microstresses m_j and $\boldsymbol{\mathcal{P}}_i$ associated with the anisotropy parameters n_j and the internal state variables $\boldsymbol{\mathcal{U}}^{\mathcal{A}_i}$ are along the normal to the dissipation function at their corresponding kinematic conjugates. For materials that exhibit a yielding behavior, the dissipation function is no longer differentiable at $l_{km} = \mathbf{0}$. Therefore, a Lagrange multiplier method cannot be used to maximize the rate of dissipation function for those materials. In that case, a standard method of convex analysis can be applied to show that the kinetic variables l_{kt} are along the normal cone to the convex hull $\mathbb{C}_{l_{km}}$ at $\hat{l}_{km}$ where $\hat{l}_{km}$ denotes the set of kinematic variables that satisfies the yield condition $Y(\hat{l}_{km}) = 1$ and the convex hull $\mathbb{C}_{l_{km}}$ is defined as

$$\mathbb{C}_{l_{km}} := \lambda_0\,\dot{\delta}^p + \sum_{j=1}^{3} \left(\lambda_j\,\dot{\varepsilon}_j^p + \lambda_{j+3}\,\dot{\gamma}_j^p + \lambda_{j+6}\,n_j\right) + \lambda_{10}\,\overset{\circ}{\boldsymbol{\mathcal{U}}}^{\mathcal{A}_i}.$$

If l_{km} is another set of kinematic variables satisfying $Y(l_{km}) < 1$, then the flow rule can be written as

$$\pi(\dot{\hat{\delta}}^p - \dot{\delta}^p) + \sum_{j=1}^{3} \Big[\sigma_j\,(\dot{\hat{\varepsilon}}_j - \dot{\varepsilon}_j) + \tau_j\,(\dot{\hat{\gamma}}_j - \dot{\gamma}_j) + m_j(\hat{n}_j - n_j) + \boldsymbol{\mathcal{P}} : (\overset{\circ}{\hat{\boldsymbol{\mathcal{U}}}}{}^{\mathcal{A}_i} - \overset{\circ}{\boldsymbol{\mathcal{U}}}{}^{\mathcal{A}_i})\Big] \geq 0. \quad (6.33)$$

Since it can be shown that the yield function is convex in the kinetic variable-space, it is also possible to obtain the normality rule in terms of the kinetic variables.

6.3 Summary

In this chapter, we studied the concept of plastic spin using an upper-triangular decomposition of the deformation gradient. This upper-triangular decomposition results in an orthogonal rotation, $\boldsymbol{\mathcal{R}}$ and an upper-triangular Laplace stretch $\boldsymbol{\mathcal{U}}$ which is further decomposed into an elastic and a plastic component. It has been shown that the intermediate configuration $\tilde{\kappa}_p$ which is related to the reference configuration of the body through the plastic Laplace stretch $\boldsymbol{\mathcal{U}^p}$, represents a macroscopic manifestation of the substructure of the constituent material. Thus, the substructural spin has been obtained as $\boldsymbol{\omega}_s^p = \dot{\boldsymbol{\mathcal{R}}}^{\boldsymbol{p}}\,\boldsymbol{\mathcal{R}}^{\boldsymbol{p}^{\boldsymbol{T}}}$ where $\boldsymbol{\mathcal{R}^p}$ is the plastic component of the rotation tensor $\boldsymbol{\mathcal{R}}$, obtained through an elastic unloading. A kinematic internal state variable $\boldsymbol{\mathcal{A}}_i$ (in the configuration $\tilde{\kappa}_p$) has been considered to represent a macroscopic manifestation of the microstructural properties. A plastic spin for this internal state variable has been obtained. This plastic spin enters into the constitutive model through an appropriate definition of the co-rotational rate of the internal state variable that has been used in subsequent analysis. Due to its importance in the context of plastically-induced anisotropy, here we have also considered the evolution of anisotropy during plastic deformation in our constitutive model. Traditionally, such evolution is considered through the internal state variable whereas in our case, this evolution is incorporated by considering the anisotropy parameters, used in encoding/decoding map, as variables. Finally, a constitutive model for all the plastic strain attributes, anisotropy parameters and internal state variables has been obtained by using a maximum rate of dissipation criterion.

7. SUMMARY

With the recent developments of **QR** kinematics and the associated constitutive model, in this dissertation, we address some of the fundamental issues in **QR** kinematics and extend this method to study some problems in elasto-plasticity. In this framework, the matrix of the deformation gradient is decomposed into an orthogonal rotation $\mathcal{R}$ and an upper-triangular matrix $\mathcal{U}$, called the Laplace stretch [36]. The primary advantage of using this new decomposition is its utility regarding experiments. Due to the direct physical interpretation of the components of Laplace stretch, one can directly and unambiguously measure the deformations in all six degrees of freedom within a specific coordinate frame [34] by performing experiments.

This decomposition can be achieved using different techniques, of which a Gram-Schmidt procedure is most suitable for our application. A Gram-Schmidt procedure requires the specification of a particular coordinate direction and a specific coordinate plane, which includes this particular coordinate direction, given some coordinate systems of interest. Unfortunately, this coordinate direction and associated coordinate plane are not known *a priori*, because they require information from both the triad of base vectors and the deformation in question. Hence, in a three-dimensional space, one has been left with making what amounts to being an ad hoc selection for these coordinate direction and coordinate plane. There are six potential re-indexings of a Cartesian base triad that one can choose to orient this coordinate direction and coordinate surface. This arbitrariness in coordinate system choice can cause differences between potential Laplace stretches obtained from this set of coordinate systems, even if the deformation of a body is physically the same. This issue can be resolved by introducing a strategy whereby that edge of a representative cube undergoing the least amount of transverse shear under a given deformation, and the adjoining coordinate plane that experiences the least amount of in-plane shear are selected. With this strategy in place, the construction of the Laplace stretch now becomes unambiguous, and therefore, Laplace stretch can be used as a kinematic variable in constitutive constructions.

Next, a compatibility condition for the Laplace stretch is derived, whenever a right Cauchy-

Green tensor $\mathbf{C} = \mathbf{F}^T\mathbf{F}$ is prescribed. It is well-known that under this condition a vanishing of the Riemann curvature tensor $\mathbb{R}$ ensures compatibility of a finite deformation field. This problem has been attempted previously by Lembo (2017) [53] where they derived a compatibility condition by considering the rotation tensor as a primary variable. However, we choose the right Cauchy-Green tensor as our primary kinematic variable and show that a vanishing of the Riemann curvature tensor imposes restrictions on the spatial variations of certain elements of the Laplace stretch $\boldsymbol{\mathcal{U}}$. Moreover, these conditions corroborate the fact that the chosen coordinate direction and ccordinate plane for Gram-Schmidt procedure remains invariant under the transformation of Laplace stretch. The derived condition on Laplace stretch is unambiguous, because a Cholesky factorization of the right Cauchy-Green tensor ensures the existence of a unique Laplace stretch. Although a vanishing of the Riemann curvature tensor provides a necessary and sufficient compatibility condition from a purely geometric point of view, this condition lacks a direct physical interpretation in a sense that one cannot identify the restrictions imposed by this condition on a quantity that can be readily measured from experiments. On the other hand, our compatibility condition restricts dependence of components of a Laplace stretch on certain spatial variables in a reference configuration. Unlike the symmetric right- Cauchy stretch tensor $\mathbf{U}$ obtained from a traditional polar decomposition of $\mathbf{F}$, the components of Laplace stretch can be measured from experiments. Thus, this newly derived compatibility condition provides a physical meaning to the somewhat abstract idea of the traditionally used compatibility condition, viz., a vanishing of the Riemann curvature tensor. Couplings between certain components of the Laplace stretch representing shear and elongation play a crucial role in deriving this condition.

A natural extension of our work on compatibility is to study the incompatibility of a pertient space when the **QR** kinematics is applied to elastoplasticity. Using the property that the set of all upper-triangular matrices form a group under multiplication, Freed *et al.* (2019) [36] proposed an elastic-plastic decomposition of Laplace stretch, i.e., $\boldsymbol{\mathcal{U}} = \boldsymbol{\mathcal{U}}^e\,\boldsymbol{\mathcal{U}}^p$. Just like its elastic counterpart, one can measure the elements of $\boldsymbol{\mathcal{U}}^p$ through EBSD experiments. Usually such direct physical interpretations cannot be obtained for elastic or plastic components of the deformation gradient, arising from a Kröner–Lee decomposition, owing to the incompatibility of these fields. Using this decomposition, we study the geometric dislocation density tensor and Burgers vector. The geometric dislocation density tensor $\tilde{\mathbf{G}}$ is obtained using the classical argument of failure of a Burgers circuit in a suitable configuration $\tilde{\kappa}_p$ where the deformation of a body is solely due to the movement of dislocations. The geometric features of space $\tilde{\kappa}_p$ are explored and it has been shown that the derived geometric dislocation tensor is related to the torsion of $\tilde{\kappa}_p$, which serves as a measure of incompatibility in this space. Additionally, $\tilde{\mathbf{G}}$ vanishes only when the space $\tilde{\kappa}_p$ is compatible. In this decomposition, the deformation of a body in all six degrees of freedom can be *fully* described by Laplace stretch whereas the rotation tensor $\boldsymbol{\mathcal{R}}$ plays an important role in coordinate transformation. Therefore, the total dislocation density can be additively decomposed into the dislocation density due to plastic "straining" and a term representing the incompatibility of rotation field. The latter of which is physically similar to Nye's definition of dislocation density tensor. A balance law for geometric dislocations is derived taking into account the effect of the dislocation flux and source dislocations. The physical meaning of the plastic Laplace stretch, and consequently, of the derived geometric dislocation tensor proves to be particularly useful in the classification of dislocations. The derived geometric dislocation density tensor could be specifically useful in developing a strain-gradient and size-dependent theory of plasticity.

As mentioned earlier, it is possible to construct constitutive models using scalar conjugate stress/strain base pairs, instead of traditionally used tensor invariants. Adopting this approach, a constitutive model has been developed for elastic-plastic materials. Interestingly, the multiplicative elastic-plastic decomposition of Laplace stretch leads to an additive decomposition of the total strain attributes into their corresponding elastic and plastic components. Although an additive strain decomposition is commonly used in small-strain theory, here such a decomposition is possible even for finite deformation. The additive decomposition of the strain attributes has a deeper consequence in the construction of our constitutive model. A maximum rate of dissipation criterion has been used in deriving the constitutive equations as this criterion is valid for a wider class of materials. This criterion requires constitutive assumptions for the Helmholtz potential and a non-negative rate of dissipation function; the non-negativity of the latter ensures that the second law of thermodynamics is automatically satisfied. This theory does not presuppose any yield criterion as is commonly used in plasticity. In fact, it has been shown that whether a material exhibits a yielding or a creep-like behavior depends on the differentiability of the rate of dissipation function. Two cases of plastic deformation – volume-preserving and dilatant-pressure dependent deformations have been considered. As illustration of the proposed model, the classical J_2 plastcity and Drucker-Prager model has been derived.

Another crucial aspect of the plasticity theory, the concept of plastic spin, has also been investigated in this framework. It has been shown that the intermediate configuration $\tilde{\kappa}_p$ which is related to the reference configuration of the body through the plastic Laplace stretch, acts as a macroscopic manifestation of the material substructure. Expressions for a substructural spin and a material spin have been obtained using appropriate physical arguments based on this configuration. An internal state variable has been considered to represent the macroscopic manifestation of the microstructural properties. Considering the orientational properties of this internal variable with respect to the material substructure, an expression for the plastic spin has been obtained and its implication in the context of single crystal plasticity has been shown. Finally, this plastic spin has been incorporated into a constitutive model by means of an appropriate definition of the corotational rate of the internal state variable. This material model also captures plastically-induced anisotropy by considering the anisotropy parameters, associated with encoding/decoding maps, as variables. Evolution equations for the plastic strain attributes, internal state variables and the anisotropy parameters have been derived.

7.1 Future works

Based on the current development of this dissertation, a list of possible future works are envisaged in this section. In chapter 2, a strategy to re-index the base vectors has been provided in order to resolve the issue of ambiguity regarding the representation of Laplace stretch. In this work, only a Cartesian coordinate system for the reference configuration has been considered. However, the issue regarding the representation of Laplace stretch persists in case of other coordinate systems as well. These coordinate systems are extensively used by experimenters, e.g., a spherical polar coordinate system is used in cone and plate rheometer experiments. Hence, the issue of representation of Laplace stretch, involving these coordinate systems must be resolved to utilize the **QR** framework in its full potential.

In chapter 3, a compatibility condition for the Laplace stretch has been developed for a simply-connected body. Another interesting and more complex problem in this context is derivation of the compatibility conditions for a non-simply connected body. Given the physical meanings of the components of Laplace stretch, it is expected that these compatibility conditions will be simpler than the ones found in literature and will likely be more physically intuitive. In chapter 4, the incompatibility of a relevant intermediate configuration has been studied to provide a measure for the geometrically necessary dislocations. A natural extension of this work will be to characterize other material defects such as disclinations, deformation twins etc. from a geometric point of view. Again in this case, the physical meanings of the components of Laplace stretch will play a prominent role. As mentioned in chapter 4, the study of geometrically necessary dislocations will be particularly useful in developing a strain-gradient and size-dependent theory of plasticity. Chapters 5 and 6 have been devoted to develop constitutive models based on the **QR** kinematics and study some of the fundamental issues in plasticity in the process. These works can be extended to capture specific material behaviors and develop relevant material models keeping the physical significance of the kinematic quantities in mind. Moreover, it is also possible to extend the study on single crystal plasticity to develop specific constitutive models.

The focus of this dissertation has been to develop a novel framework for elasticity and plasticity that is more amenable to an experimenter. In fact, it has been pointed out that the proposed experimental procedure to measure the components of a plastic velocity gradient $\mathbf{F}^p$ suffers from a fundamental theoretical issue. On the other hand, an appropriate experimental procedure has been delineated to measure the components of the plastic Laplace stretch, at least, for a homogeneous rotation field. However, only a small amount of work has been done to actually carry out these experiments. Therefore, this field provides a greater scope of future research.

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APPENDIX A

SCHEME TO RE-INDEX THE MATRIX OF A DEFORMATION GRADIENT FOR AN UNAMBIGUOUS REPRESENTATION OF THE LAPLACE STRETCH

The following table provides a list of possible cases for coordinate indexing and their corresponding orthogonal re-indexing matrices.

The re-indexing scheme described in chapter 2 is generalized in the following algorithm for all six potential cases.

Algorithm 1: Pivoting the coordinate system for our experimenter's frame of reference.

Input: Deformation gradient $\mathbf{F}$ evaluated in Lagrangian basis $(\vec{\boldsymbol{E}}_1, \vec{\boldsymbol{E}}_2, \vec{\boldsymbol{E}}_3)$
if $\mathcal{G}_1 \leq \mathcal{G}_2$ **and** $\mathcal{G}_1 \leq \mathcal{G}_3$ **then**
  if $\boldsymbol{f}_1 \cdot \boldsymbol{f}_2 \leq \boldsymbol{f}_1 \cdot \boldsymbol{f}_3$ **then**
    $\boldsymbol{\mathcal{F}} = \mathbf{P}_1^{\mathsf{T}} \mathbf{F} \mathbf{P}_1, \quad \mathbf{P} = \mathbf{P}_1$
  else
    $\boldsymbol{\mathcal{F}} = \mathbf{P}_2^{\mathsf{T}} \mathbf{F} \mathbf{P}_2, \quad \mathbf{P} = \mathbf{P}_2$
  end
else if $\mathcal{G}_2 \leq \mathcal{G}_1$ **and** $\mathcal{G}_2 \leq \mathcal{G}_3$ **then**
  if $\boldsymbol{f}_1 \cdot \boldsymbol{f}_2 \leq \boldsymbol{f}_2 \cdot \boldsymbol{f}_3$ **then**
    $\boldsymbol{\mathcal{F}} = \mathbf{P}_3^{\mathsf{T}} \mathbf{F} \mathbf{P}_3, \quad \mathbf{P} = \mathbf{P}_3$
  else
    $\boldsymbol{\mathcal{F}} = \mathbf{P}_4^{\mathsf{T}} \mathbf{F} \mathbf{P}_4, \quad \mathbf{P} = \mathbf{P}_4$
  end
else
  if $\boldsymbol{f}_1 \cdot \boldsymbol{f}_3 \leq \boldsymbol{f}_2 \cdot \boldsymbol{f}_3$ **then**
    $\boldsymbol{\mathcal{F}} = \mathbf{P}_5^{\mathsf{T}} \mathbf{F} \mathbf{P}_5, \quad \mathbf{P} = \mathbf{P}_5$
  else
    $\boldsymbol{\mathcal{F}} = \mathbf{P}_6^{\mathsf{T}} \mathbf{F} \mathbf{P}_6, \quad \mathbf{P} = \mathbf{P}_6$
  end
end
Output: Re-indexed deformation gradient $\boldsymbol{\mathcal{F}}$ evaluated in $(\vec{\boldsymbol{\mathcal{E}}}_1, \vec{\boldsymbol{\mathcal{E}}}_2, \vec{\boldsymbol{\mathcal{E}}}_3)$ and re-indexer $\mathbf{P}$

(1 direction, 12 plane)	coordinate mapping	Re-indexing tensor	Re-indexed deformation gradient
$(\vec{\boldsymbol{E}}_1, \pi_3)$	$(\vec{\boldsymbol{E}}_1, \vec{\boldsymbol{E}}_2, \vec{\boldsymbol{E}}_3) \mapsto (\vec{\boldsymbol{\mathcal{E}}}_1, \vec{\boldsymbol{\mathcal{E}}}_2, \vec{\boldsymbol{\mathcal{E}}}_3)$	$\mathbf{P}_1 = \begin{bmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 1 \end{bmatrix}$	$\boldsymbol{\mathcal{F}} = \begin{bmatrix} F_{11} & F_{12} & F_{13} \\ F_{21} & F_{22} & F_{23} \\ F_{31} & F_{32} & F_{33} \end{bmatrix}$
$(\vec{\boldsymbol{E}}_1, \pi_2)$	$(\vec{\boldsymbol{E}}_1, \vec{\boldsymbol{E}}_2, \vec{\boldsymbol{E}}_3) \mapsto (\vec{\boldsymbol{\mathcal{E}}}_1, \vec{\boldsymbol{\mathcal{E}}}_3, \vec{\boldsymbol{\mathcal{E}}}_2)$	$\mathbf{P}_2 = \begin{bmatrix} 1 & 0 & 0 \\ 0 & 0 & 1 \\ 0 & 1 & 0 \end{bmatrix}$	$\boldsymbol{\mathcal{F}} = \begin{bmatrix} F_{11} & F_{13} & F_{12} \\ F_{31} & F_{33} & F_{32} \\ F_{21} & F_{23} & F_{22} \end{bmatrix}$
$(\vec{\boldsymbol{E}}_2, \pi_3)$	$(\vec{\boldsymbol{E}}_1, \vec{\boldsymbol{E}}_2, \vec{\boldsymbol{E}}_3) \mapsto (\vec{\boldsymbol{\mathcal{E}}}_2, \vec{\boldsymbol{\mathcal{E}}}_1, \vec{\boldsymbol{\mathcal{E}}}_3)$	$\mathbf{P}_3 = \begin{bmatrix} 0 & 1 & 0 \\ 1 & 0 & 0 \\ 0 & 0 & 1 \end{bmatrix}$	$\boldsymbol{\mathcal{F}} = \begin{bmatrix} F_{22} & F_{21} & F_{23} \\ F_{12} & F_{11} & F_{13} \\ F_{32} & F_{31} & F_{33} \end{bmatrix}$
$(\vec{\boldsymbol{E}}_2, \pi_1)$	$(\vec{\boldsymbol{E}}_1, \vec{\boldsymbol{E}}_2, \vec{\boldsymbol{E}}_3) \mapsto (\vec{\boldsymbol{\mathcal{E}}}_2, \vec{\boldsymbol{\mathcal{E}}}_3, \vec{\boldsymbol{\mathcal{E}}}_1)$	$\mathbf{P}_4 = \begin{bmatrix} 0 & 0 & 1 \\ 1 & 0 & 0 \\ 0 & 1 & 0 \end{bmatrix}$	$\boldsymbol{\mathcal{F}} = \begin{bmatrix} F_{22} & F_{23} & F_{21} \\ F_{32} & F_{33} & F_{31} \\ F_{12} & F_{13} & F_{11} \end{bmatrix}$
$(\vec{\boldsymbol{E}}_3, \pi_2)$	$(\vec{\boldsymbol{E}}_1, \vec{\boldsymbol{E}}_2, \vec{\boldsymbol{E}}_3) \mapsto (\vec{\boldsymbol{\mathcal{E}}}_3, \vec{\boldsymbol{\mathcal{E}}}_1, \vec{\boldsymbol{\mathcal{E}}}_2)$	$\mathbf{P}_5 = \begin{bmatrix} 0 & 1 & 0 \\ 0 & 0 & 1 \\ 1 & 0 & 0 \end{bmatrix}$	$\boldsymbol{\mathcal{F}} = \begin{bmatrix} F_{33} & F_{31} & F_{32} \\ F_{13} & F_{11} & F_{12} \\ F_{23} & F_{21} & F_{22} \end{bmatrix}$
$(\vec{\boldsymbol{E}}_3, \pi_1)$	$(\vec{\boldsymbol{E}}_1, \vec{\boldsymbol{E}}_2, \vec{\boldsymbol{E}}_3) \mapsto (\vec{\boldsymbol{\mathcal{E}}}_3, \vec{\boldsymbol{\mathcal{E}}}_2, \vec{\boldsymbol{\mathcal{E}}}_1)$	$\mathbf{P}_6 = \begin{bmatrix} 0 & 0 & 1 \\ 0 & 1 & 0 \\ 1 & 0 & 0 \end{bmatrix}$	$\boldsymbol{\mathcal{F}} = \begin{bmatrix} F_{33} & F_{32} & F_{31} \\ F_{23} & F_{22} & F_{21} \\ F_{13} & F_{12} & F_{11} \end{bmatrix}$

Table A.1: A scheme to re-index the deformation gradient needed to get a physically consistent Laplace stretch, viz., $\boldsymbol{\mathcal{F}} = \mathbf{P}^{\mathsf{T}}\mathbf{F}\mathbf{P}$ where $\mathbf{P}^{-1} = \mathbf{P}^{\mathsf{T}}$. In the first set of two rows, $\mathcal{G}_1$ is minimum; in the second set of two rows, $\mathcal{G}_2$ is minimum; and in the last set of two rows, $\mathcal{G}_3$ is minimum.

APPENDIX B

TRANSPOSITION OF TENSORS AND EQUATIONS PERTINENT TO THE COMPATIBILITY CONDITION

B.1 Transpositions of tensors

Fourth-order tensor

$$
\begin{aligned}
\mathbb{A}^T &= (\mathbb{A}^{ijkl} e_i \otimes e_j \otimes e_k \otimes e_l)^T = \mathbb{A}^{ijkl} e_j \otimes e_i \otimes e_l \otimes e_k = \mathbb{A}^{jilk} e_i \otimes e_j \otimes e_k \otimes e_l \\
\mathbb{A}^{ti} &= (\mathbb{A}^{ijkl} e_i \otimes e_k \otimes e_j \otimes e_l)^{ti} = \mathbb{A}^{ikjl} e_j \otimes e_i \otimes e_l \otimes e_k = \mathbb{A}^{ikjl} e_i \otimes e_j \otimes e_k \otimes e_l \\
\mathbb{A}^{to} &= (\mathbb{A}^{ijkl} e_i \otimes e_j \otimes e_k \otimes e_l)^{to} = \mathbb{A}^{ijkl} e_l \otimes e_j \otimes e_k \otimes e_i = \mathbb{A}^{ljki} e_i \otimes e_j \otimes e_k \otimes e_l \\
\mathbb{A}^{t} &= (\mathbb{A}^{ijkl} e_i \otimes e_j \otimes e_k \otimes e_l)^{t} = \mathbb{A}^{ijkl} e_l \otimes e_k \otimes e_j \otimes e_i = \mathbb{A}^{lkji} e_i \otimes e_j \otimes e_k \otimes e_l \\
\mathbb{A}^{D} &= (\mathbb{A}^{ijkl} e_i \otimes e_j \otimes e_k \otimes e_l)^{D} = \mathbb{A}^{ijkl} e_k \otimes e_l \otimes e_i \otimes e_j = \mathbb{A}^{klij} e_i \otimes e_j \otimes e_k \otimes e_l \\
\mathbb{A}^{dl} &= (\mathbb{A}^{ijkl} e_i \otimes e_j \otimes e_k \otimes e_l)^{dl} = \mathbb{A}^{ijkl} e_j \otimes e_i \otimes e_k \otimes e_l = \mathbb{A}^{jikl} e_i \otimes e_j \otimes e_k \otimes e_l \\
\mathbb{A}^{dr} &= (\mathbb{A}^{ijkl} e_i \otimes e_j \otimes e_k \otimes e_l)^{dr} = \mathbb{A}^{ijkl} e_i \otimes e_j \otimes e_l \otimes e_k = \mathbb{A}^{ijlk} e_i \otimes e_j \otimes e_k \otimes e_l \\
\mathbb{A}^{d} &= (\mathbb{A}^{ijkl} e_i \otimes e_j \otimes e_k \otimes e_l)^{d} = \mathbb{A}^{ijkl} e_j \otimes e_i \otimes e_l \otimes e_k = \mathbb{A}^{jilk} e_i \otimes e_j \otimes e_k \otimes e_l
\end{aligned} \tag{B.1.1}
$$

Third-order tensor

$$
\begin{aligned}
\mathtt{A}^T &= (\mathtt{A}^{ijk} e_i \otimes e_j \otimes e_k)^T = \mathtt{A}^{ijk} e_i \otimes e_k \otimes e_j = \mathtt{A}^{ikj} e_i \otimes e_j \otimes e_k \\
\mathtt{A}^t &= (\mathtt{A}^{ijk} e_i \otimes e_j \otimes e_k)^t = \mathtt{A}^{ijk} e_k \otimes e_j \otimes e_i = \mathtt{A}^{kji} e_i \otimes e_j \otimes e_k \\
\mathtt{A}^D &= (\mathtt{A}^{ijk} e_i \otimes e_j \otimes e_k)^D = \mathtt{A}^{ijk} e_j \otimes e_k \otimes e_i = \mathtt{A}^{jki} e_i \otimes e_j \otimes e_k
\end{aligned} \tag{B.1.2}
$$

Second-order tensor

$$\mathbf{A}^T = (\mathbf{A}^{ij} e_i \otimes e_j)^T = \mathbf{A}^{ij} e_j \otimes e_i = \mathbf{A}^{ji} e_i \otimes e_j \tag{B.1.3}$$

B.2 Symmetries of $\mathbb{R}_m$

$\mathbb{R}_1$:

$$\begin{gathered}\mathbb{R}_1^{dr} = -\mathbb{R}_1; \quad [\mathbb{R}_1^{dl}]^{dr} = -\mathbb{R}_1^{dl}; \quad [[\mathbb{R}_1^{D}]^{dr}] = -\mathbb{R}_1^{D}; \\ [[\mathbb{R}_1^{D}]^{dl}]^{dr} = -[\mathbb{R}_1^{D}]^{dl}; \quad [\mathbb{R}_1^{D}]^{dr} = [\mathbb{R}_1^{dl}]^{D}\end{gathered} \tag{B.2.1}$$

$\mathbb{R}_2$:

$$\mathbb{R}_2^{dr} = -\mathbb{R}_2; \quad \mathbb{R}_2^{D} = \mathbb{R}_2; \quad \mathbb{R}_2^{ti} = [\mathbb{R}_2^{ti}]^{D}; \quad [\mathbb{R}_2^{ti}]^{dr} = [[\mathbb{R}_2^{ti}]^{dr}]^{D} \tag{B.2.2}$$

$\mathbb{R}_3$:

$$\begin{gathered}\mathbb{R}_3^{dr} = \mathbb{R}_3; \quad [\mathbb{R}_3^{to}]^{T} = [\mathbb{R}_3^{dl}]^{ti}; \quad [\mathbb{R}_3^{ti}]^{T} = [\mathbb{R}_3^{dl}]^{to}; \\ [[\mathbb{R}_3^{ti}]^{T}]^{dr} = [\mathbb{R}_3^{ti}]^{dl}; \quad [[\mathbb{R}_3^{to}]^{dl}]^{dr} = [\mathbb{R}_3^{to}]^{T}; \quad [[\mathbb{R}_3^{to}]^{dl}]^{D} = [\mathbb{R}_3^{ti}]^{dl}; \quad [[\mathbb{R}_3^{ti}]^{dl}]^{D} = [\mathbb{R}_3^{to}]^{dl}; \\ [[\mathbb{R}_3^{ti}]^{dr}]^{D} = [\mathbb{R}_3^{to}]^{dr} \quad [[\mathbb{R}_3^{to}]^{dr}]^{D} = [\mathbb{R}_3^{ti}]^{dr}; \quad [[\mathbb{R}_3^{to}]^{T}]^{D} = [\mathbb{R}_3^{dr}]^{ti}; \quad [[\mathbb{R}_3^{ti}]^{T}]^{D} = [\mathbb{R}_3^{dr}]^{to};\end{gathered} \tag{B.2.3}$$

$\mathbb{R}_4$:

$$\begin{gathered}\mathbb{R}_4^{t} = \mathbb{R}_4; \quad [[\mathbb{R}_4^{to}]^{T}]^{dr} = [\mathbb{R}_4^{to}]^{dl}; \quad [[[\mathbb{R}_4^{dr}]^{ti}]^{dr}]^{D} = [[\mathbb{R}_4^{dl}]^{ti}]^{dr}; \\ [[\mathbb{R}_4^{to}]^{dl}]^{D} = [\mathbb{R}_4^{to}]^{dl}; \quad [[\mathbb{R}_4^{dr}]^{ti}]^{D} = [\mathbb{R}_4^{dl}]^{ti}; \quad [[\mathbb{R}_4^{ti}]^{dr}]^{D} = [\mathbb{R}_4^{ti}]^{dr}; \quad [\mathbb{R}_4^{ti}]^{D} = [\mathbb{R}_4^{to}]^{T}\end{gathered} \tag{B.2.4}$$

B.3 System of equations

B.3.1 Equations arising from symmetries of $f_1(\mathbb{R}_1)$

Because the diagonal blocks of $f_1(\mathbb{R})$ are zero, we obtain:

$$aW_{1,1} = 0; \tag{B.3.1.1}$$

$$aW_{3,1} = 0 \tag{B.3.1.2}$$

$$\beta W_{1,1} + \gamma W_{2,1} = \tilde{\alpha} W_{3,1} + bW_{4,1} \tag{B.3.1.3}$$

$$\tilde{\alpha} W_{1,2} + bW_{2,2} = 0; \tag{B.3.1.4}$$

$$\tilde{\alpha} W_{6,2} + bW_{7,2} = 0; \tag{B.3.1.5}$$

$$\tilde{\beta} W_{1,2} = -aW_{6,2} \tag{B.3.1.6}$$

$$\tilde{\beta} W_{6,3} + \tilde{\gamma} W_{7,3} + cW_{8,3} = 0; \tag{B.3.1.7}$$

$$\tilde{\beta} W_{3,3} + \tilde{\gamma} W_{4,3} + cW_{5,3} = 0; \tag{B.3.1.8}$$

$$\tilde{\alpha} W_{3,3} + bW_{4,3} = aW_{6,3} \tag{B.3.1.9}$$

From skew-symmetry of $f_1(\mathbb{R}_1)$, we get

$$aW_{1,2} = -\tilde{\gamma}W_{1,1} - bW_{2,1} \tag{B.3.1.10}$$

$$aW_{3,2} = -\tilde{\beta}W_{1,1} - \tilde{\alpha}W_{2,1} \tag{B.3.1.11}$$

$$\tilde{\gamma}W_{6,1} + bW_{7,1} = \tilde{\alpha}W_{1,2} + \tilde{\alpha}W_{2,2} - \tilde{\gamma}W_{3,2} - bW_{4,2} \tag{B.3.1.12}$$

$$aW_{1,3} = aW_{6,1} - \tilde{\gamma}W_{1,3} - bW_{4,1} \tag{B.3.1.13}$$

$$aW_{3,3} = -\tilde{\beta}W_{3,1} - \tilde{\alpha}W_{4,1} - cW_{5,1} \tag{B.3.1.14}$$

$$\tilde{\gamma}W_{3,3} + bW_{4,3} = \tilde{\beta}W_{1,3} + \tilde{\alpha}W_{2,3} - \tilde{\beta}W_{6,1} - \tilde{\alpha}W_{7,1} - cW_{8,1} \tag{B.3.1.15}$$

$$aW_{6,2} = \tilde{\gamma}W_{2,3} + bW_{2,3} + \tilde{\gamma}W_{3,2} + bW_{4,2} \tag{B.3.1.16}$$

$$aW_{6,3} = -\tilde{\beta}W_{1,3} - \tilde{\alpha}W_{2,3} - \tilde{\beta}W_{3,2} - \tilde{\alpha}W_{4,2} - cW_{5,2} \tag{B.3.1.17}$$

$$\tilde{\gamma}W_{6,3} + bW_{7,3} = -\tilde{\beta}W_{6,2} - \tilde{\alpha}W_{7,2} - cW_{8,2} \tag{B.3.1.18}$$

Because $a, \tilde{\gamma}, \tilde{\beta}$ and $b, \tilde{\alpha}$ are the only coupled elements of $\boldsymbol{\mathcal{U}}$, we conclude that

$$\begin{aligned} &W_{1,1} = W_{2,1} = W_{1,2} = W_{3,3} = W_{4,3} = W_{3,1} = W_{6,2} = W_{6,3} = W_{7,3} = W_{2,2} = W_{5,3} = W_{7,2} \\ &= W_{8,3} = W_{4,1} = W_{5,1} = W_{8,2} = W_{3,2} + W_{6,1} = W_{4,2} + W_{7,1} = W_{1,3} - W_{6,1} = W_{8,1} \\ &= W_{5,2} = W_{2,3} - W_{7,1} = 0 \end{aligned} \tag{B.3.1.19}$$

Thus, no term involving derivatives of W_p, $p = 1, ..., 8$, appears in the 6 equations arising from equating off-diagonal elements of $\mathbb{R}$ to zero.

B.3.2 Equations arising from vanishing of Riemann curvature tensor

$\mathbb{R}_{1313} = 0$ leads to:

$$
\begin{aligned}
&a\cancel{W_{3,3}} + \tilde{\beta}\cancel{W_{3,1}} - \left(\frac{\tilde{\beta}^2}{b^2} + \frac{\tilde{\beta}^2\tilde{\alpha}^2}{b^2c^2}\right)W_1^2 - \frac{2\tilde{\alpha}^4}{b^2c^2}W_2^2 + \left(2 + \frac{4a\tilde{\alpha}\tilde{\gamma}\tilde{\beta}}{b^2c^2} - \frac{4a\tilde{\beta}^2}{bc^2} - \frac{\tilde{\alpha}^2}{b^2} - \frac{\tilde{\gamma}^2}{b^2} - \frac{\tilde{\alpha}^2\tilde{\gamma}^2}{b^2c^2}\right)W_3^2 \\
&+ 2W_5^2 - \left(\frac{\tilde{\alpha}^2\tilde{\gamma}^2}{b^2c^2} + \frac{a^2}{b^2}\right)W_6^2 - \frac{2\tilde{\beta}\tilde{\alpha}^3}{b^2c^2}W_1W_2 + \left(\frac{2\tilde{\gamma}\tilde{\beta}}{b^2} - \frac{2\tilde{\beta}\tilde{\alpha}}{b^2} - \frac{2\tilde{\gamma}\tilde{\beta}\tilde{\alpha}^2}{b^2c^2} + \frac{4\tilde{\beta}^2\tilde{\alpha}}{bc^2}\right)W_1W_3 - \frac{4a\tilde{\alpha}}{b^2}W_1W_7 \\
&+ \left(-\frac{2\tilde{\beta}}{b} + \frac{4\tilde{\alpha}\tilde{\gamma}}{b^2} - \frac{4\tilde{\gamma}\tilde{\alpha}^3}{b^2c^2} + \frac{6\tilde{\beta}\tilde{\alpha}^2}{bc^2}\right)W_1W_4 + \left(\frac{8\tilde{\beta}\tilde{\alpha}}{bc} + \frac{4\tilde{\gamma}c}{b^2} - \frac{4\tilde{\gamma}\tilde{\alpha}^2}{b^2c}\right) + \left(\frac{2\tilde{\gamma}\tilde{\beta}\tilde{\alpha}^2}{b^2c^2} - \frac{4a\tilde{\beta}}{b^2}\right)W_1W_6 \\
&- \frac{4ac}{b^2}W_1W_8 + \left(\frac{2\tilde{\gamma}\tilde{\alpha}^3}{b^2c^2} - \frac{4\tilde{\gamma}\tilde{\alpha}}{b^2}\right)W_2W_3 + \left(\frac{2\tilde{\alpha}^3}{bc^2} - \frac{2\tilde{\alpha}}{b}\right)W_2W_4 + \frac{4\tilde{\alpha}^2}{bc}W_2W_5 + \left(\frac{2\tilde{\gamma}\tilde{\alpha}^2}{bc^2} - 2\tilde{\gamma}\right)W_3W_4 \\
&+ \left(\frac{2a\tilde{\alpha}}{b^2} + \frac{2a\tilde{\alpha}^3}{b^2c^2}\right)W_2W_6 + \frac{2\tilde{\beta}}{c}W_3W_5 + \left(\frac{2\tilde{\alpha}\tilde{\beta}\tilde{\gamma}}{bc^2} + \frac{4a\tilde{\beta}\tilde{\alpha}}{bc^2} + \frac{4a\tilde{\gamma}}{b^2} - \frac{4a^2\tilde{\alpha}^2}{b^2c^2}\right)W_3W_6 + \frac{4a\tilde{\alpha}^2}{bc^2}W_3W_7 \\
&+ \frac{4a\tilde{\alpha}}{bc}W_3W_8 + \frac{2\tilde{\alpha}}{c}W_4W_5 - \frac{2a\tilde{\alpha}^2}{bc^2}W_4W_6 + \left(\frac{2a}{b} - \frac{2a\tilde{\alpha}}{bc}\right)W_5W_6 + \left(\frac{4a\tilde{\alpha}_{,3}}{b} - \frac{4a\tilde{\alpha}c_{,3}}{bc}\right)W_1 \\
&- \frac{4\tilde{\alpha}a_{,1}}{a}W_4 + \left(\frac{4ac_{,3}}{c} - \frac{4\tilde{\beta}a_{,1}}{a}\right)W_3 - \frac{4ca_{,1}}{a}W_5 + \left(3 - \frac{\tilde{\alpha}^2}{c^2}\right)W_4^2 = 0
\end{aligned}
\tag{B.3.2.1}
$$

$\mathbb{R}_{2323} = 0$ yields:

$$
\begin{aligned}
&\tilde{\alpha}\cancel{W_{6,3}} + b\cancel{W_{7,3}} + \left(\frac{\tilde{\beta}^2}{a^2} + \frac{\tilde{\beta}^2\xi^2}{a^2b^2c^2}\right)W_1^2 - \left(\frac{\tilde{\alpha}^2}{a^2} + \frac{\tilde{\alpha}^2\xi^2}{a^2b^2c^2}\right)W_2^2 - \frac{2\tilde{\beta}^2\xi}{abc^2}W_3^2 - \left(\frac{b^2}{a^2} + \frac{2\tilde{\alpha}^2\xi}{abc}\right)W_4^2 - \frac{\tilde{\alpha}\xi}{abc}W_5^2 \\
&+ \left(3 - \frac{3\tilde{\alpha}^2}{c^2}\right)W_7^2 + \left(3 - \frac{2\tilde{\alpha}\tilde{\beta}\tilde{\gamma}}{bc^2} - \frac{\tilde{\beta}^2}{c^2}\right)W_6^2 - \left(\frac{2\tilde{\beta}\tilde{\alpha}}{a^2} + \frac{2\tilde{\beta}\tilde{\alpha}\xi^2}{a^2b^2c^2}\right)W_1W_2 + \left(\frac{2b\tilde{\alpha}}{a^2} + \frac{2\tilde{\alpha}\xi^2}{a^2bc^2} + \frac{2\tilde{\alpha}^3\xi}{ab^2c}\right)W_2W_4 \\
&+ \left(\frac{4\tilde{\alpha}\tilde{\gamma}}{a^2} + \frac{4\tilde{\alpha}\tilde{\gamma}\xi^2}{a^2b^2c^2} - \frac{2\tilde{\beta}b}{a^2} + \frac{2\tilde{\beta}\tilde{\alpha}^2\xi}{ab^2c^2}\right)W_1W_4 + \left(\frac{4\tilde{\gamma}^3c}{a^2b^2} - \frac{2\tilde{\gamma}\tilde{\beta}\tilde{\alpha}\xi}{ab^2c}\right)W_1W_5 + \left(-\frac{2\tilde{\beta}\tilde{\alpha}\xi}{abc^2} + \frac{2\tilde{\beta}\tilde{\alpha}^3}{b^2c^2}\right)W_1W_7 \\
&+ \left(\frac{2\tilde{\gamma}^2\tilde{\beta}}{ab^2} - \frac{2\tilde{\beta}^2\xi}{abc^2} + \frac{2\tilde{\beta}^2\tilde{\alpha}^2}{b^2c^2}\right)W_1W_6 + \left(\frac{4\tilde{\beta}b}{a^2} + \frac{2\tilde{\alpha}^2\tilde{\beta}\xi}{ab^2c^2}\right)W_2W_3 - \left(-\frac{4\tilde{\beta}\xi}{ac^2} + \frac{2\tilde{\beta}\tilde{\alpha}^2}{bc^2} + \frac{2\tilde{\alpha}\tilde{\gamma}\xi}{abc^2}\right)W_3W_7 \\
&+ \left(\frac{2\tilde{\gamma}\tilde{\beta}}{a^2} + \frac{2\tilde{\gamma}^3\tilde{\beta}}{a^2b^2} + \frac{2\tilde{\beta}^2\tilde{\alpha}\xi}{ab^2c^2} + \frac{4\tilde{\gamma}\tilde{\beta}\xi^2}{a^2b^2c^2}\right)W_1W_3 + \left(\frac{4bc}{a^2} + \frac{4\xi^2}{a^2bc} + \frac{2\tilde{\alpha}^2\xi}{ab^2c}\right)W_2W_5 - \frac{4cb_{,2}}{b}W_8 \\
&+ \left(\frac{2\tilde{\beta}\tilde{\alpha}^3}{b^2c^2} - \frac{2\tilde{\gamma}\tilde{\alpha}^2\xi}{ab^2c^2} - \frac{2\tilde{\beta}\tilde{\alpha}\xi}{a^2bc^2}\right)W_2W_6 + \left(\frac{2\tilde{\alpha}\tilde{\gamma}}{ab} + \frac{2\tilde{\alpha}^4}{b^2c^2}\right)W_2W_7 - \frac{6\tilde{\alpha}}{c}W_7W_8 - \frac{2\tilde{\alpha}\xi}{abc}W_2W_8 - \frac{2\tilde{\beta}\xi}{abc}W_3W_5 \\
&- \left(\frac{2\tilde{\gamma}\tilde{\beta}\xi}{abc^2} + \frac{2\tilde{\beta}^2\tilde{\alpha}}{bc^2}\right)W_3W_6 - \frac{2\tilde{\beta}\tilde{\alpha}\xi}{abc^2}W_3W_4 + \left(\frac{4bc_{,3}}{c} - \frac{4\tilde{\alpha}b_{,2}}{b}\right)W_7 + \left(\frac{2\tilde{\alpha}^3}{b^2c} - \frac{4\tilde{\gamma}\xi}{abc}\right)W_3W_8 - \frac{4\tilde{\alpha}\xi}{abc}W_4W_5 \\
&+ \left(\frac{4\tilde{\alpha}\tilde{\gamma}\xi}{abc^2} - \frac{2\tilde{\beta}\tilde{\alpha}^2}{bc^2} - \frac{2\tilde{\beta}\xi}{abc}\right)W_4W_6 + \left(\frac{2\tilde{\alpha}\xi}{ac^2} - \frac{2\tilde{\alpha}^3}{bc^2}\right)W_4W_7 - \left(\frac{2\tilde{\gamma}\xi}{ac^2} + \frac{2\xi}{ac}\right)W_4W_8 + \left(\frac{4\tilde{\gamma}\xi}{abc} - \frac{4\tilde{\beta}\tilde{\alpha}}{bc}\right)W_5W_6 \\
&+ \frac{4\xi}{ac}W_5W_7 - \frac{2\tilde{\alpha}}{b}W_5W_8 - \left(\frac{4\tilde{\beta}\tilde{\alpha}}{c^2} + \frac{2\tilde{\beta}}{c}\right)W_6W_7 - \left(\frac{2\tilde{\alpha}\tilde{\gamma}}{bc} + \frac{2\tilde{\beta}}{c} + \frac{2\tilde{\gamma}}{b}\right)W_6W_8 - 4c\left(\frac{\tilde{\gamma}_{,2}}{a} - \frac{\tilde{\gamma}b_{,2}}{ab}\right)W_5 \\
&+ \left(\frac{2\tilde{\beta}(\tilde{\gamma}_{,3} + \tilde{\beta}_{,2})}{a} - \frac{2\tilde{\beta}_{,3}\tilde{\gamma}}{a} + \frac{4\tilde{\gamma}^2\tilde{\alpha}_{,3}}{ab} + \frac{4\tilde{\gamma}\xi c_{,3}}{abc}\right)W_1 + \left(\frac{2\tilde{\alpha}(\tilde{\gamma}_{,3} + \tilde{\beta}_{,2})}{a} - \frac{4\tilde{\beta}_{,3}\tilde{\gamma}}{a} + \frac{4\tilde{\gamma}^2\tilde{\alpha}_{,3}}{ab} + \frac{4\tilde{\gamma}\xi c_{,3}}{ac}\right)W_2 \\
&+ \left(\frac{2b(\tilde{\gamma}_{,3} + \tilde{\beta}_{,2})}{a} - \frac{2\tilde{\gamma}(b_{,3} + \tilde{\gamma}_{,2})}{b} - 4\tilde{\alpha}\left(\frac{\tilde{\gamma}_{,2}}{a} - \frac{\tilde{\gamma}b_{,2}}{ab}\right)\right)W_4 + \left(\frac{4\tilde{\gamma}c_{,3}}{c} - \frac{4\tilde{\beta}b_{,2}}{b}\right)W_6 \\
&+ \left(\frac{2\tilde{\gamma}(\tilde{\gamma}_{,3} + \tilde{\beta}_{,2})}{a} - \frac{2\tilde{\gamma}^2(b_{,3} + \tilde{\alpha}_{,2})}{ab} - 4\tilde{\beta}\left(\frac{\tilde{\gamma}_{,2}}{a} - \frac{\tilde{\gamma}\tilde{\beta}_{,2}}{ab}\right)\right)W_3 = 0
\end{aligned}
\tag{B.3.2.2}
$$

where $\xi = \tilde{\alpha}\tilde{\gamma} - \tilde{\beta}b$

APPENDIX C

DERIVATION OF CONVEXITY CONDITION IN STRESS AND STRAIN SPACE AND ILLUSTRATION OF THE DEVELOPED CONSTITUTIVE MODEL

C.1 Convexity of yield function

Let us consider the case where the stress attributes are held constant and the plastic strain-rate attributes are allowed to vary in order to maximize the rate of dissipation function ξ. Consider two sets of plastic strain-rate attributes $\bar{l}_{\dot{\mathcal{U}}^p} = \{\dot{\bar{\delta}}^p \quad \dot{\bar{\varepsilon}}_1^p \quad \dot{\bar{\varepsilon}}_2^p \quad \dot{\bar{\varepsilon}}_3^p \quad \dot{\bar{\gamma}}_1^p \quad \dot{\bar{\gamma}}_2^p \quad \dot{\bar{\gamma}}_3^p\}$ and $\hat{l}_{\dot{\mathcal{U}}^p} = \{\dot{\hat{\delta}}^p \quad \dot{\hat{\varepsilon}}_1^p \quad \dot{\hat{\varepsilon}}_2^p \quad \dot{\hat{\varepsilon}}_3^p \quad \dot{\hat{\gamma}}_1^p \quad \dot{\hat{\gamma}}_2^p \quad \dot{\hat{\gamma}}_3^p\}$ along with a prescribed set of values for the stress attributes $\bar{l}_\sigma = \{\overline{\pi} \quad \overline{\sigma}_1 \quad \overline{\sigma}_2 \quad \overline{\sigma}_3 \quad \overline{\tau}_1 \quad \overline{\tau}_2 \quad \overline{\tau}_3\}$. Now, from the definition of our yield function, we can say that for any arbitrary plastic strain-rate attributes $\bar{l}_{\dot{\mathcal{U}}^p}$ and $\hat{l}_{\dot{\mathcal{U}}^p}$, the following conditions hold:

$$\frac{\overline{\pi}\,\dot{\bar{\delta}}^p + \overline{\sigma}_1\,\dot{\bar{\varepsilon}}_1^p + \overline{\sigma}_2\,\dot{\bar{\varepsilon}}_2^p + \overline{\sigma}_3\,\dot{\bar{\varepsilon}}_3^p + \overline{\tau}_1\,\dot{\bar{\gamma}}_1^p + \overline{\tau}_2\,\dot{\bar{\gamma}}_2^p + \overline{\tau}_3\,\dot{\bar{\gamma}}_3^p}{\overline{\xi}(l_{\dot{\mathcal{U}}^p})} \leq Y(\bar{l}_{\dot{\mathcal{U}}^p}) \tag{C.1a}$$

and

$$\frac{\overline{\pi}\,\dot{\hat{\delta}}^p + \overline{\sigma}_1\,\dot{\hat{\varepsilon}}_1^p + \overline{\sigma}_2\,\dot{\hat{\varepsilon}}_2^p + \overline{\sigma}_3\,\dot{\hat{\varepsilon}}_3^p + \overline{\tau}_1\,\dot{\hat{\gamma}}_1^p + \overline{\tau}_2\,\dot{\hat{\gamma}}_2^p + \overline{\tau}_3\,\dot{\hat{\gamma}}_3^p}{\overline{\xi}(l_{\dot{\mathcal{U}}^p})} \leq Y(\hat{l}_{\dot{\mathcal{U}}^p}). \tag{C.1b}$$

The yield function for the plastic strain-rate attributes

$$\bar{l}_{\dot{\mathcal{U}}^p} + \hat{l}_{\dot{\mathcal{U}}^p} = \{\dot{\bar{\delta}}^p + \dot{\hat{\delta}}^p \quad \dot{\bar{\varepsilon}}_1^p + \dot{\hat{\varepsilon}}_1^p \quad \dot{\bar{\varepsilon}}_2^p + \dot{\hat{\varepsilon}}_2^p \quad \dot{\bar{\varepsilon}}_3^p + \dot{\hat{\varepsilon}}_3^p \quad \dot{\bar{\gamma}}_1^p + \dot{\hat{\gamma}}_1^p \quad \dot{\bar{\gamma}}_2^p + \dot{\hat{\gamma}}_2^p \quad \dot{\bar{\gamma}}_3^p + \dot{\hat{\gamma}}_3^p\}$$

can be written in the same manner as

$$
\begin{aligned}
Y(\bar{l}_{\dot{\mathcal{U}}^p} + \hat{l}_{\dot{\mathcal{U}}^p}) &= \max_{\bar{l}_{\dot{\mathcal{U}}^p} \neq \mathbf{0}} \frac{(\dot{\bar{\delta}}^p + \dot{\hat{\delta}}^p)\,\overline{\pi} + \sum_{i=1}^{3}\left((\dot{\bar{\varepsilon}}_i^p + \dot{\hat{\varepsilon}}_i^p)\,\overline{\sigma}_i + (\dot{\bar{\gamma}}_i^p + \dot{\hat{\gamma}}_i^p)\,\overline{\tau}_i\right)}{\overline{\xi}(l_{\dot{\mathcal{U}}^p})} \\
&= \max_{\bar{l}_{\dot{\mathcal{U}}^p} \neq \mathbf{0}} \frac{\dot{\bar{\delta}}^p\,\overline{\pi} + \sum_{i=1}^{3}\left(\dot{\bar{\varepsilon}}_i^p\,\overline{\sigma}_i + \dot{\bar{\gamma}}_i^p\,\overline{\tau}_i\right)}{\overline{\xi}(l_{\dot{\mathcal{U}}^p})} + \frac{\dot{\hat{\delta}}^p\,\overline{\pi} + \sum_{i=1}^{3}\left(\dot{\hat{\varepsilon}}_i^p\,\overline{\sigma}_i + \dot{\hat{\gamma}}_i^p\,\overline{\tau}_i\right)}{\overline{\xi}(l_{\dot{\mathcal{U}}}{}^p)} \leq Y(\bar{l}_{\dot{\mathcal{U}}^p}) + Y(\hat{l}_{\dot{\mathcal{U}}^p}).
\end{aligned}
\tag{C.2}
$$

The last of Eqn. (C.2) is derived by using Eqn. (C.1). Therefore, from Eqn. (C.2), we conclude that *the yield function is convex in the plastic strain-rate space.*

Now, alternatively, one can choose to allow the stress attributes to vary while keeping the plastic strain rates fixed. In that case, if we consider two different sets of values for the stress attributes $\bar{l}_\sigma$ and $\hat{l}_\sigma$ with a fixed set of plastic strain-rate attributes $\bar{l}_{\dot{\mathcal{U}}^p}$, then following the similar procedure, we can easily conclude that *the yield function is also convex in stress space.*

C.2 Illustration

With the constitutive model based on **QR** kinematics established, we now focus on some important examples. As mentioned earlier, a key advantage of using **QR** kinematics is an additive decomposition of the strain attributes into their respective elastic and plastic components. In general, such a decomposition is a key feature of the small-displacement gradient theory. However, in our case, an additive strain decomposition follows from the upper-triangular decomposition of the deformation gradient, even in the finite deformation setting. Therefore, we pick up some important models widely used in the small-strain plasticity theory and extend them in the finite deformation setting using our developed constitutive model.

C.2.1 J_2 plasticity

The von Mises criterion[1] is possibly the most commonly used yield criterion for metal plasticity. According to this criterion, a material exhibits inelastic behavior when a quantity $\sqrt{J_2}$, associated with the Cauchy stress components σ_{ij} reach the current yield stress in shear, i.e., k.

[1]This yield criterion and associated flow rule were first introduced by Lévy and later developed by von Mises. Their theory is applicable whenever the elastic strains are negligible. An extension of their theory to capture nonzero elastic strains was later proposed, the outcome being commonly known as the Prandtl-Reuss equations.

The quantity J_2 is defined as

$$J_2 := \frac{1}{2}\,\mathrm{tr}(\hat{\boldsymbol{S}} \cdot \hat{\boldsymbol{S}}) = \frac{1}{2}\,\hat{S}_{ij}\,\hat{S}_{ij} \tag{C.3}$$

where $\hat{\boldsymbol{S}}$ is the deviatoric stress defined as

$$\hat{\boldsymbol{S}} = \boldsymbol{\sigma} - \frac{1}{3}\,\mathrm{tr}(\boldsymbol{\sigma})\,\boldsymbol{I}. \tag{C.4}$$

Therefore, the yield function can be written as

$$f(\boldsymbol{\sigma}) = J_2 - k^2. \tag{C.5}$$

The flow rule associated with this yield criterion is given by

$$\dot{\epsilon}^p_{ij} = \dot{\lambda}\,\frac{\partial f}{\partial \sigma_{ij}} \tag{C.6}$$

where ϵ^p_{ij} denote the plastic components of the strain tensor in a small displacement gradient theory.

In our theory, the constitutive assumption for two functions, namely, the Helmholtz potential function ψ and the rate of dissipation function ξ, must be specified at the beginning. Here we assume that the elastic response of the material is that of a Green elastic solid. Therefore, the form for the Helmholtz potential function is same as that in Eqn. (5.15). Note that J_2 plasticity results in an *associative* plastic flow rule. In order to obtain associative flow rules in our framework, the rate of dissipation function must be a function of the plastic strain-rate attributes alone. Because the J_2 theory was developed based on an assumption that plastic deformation is volume-preserving, we further assume that the plastic dilatational strain-rate $\dot{\delta}^p$ is zero. Let us choose a rate of dissipation function ξ of the form

$$\xi = k\sqrt{\sum_{i=1}^{3}\big(\dot{\varepsilon}_i^{p^2} + \dot{\gamma}_i^{p^2}\big)}. \tag{C.7}$$

With this assumed form for the rate of dissipation function ξ, while employing Eqn. (5.16), the stress attributes can be obtained as

$$\sigma_i = \mu k \, \frac{\dot{\varepsilon}_i^p}{\sqrt{\sum_{i=1}^{3}\big(\dot{\varepsilon}_i^{p^2} + \dot{\gamma}_i^{p^2}\big)}} \quad \text{and} \quad \tau_i = \mu k \, \frac{\dot{\gamma}_i^p}{\sqrt{\sum_{i=1}^{3}\big(\dot{\varepsilon}_i^{p^2} + \dot{\gamma}_i^{p^2}\big)}}. \tag{C.8}$$

The consistency parameter μ is determined by satisfaction of the reduced rate of dissipation equation (5.29). By substituting the stress attributes from Eqn. (C.8) into Eqn. (5.29), we find that $\mu = 1$. In our theory, physically, the quantity J_2 is equivalent to

$$\mathcal{J}_2 \coloneqq \sum_{i=1}^{3}\big(\sigma_i^2 + \tau_i^2\big). \tag{C.9}$$

In the classical J_2 theory, the independence of the yield function on the volumetric (or mean) stress is achieved by defining J_2 based on the deviatoric stress $\hat{\boldsymbol{S}}$, instead of the Cauchy stress $\boldsymbol{\sigma}$; whereas in our theory, this independence is manifested by simply avoiding the volumetric stress π in the definition of $\mathcal{J}_2$. Substituting the expressions for stress attributes from Eqn. (C.8), one can easily compute $\mathcal{J}_2$ as

$$\mathcal{J}_2 = \sum_{i=1}^{3}\big(\sigma_i^2 + \tau_i^2\big) = k^2 \implies \frac{\mathcal{J}_2}{k^2} = 1. \tag{C.10}$$

Now the yield function in this case is given as

$$Y = \frac{\sum_{i=1}^{3}(\sigma_i \, \dot{\varepsilon}_i + \tau_i \, \dot{\gamma}_i)}{\xi}. \tag{C.11}$$

By substituting the stress and plastic strain-rate attributes, and the assumed form for the rate of dissipation function ξ, one can easily show that the yield function Y is equal to the quantity $\mathcal{J}_2/k^2$. Therefore, Eqn. (C.10) serves as the yield criterion in this case.

C.2.2 Drucker–Prager criterion

For materials like soils, rocks, foams, etc., the plastic deformation also depends on the volumetric stress π. To incorporate this in a plasticity model, Drucker and Prager (1952) [26] came up with an extended version of the Mohr-Coulomb model and combined it with the von Mises yield criterion in such a way that the yield function f also depends upon the mean stress. Moreover, unlike the von Mises criterion, in this model, the plastic flow rules are derived from a separate plastic potential function G ($\neq f$), i.e., the flow rules are non-associative. In this model, the yield function is given as

$$f(\boldsymbol{\sigma}) := \sqrt{J_2} + \alpha\, p - k = 0 \tag{C.12}$$

whereas the plastic potential is given as

$$G(\boldsymbol{\sigma}) := \sqrt{J_2} + \beta p. \tag{C.13}$$

Here p is the mean stress which is given as $p = \frac{1}{3}\,\mathrm{tr}(\boldsymbol{\sigma})$ while α, β are material parameters. This flow rule can be obtained from a plastic potential as

$$\dot{\epsilon}^p = \dot{\lambda}\, \frac{\partial G(\boldsymbol{\sigma})}{\partial \boldsymbol{\sigma}}. \tag{C.14}$$

To derive the Drucker-Prager model in our framework, we assume the same form for the Helmholtz potential function as in Eqn. (5.15). The rate of dissipation function must be chosen in a way such that the plastic volumetric strain rate is also taken into account. Let us choose a rate of dissipation function ξ of the form

$$\xi(\pi, l_{\dot{\mathcal{U}}^p}) = m_1(\pi)\, \sqrt{\sum_{i=1}^{3} \left(\dot{\varepsilon}_i^{p^2} + \dot{\gamma}_i^{p^2}\right)} + m_2(\pi)\, \frac{\dot{\delta}^{p^2}}{\sqrt{\sum_{i=1}^{3} \left(\dot{\varepsilon}_i^{p^2} + \dot{\gamma}_i^{p^2}\right)}}. \tag{C.15}$$

Now employing Eqn. (5.30), the stress attributes are obtained as

$$\pi = \frac{2m_1(\pi)\dot{\delta}^p}{\sqrt{\sum_{i=1}^{3}\left(\dot{\varepsilon}_i^{p^2} + \dot{\gamma}_i^{p^2}\right)}}, \tag{C.16a}$$

$$\sigma_i = \left(m_1 - \frac{m_2\,\dot{\delta}^{p^2}}{\sum_{i=1}^{3}\left(\dot{\varepsilon}_i^{p^2} + \dot{\gamma}_i^{p^2}\right)}\right)\frac{\dot{\varepsilon}_i^p}{\sqrt{\sum_{i=1}^{3}\left(\dot{\varepsilon}_i^{p^2} + \dot{\gamma}_i^{p^2}\right)}}, \tag{C.16b}$$

$$\tau_i = \left(m_1 - \frac{m_2\,\dot{\delta}^{p^2}}{\sum_{i=1}^{3}\left(\dot{\varepsilon}_i^{p^2} + \dot{\gamma}_i^{p^2}\right)}\right)\frac{\dot{\gamma}_i^p}{\sqrt{\sum_{i=1}^{3}\left(\dot{\varepsilon}_i^{p^2} + \dot{\gamma}_i^{p^2}\right)}}. \tag{C.16c}$$

Now let us compute the equivalent Mises stress $\mathcal{J}_2$. Substituting the expressions for σ_i and τ_i from Eqns. (C.16b and C.16c), $\mathcal{J}_2$ can be computed as

$$\mathcal{J}_2 = \left(m_1(\pi) - m_2(\pi)\frac{\dot{\delta}^{p^2}}{\sum_{i=1}^{3}\left(\dot{\varepsilon}_i^{p^2} + \dot{\gamma}_i^{p^2}\right)}\right)^2. \tag{C.17}$$

Let us define the material dependent parameters k and α as $k = m_1$ and $\alpha(\pi) = \pi/4m_2(\pi)$. Note that parameter m_1 in Eqn. (C.15) is equal to k and thus, no longer needs to be a function of π. Therefore, if the material parameter k is not considered to be a function of π, then the Eqn. (C.16a) provides an explicit expression for the dilatant pressure π. Substituting k and α in Eqn. (C.17), one can write

$$\sqrt{\mathcal{J}_2} + \alpha\,\pi - k = 0 \implies \frac{\sqrt{\mathcal{J}_2} + \alpha\,\pi}{k} = 1. \tag{C.18}$$

From the definition of the yield function (5.19), one can easily show that the Eqn. (C.18) acts as the yield condition in this case. Therefore, we can conclude that with the proper choice of a Helmholtz potential ψ and a rate of dissipation function ξ, it is possible to recover the classical models for plasticity, even in a finite deformation setting.

APPENDIX D

DERIVATION OF FLOW RULES USING A MAXIMUM RATE OF DISSIPATION CRITERION

From Eqn. (1.41), we observe that the anisotropy parameters are only associated with the dilatational and squeeze strain rates when they are expressed in terms of the components of the plastic velocity gradient, $\boldsymbol{\mathcal{L}^p}$ or vice versa. Moreover, these strain rates are related to only three components of plastic Laplace stretch, $\mathcal{L}^p_{11}$, $\mathcal{L}^p_{22}$ and $\mathcal{L}^p_{33}$. Therefore, it is reasonable to carry out the maximization process with respect to these three components of the plastic Laplace stretch, the shear strain rates $\dot{\gamma}_j$ and the co-rotational rate of the internal state variable.

Now, from Eqn. (6.24), the components of Laplace stretch in terms of the dilatational and squeeze strain rates and the anisotropy parameters can be written as

$$\mathcal{L}^p_{11} = n_1(\dot{\delta}^p + 2\dot{\varepsilon}^p_1 + \dot{\varepsilon}^p_2), \tag{D.1a}$$

$$\mathcal{L}^p_{22} = n_2(\dot{\delta}^p - \dot{\varepsilon}^p_1 + \dot{\varepsilon}^p_2), \tag{D.1b}$$

$$\mathcal{L}^p_{33} = n_3(\dot{\delta}^p - \dot{\varepsilon}^p_1 - 2\dot{\varepsilon}^p_2). \tag{D.1c}$$

The Lagrangian for our constrained optimization problem can be written as

$$\mathbb{L} := \xi + \overline{\lambda}\left(\hat{\xi} + \rho_0 \frac{\partial\hat{\psi}}{\partial\delta^p}\dot{\delta}^p + \rho_0 \sum_{j=1}^{3}\left[\frac{\partial\hat{\psi}}{\partial\varepsilon^p_j}\dot{\varepsilon}^p_j + \rho_0\frac{\partial\hat{\psi}}{\partial\gamma_j}\dot{\gamma}_j + \frac{\partial\hat{\psi}}{\partial\overline{n}_j}\, n_j\right] + \boldsymbol{\mathcal{P}}_i : \overset{\circ}{\boldsymbol{\mathcal{U}}}^{\mathcal{A}_i}\right). \tag{D.2}$$

Now the condition for maximizing the Lagrangian $\mathbb{L}$ with respect to the component of plastic velocity gradient $\mathcal{L}^p_{11}$ is given as

$$\frac{\partial\mathbb{L}}{\partial\mathcal{L}^p_{11}} = 0 \implies (1+\overline{\lambda})\,\frac{\partial\xi}{\partial\mathcal{L}^p_{11}} + \rho_0\,\overline{\lambda}\left(\frac{\partial\hat{\psi}}{\partial\delta^p}\,\frac{\partial\dot{\delta}^p}{\partial\mathcal{L}^p_{11}} + \frac{\partial\hat{\psi}}{\partial\varepsilon^p_1}\,\frac{\partial\dot{\varepsilon}^p_1}{\partial\mathcal{L}^p_{11}} + \frac{\partial\hat{\psi}}{\partial\varepsilon^p_2}\,\frac{\partial\dot{\varepsilon}^p_2}{\partial\mathcal{L}^p_{11}} + \frac{\partial\hat{\psi}}{\partial\overline{n}_1}\,\frac{\partial n_1}{\partial\mathcal{L}^p_{11}}\right) = 0. \tag{D.3}$$

Note that the components $\mathcal{L}^p_{11}, \mathcal{L}^p_{22}$ and $\mathcal{L}^p_{33}$ do not explicitly depend upon the third squeeze strain rate $\dot{\varepsilon}_3^p$. This is due to the fact that the squeeze strain rate $\dot{\varepsilon}_3^p$ can be expressed as the linear combination of the other two. However, it does not pose any issue regarding the determination of an evolution equation for ε_3^p. Now since $\mathcal{L}_{11}^p$ depends upon the strain rates and the anisotropy parameter n_1, Eqn. (D.3) reduces to

$$\begin{aligned}(1+\overline{\lambda})\left[\frac{\partial \xi}{\partial \dot{\delta}^p}\frac{\partial \dot{\delta}^p}{\partial \mathcal{L}_{11}^p}+\frac{\partial \xi}{\partial \dot{\varepsilon}_1}\frac{\partial \dot{\varepsilon}_1^p}{\partial \mathcal{L}_{11}^p}+\frac{\partial \xi}{\partial \dot{\varepsilon}_2}\frac{\partial \dot{\varepsilon}_2^p}{\partial \mathcal{L}_{11}^p}+\frac{\partial \xi}{\partial n_1}\frac{\partial n_1}{\partial \mathcal{L}_{11}^p}\right]+\rho_0\,\overline{\lambda}\,\frac{\partial \hat{\psi}}{\partial \delta^p}\frac{\partial \dot{\delta}^p}{\partial \mathcal{L}_{11}^p}\\ +\rho_0\,\overline{\lambda}\,\frac{\partial \hat{\psi}}{\partial \varepsilon_1^p}\frac{\partial \dot{\varepsilon}_1^p}{\partial \mathcal{L}_{11}^p}+\rho_0\,\overline{\lambda}\,\frac{\partial \hat{\psi}}{\partial \varepsilon_2^p}\frac{\partial \dot{\varepsilon}_2^p}{\partial \mathcal{L}_{11}^p}+\rho_0\,\overline{\lambda}\,\frac{\partial \hat{\psi}}{\partial \overline{n}_1}\frac{\partial n_1}{\partial \mathcal{L}_{11}^p}=0.\end{aligned} \tag{D.4}$$

Now substituting the derivatives of the strain rates and anisotropy parameter with respect to $\mathcal{L}_{11}^p$ into Eqn. (D.4), we obtain

$$\begin{aligned}\frac{1}{n_1}\left[(1+\overline{\lambda})\frac{\partial \xi}{\partial \dot{\delta}^p}+\rho_0\,\overline{\lambda}\,\frac{\partial \psi}{\partial \delta^p}\right]+\frac{1}{2n_1}\left[(1+\overline{\lambda})\frac{\partial \xi}{\partial \dot{\varepsilon}_1^p}+\rho_0\,\overline{\lambda}\,\frac{\partial \psi}{\partial \varepsilon_1^p}\right]\\ +\frac{1}{n_1}\left[(1+\overline{\lambda})\frac{\partial \xi}{\partial \dot{\varepsilon}_2^p}+\rho_0\,\overline{\lambda}\,\frac{\partial \psi}{\partial \varepsilon_2^p}\right]+\frac{1}{\dot{\delta}^p+2\dot{\varepsilon}_1^p+\dot{\varepsilon}_2}\left[(1+\overline{\lambda})\frac{\partial \xi}{\partial n_1}+\rho_0\,\overline{\lambda}\frac{\partial \psi}{\partial \overline{n}_1}\right]=0.\end{aligned} \tag{D.5}$$

Similarly, the condition for maximizing the Lagrangian $\mathbb{L}$ with respect to $\mathcal{L}_{22}^p$ and $\mathcal{L}_{33}^p$ are given as

$$\begin{aligned}\frac{1}{n_2}\left[(1+\overline{\lambda})\frac{\partial \xi}{\partial \dot{\delta}^p}+\rho_0\,\overline{\lambda}\,\frac{\partial \psi}{\partial \delta^p}\right]-\frac{1}{n_2}\left[(1+\overline{\lambda})\frac{\partial \xi}{\partial \dot{\varepsilon}_1^p}+\rho_0\,\overline{\lambda}\,\frac{\partial \psi}{\partial \varepsilon_1^p}\right]\\ +\frac{1}{n_2}\left[(1+\overline{\lambda})\frac{\partial \xi}{\partial \dot{\varepsilon}_2^p}+\rho_0\,\overline{\lambda}\,\frac{\partial \psi}{\partial \varepsilon_2^p}\right]+\frac{1}{\dot{\delta}^p-\dot{\varepsilon}_1^p+\dot{\varepsilon}_2}\left[(1+\overline{\lambda})\frac{\partial \xi}{\partial n_1}+\rho_0\,\overline{\lambda}\frac{\partial \psi}{\partial \overline{n}_2}\right]=0\end{aligned} \tag{D.6}$$

and

$$\begin{aligned}\frac{1}{n_3}\left[(1+\overline{\lambda})\frac{\partial \xi}{\partial \dot{\delta}^p}+\rho_0\,\overline{\lambda}\,\frac{\partial \psi}{\partial \delta^p}\right]-\frac{1}{n_3}\left[(1+\overline{\lambda})\frac{\partial \xi}{\partial \dot{\varepsilon}_1^p}+\rho_0\,\overline{\lambda}\,\frac{\partial \psi}{\partial \varepsilon_1^p}\right]\\ -\frac{1}{2n_3}\left[(1+\overline{\lambda})\frac{\partial \xi}{\partial \dot{\varepsilon}_2^p}+\rho_0\,\overline{\lambda}\,\frac{\partial \psi}{\partial \varepsilon_2^p}\right]+\frac{1}{\dot{\delta}^p-\dot{\varepsilon}_1^p-2\dot{\varepsilon}_2}\left[(1+\overline{\lambda})\frac{\partial \xi}{\partial n_1}+\rho_0\,\overline{\lambda}\frac{\partial \psi}{\partial \overline{n}_2}\right]=0.\end{aligned} \tag{D.7}$$

The maximization process for the shear strain rates are rather straightforward. Since they are not related to the components of $\boldsymbol{\mathcal{L}}^p$ through the anisotropy parameters, one can carry out the maximization process directly with respect to the shear strain rates $\dot{\gamma}_j^p$. A routine calculation leads to

$$(1+\overline{\lambda})\frac{\partial \xi}{\partial \dot{\gamma}_j^p} = -\overline{\lambda}\,\rho_0\,\frac{\partial \psi}{\partial \gamma_j^p}. \tag{D.8}$$

Similarly, an evolution equation for the anisotropy parameters and the internal state variables are obtained as

$$(1+\overline{\lambda})\,\frac{\partial \xi}{\partial n_j} = -\overline{\lambda}\,\rho_0\,\frac{\partial \psi}{\partial \overline{n}_j} \tag{D.9}$$

and

$$(1+\overline{\lambda})\,\frac{\partial \xi}{\partial \overset{\circ}{\boldsymbol{\mathcal{U}}}^{\mathcal{A}_i}} = -\overline{\lambda}\,\boldsymbol{\mathcal{P}}. \tag{D.10}$$

Now in view of Eqn. (D.9), Eqns. (D.5), (D.6) and (D.7) can be collectively written as

$$\begin{aligned} f_{1j}(n_j)\underbrace{\left[(1+\overline{\lambda})\,\frac{\partial \xi}{\partial \dot{\delta}^p} + \rho_0\,\overline{\lambda}\,\frac{\partial \psi}{\partial \delta^p}\right]}_{q_1(\delta^p,\dot{\delta}^p)} + f_{2j}(n_j)\underbrace{\left[(1+\overline{\lambda})\,\frac{\partial \xi}{\partial \dot{\varepsilon}_1^p} + \rho_0\,\overline{\lambda}\,\frac{\partial \psi}{\partial \varepsilon_1^p}\right]}_{q_2(\varepsilon_1^p,\dot{\varepsilon}_1^p)} \\ + f_{3j}(n_j)\underbrace{\left[(1+\overline{\lambda})\,\frac{\partial \xi}{\partial \dot{\varepsilon}_2^p} + \rho_0\,\overline{\lambda}\,\frac{\partial \psi}{\partial \varepsilon_2^p}\right]}_{q_3(\varepsilon_2^p,\dot{\varepsilon}_2^p)} = 0 \end{aligned} \tag{D.11}$$

where f_{ij}'s are functions of n_j in accordance with Eqn. (6.24). Notice that for the reduced equations (D.5), (D.6) and (D.7), their constituents q_i's remain the same. Moreover, it is evident that Eqn. (D.11) must be satisfied for any variation of the dilatational and squeeze strain attributes and their rates in order to maximize the Lagrangian $\mathbb{L}$. Moreover, each of the constituents of Eqn. (D.11), q_i depends on a certain mode of deformation, for example, the constituent q_1 depends only on the dilatational mode of deformation. Since the dilatation and these squeeze mode of deformations are independent of each other, one can vary the functions q_1, q_2 and q_3 arbitrarily such that Eqn. (D.11) is always satisfied. This is possible if and only if these constituents are individually zero, i.e., $q_1(\delta^p,\dot{\delta}^p) = q_2(\varepsilon_1^p,\dot{\varepsilon}_1^p) = q_3(\varepsilon_3^p,\dot{\varepsilon}_3^p) = 0$. Thus, the condition to maximize the

Lagrangian $\mathbb{L}$ with respect to $\mathcal{L}^p_{11}$, $\mathcal{L}^p_{22}$ and $\mathcal{L}^p_{33}$ can be written as

$$
\begin{aligned}
(1+\overline{\lambda})\,\frac{\partial\xi}{\partial\dot{\delta}^p} &= -\rho_0\,\overline{\lambda}\,\frac{\partial\psi}{\partial\delta^p},\\
(1+\overline{\lambda})\,\frac{\partial\xi}{\partial\dot{\varepsilon}^p_1} &= -\rho_0\,\overline{\lambda}\,\frac{\partial\psi}{\partial\varepsilon^p_1},\\
(1+\overline{\lambda})\,\frac{\partial\xi}{\partial\dot{\varepsilon}^p_2} &= -\rho_0\,\overline{\lambda}\,\frac{\partial\psi}{\partial\varepsilon^p_2}.
\end{aligned} \tag{D.12}
$$

Since the third squeeze mode satisfies the condition $\varepsilon^p_3 = -(\varepsilon^p_1 + \varepsilon^p_2)$ and $\dot{\varepsilon}^p_3 = -(\dot{\varepsilon}^p_1 + \dot{\varepsilon}^p_2)$, the evolution equation for ε^p_3 can be written as

$$
(1+\overline{\lambda})\,\frac{\partial\xi}{\partial\dot{\varepsilon}^p_3} = -\rho_0\,\overline{\lambda}\,\frac{\partial\psi}{\partial\varepsilon^p_3}. \tag{D.13}
$$