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The geometry of discombinations and its applications to semi-inverse problems in anelasticity

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The geometrical formulation of continuum mechanics provides us with a powerful approach to understand and solve problems in anelasticity where an elastic deformation is combined with a non-elastic component arising from defects, thermal stresses, growth effects or other effects leading to residual stresses. The central idea is to assume that the material manifold, prescribing the reference configuration for a body, has an intrinsic, non-Euclidean, geometrical structure. Residual stresses then naturally arise when this configuration is mapped into Euclidean space. Here, we consider the problem of discombinations (a new term that we introduce in this paper), that is, a combined distribution of fields of dislocations, disclinations and point defects. Given a discombination, we compute the geometrical characteristics of the material manifold (curvature, torsion, non-metricity), its Cartan's moving frames and structural equations. This identification provides a powerful algorithm to solve semi-inverse problems with non-elastic components. As an example, we calculate the residual stress field of a cylindrically symmetric distribution of discombinations in an infinite circular cylindrical bar made of an incompressible hyperelastic isotropic elastic solid.

1. Introduction

In a series of seminal papers, Rivlin developed a systematic approach to solve simple but fundamental

problems of nonlinear elasticity [1–3]. Rivlin’s approach is mostly based on the semi-inverse method where the geometry of the deformation is known up to a few unknown functions or constants that are obtained through simple boundary-value problems. For instance, in incompressible isotropic elasticity, one can consider the deformation of a spherical shell into another spherical shell when subjected to internal pressure. Once this deformation is known, the computation of the solution amounts to finding a single parameter (say, the internal radius of the deformed sphere) that is obtained by a single quadrature. The beauty of such solutions is that they exist for arbitrary strain-energy functions (in that case, they are known as *universal semi-inverse solutions*). Arguably, Rivlin’s work has been central in the development of nonlinear elasticity over the past 50 years as it has provided a systematic way to explore analytically the nonlinear behaviour of elastic materials [4–6].

Whereas the framework for computing solutions for semi-inverse problems in elasticity is now completely understood, the equivalent framework for systems with defects, or more generally for anelastic problems, has not yet been established. Many authors have obtained particular solutions for specific anelastic problems in different fields as they naturally arise in the theory of distributed defects (see below), finite strain plasticity [7], morpho-elasticity (the theory of growth and remodelling) [8–12] or thermoelasticity [13]. The central problem is to compute the residual stress created by the non-elastic components of the deformation. Perhaps the main reason why a general method for semi-inverse problems in anelasticity has not yet been proposed is that the characterization of the non-elastic components is a non-trivial task. However, we argue here that the geometrical approach of anelasticity provides a natural framework both to characterize non-elastic effects and to compute the residual stresses they generate. The approach presented here is suitable to describe any anelastic components but, for the sake of illustration, we discuss the problem of distributed defects. The translation to any other anelastic theory follows with a suitable change of terminology.

The mathematical study of defects in solids goes back to Volterra [14] more than a century ago. Combinations of dislocations and disclinations were originally referred to as ‘distortions’ by Volterra, but we call them line defects in this paper. Love [15] and Frank [16] called the translational and rotational line defects, dislocations and disclinations, respectively. As defects strongly affect the mechanical properties of various structural components, calculating stress fields of defects, their dynamics and understanding their interactions has been a central problem for the mechanics community. The existing stress calculations are overwhelmingly linear. In the setting of linear elasticity, Green’s functions can be used and, from the knowledge of a fundamental solution, the stress field of an arbitrary defect distribution can be computed. One can also study the interaction of defects by using the superposition principle. However, in the framework of nonlinear elasticity, superposition is not possible and each problem combining defects has to be solved separately.

In the framework of nonlinear elasticity, there are very few exact solutions for defects. We should mention [7,17–20] for dislocations, [19,21,22] for disclinations and the authors’ recent works [23,24] for point defects. For a combination of defects, we are aware only of the work of Zubov [19], who calculated the stress field of a combination of a single screw dislocation and a single wedge disclination both lying on the same line (a dispiration according to Harris [25]). By extension, we refer to *discombination* as any combination of line and point defects in nonlinear solids. We should emphasize that discombination is a new term that we introduce in this paper. As we are not aware of any calculation of stress field for general discombinations, we present here a general algorithm with application to some problems with cylindrical symmetry.

In a recent paper, Clayton [26] used a geometrical theory based on a multiplicative decomposition of deformation gradient into elastic and defect parts and presented analytical second-order solutions for a single screw dislocation, a single wedge disclination and a single point defect in isotropic compressible solids. In these approximate second-order solutions, the strain-energy function is a polynomial truncated at third order with respect to displacement gradients. Kupferman *et al.* [27] describe defects assuming only a metric structure. Bodies with isolated defects are viewed as multiply-connected affine manifolds. Both disclinations and

dislocations are characterized by the monodromy, which maps curves that surround the loci of the defects into affine transformations. They also show that two-dimensional defects with trivial monodromy (e.g. metric quadrupoles) are purely local. We should also mention the recent work of Acharya & Fressengeas [28], who present a continuum theory of interactions of dislocations and phase boundaries.

In the 1950s, Kondo [29,30] and Bilby *et al.* [31] independently discovered the close connection between non-Riemannian geometries and the mechanics of distributed defects. Their discussions were mainly kinematic. Following their seminal works, many researchers studied the geometric mechanics of defects. Unfortunately, these geometrical works remained mostly formal with very few stress calculations for distributed defects. Recently, we revisited the geometric theory of solids with distributed defects and showed that it is also suitable for the calculation of stress fields in nonlinear solids with distributed defects by computing explicitly solutions with either dislocations, disclinations or point defects [7,22,23]. To further emphasize the power of such an approach, here we first present the general geometric theory for combined defects and derive from it a general method for semi-inverse problems in anelasticity based on Cartan's moving frames and structural equations. We then illustrate this method on a cylinder with general radial defects.

2. Non-Riemannian geometries, Cartan's moving frames and the nonlinear mechanics of defects

(a) Metric-affine manifolds

The stress-free configuration of a body with distributed defects is described by a metric-affine manifold, which is a triple $(\mathcal{B}, \nabla, \mathbf{G})$, where \mathcal{B} is a manifold, ∇ is a connection and \mathbf{G} is a metric. In general, ∇ and \mathbf{G} are independent geometrical entities. When ∇ is the Levi-Civita connection of \mathbf{G} , for example, $(\mathcal{B}, \nabla, \mathbf{G})$ is reduced to a Riemannian manifold. We briefly review the geometrical machinery needed for the analysis of defective solids; details are given in [7,22,23].

A linear (affine) connection on a manifold \mathcal{B} is an operation $\nabla: \mathcal{X}(\mathcal{B}) \times \mathcal{X}(\mathcal{B}) \rightarrow \mathcal{X}(\mathcal{B})$, where $\mathcal{X}(\mathcal{B})$ is the set of vector fields on \mathcal{B} , such that $\forall \mathbf{X}, \mathbf{Y}, \mathbf{X}_1, \mathbf{X}_2, \mathbf{Y}_1, \mathbf{Y}_2 \in \mathcal{X}(\mathcal{B}), \forall f, f_1, f_2 \in C^\infty(\mathcal{B}), \forall a_1, a_2 \in \mathbb{R}$: (i) $\nabla_{f_1 \mathbf{X}_1 + f_2 \mathbf{X}_2} \mathbf{Y} = f_1 \nabla_{\mathbf{X}_1} \mathbf{Y} + f_2 \nabla_{\mathbf{X}_2} \mathbf{Y}$, (ii) $\nabla_{\mathbf{X}}(a_1 \mathbf{Y}_1 + a_2 \mathbf{Y}_2) = a_1 \nabla_{\mathbf{X}}(\mathbf{Y}_1) + a_2 \nabla_{\mathbf{X}}(\mathbf{Y}_2)$, and (iii) $\nabla_{\mathbf{X}}(f \mathbf{Y}) = f \nabla_{\mathbf{X}} \mathbf{Y} + (\mathbf{X}f) \mathbf{Y}$. The vector $\nabla_{\mathbf{X}} \mathbf{Y}$ is the covariant derivative of \mathbf{Y} along \mathbf{X} . In a local chart $\{X^A\}$, $\nabla_{\partial_A} \partial_B = \Gamma^C_{AB} \partial_C$, where Γ^C_{AB} are Christoffel symbols of the connection and $\partial_A = \partial/\partial X^A$ are the natural bases for the tangent space corresponding to a coordinate chart $\{X^A\}$. A linear connection is compatible with a metric \mathbf{G} if and only if $\nabla \mathbf{G} = \mathbf{0}$. The torsion of a connection is defined as

$$T(\mathbf{X}, \mathbf{Y}) = \nabla_{\mathbf{X}} \mathbf{Y} - \nabla_{\mathbf{Y}} \mathbf{X} - [\mathbf{X}, \mathbf{Y}]. \quad (2.1)$$

The connection ∇ is symmetric if it is torsion-free, i.e. $\nabla_{\mathbf{X}} \mathbf{Y} - \nabla_{\mathbf{Y}} \mathbf{X} = [\mathbf{X}, \mathbf{Y}]$. On any Riemannian manifold $(\mathcal{B}, \mathbf{G})$, there is a unique linear connection ∇ that is compatible with \mathbf{G} and is torsion-free. This is the Levi-Civita connection. In a manifold with a connection the curvature, which quantifies the deviation of a manifold from being flat, is a map $\mathbf{R}: \mathcal{X}(\mathcal{B}) \times \mathcal{X}(\mathcal{B}) \times \mathcal{X}(\mathcal{B}) \rightarrow \mathcal{X}(\mathcal{B})$ defined by

$$\mathbf{R}(\mathbf{X}, \mathbf{Y})\mathbf{Z} = \nabla_{\mathbf{X}} \nabla_{\mathbf{Y}} \mathbf{Z} - \nabla_{\mathbf{Y}} \nabla_{\mathbf{X}} \mathbf{Z} - \nabla_{[\mathbf{X}, \mathbf{Y}]} \mathbf{Z}. \quad (2.2)$$

Finally, we quantify non-metricity. Given a manifold with a metric and an affine connection $(\mathcal{B}, \nabla, \mathbf{G})$, the non-metricity is a map $\mathbf{Q}: \mathcal{X}(\mathcal{B}) \times \mathcal{X}(\mathcal{B}) \times \mathcal{X}(\mathcal{B}) \rightarrow \mathcal{X}(\mathcal{B})$ defined as

$$\mathbf{Q}(\mathbf{U}, \mathbf{V}, \mathbf{W}) = \langle \nabla_{\mathbf{U}} \mathbf{V}, \mathbf{W} \rangle_{\mathbf{G}} + \langle \mathbf{V}, \nabla_{\mathbf{U}} \mathbf{W} \rangle_{\mathbf{G}} - \mathbf{U}[\langle \mathbf{V}, \mathbf{W} \rangle_{\mathbf{G}}]. \quad (2.3)$$

Or simply, $\mathbf{Q} = -\nabla \mathbf{G}$. As we see, from a mechanical point of view, the torsion and curvature tensors are the geometrical analogues of, respectively, the dislocation and the disclination density tensors [7,22]. In the case of distributed point defects, ∇ is not compatible with \mathbf{G} [23,24].

(b) Cartan's moving frames

Many calculations can be conveniently performed using a judicious choice of coordinate bases. However, to establish the theory, it is easier to work with non-coordinate bases. A Cartan's moving frame is an orthonormal frame field $\{\mathbf{e}_\alpha\}_{\alpha=1}^N$ that forms a basis for the tangent space at every point of a manifold \mathcal{B} . Because this frame is orthonormal, i.e. $\langle\langle \mathbf{e}_\alpha, \mathbf{e}_\beta \rangle\rangle_{\mathbf{G}} = \delta_{\alpha\beta}$, we have $\mathbf{G} = \delta_{\alpha\beta} \vartheta^\alpha \otimes \vartheta^\beta$, where $\{\vartheta^\alpha\}$ is the orthonormal coframe field. This is, in general, a non-coordinate basis for the tangent space. Connection 1-forms are defined as

$$\nabla \mathbf{e}_\alpha = \mathbf{e}_\gamma \otimes \omega^\gamma{}_\alpha. \quad (2.4)$$

The corresponding connection coefficients are defined as $\nabla_{\mathbf{e}_\beta} \mathbf{e}_\alpha = \langle \omega^\gamma{}_\alpha, \mathbf{e}_\beta \rangle \mathbf{e}_\gamma = \omega^\gamma{}_\beta \mathbf{e}_\gamma$. In other words, $\omega^\gamma{}_\alpha = \omega^\gamma{}_\beta \vartheta^\beta$. Similarly, $\nabla \vartheta^\alpha = -\omega^\alpha{}_\gamma \vartheta^\gamma$ and $\nabla_{\mathbf{e}_\beta} \vartheta^\alpha = -\omega^\alpha{}_\beta \vartheta^\gamma$.

We can now express the key geometrical parameters introduced in §2a in terms of Cartan's moving frames $\{\mathbf{e}_\alpha\}$. First, consider the non-metricity for which we have $\mathcal{Q}_{\gamma\alpha\beta} = \mathcal{Q}(\mathbf{e}_\gamma, \mathbf{e}_\alpha, \mathbf{e}_\beta)$. The non-metricity 1-forms are defined as $\mathcal{Q}_{\alpha\beta} = \mathcal{Q}_{\gamma\alpha\beta} \vartheta^\gamma$, where $\{\vartheta^\alpha\}$ is the co-frame field, so that

$$\mathcal{Q}_{\alpha\beta} = \omega_{\alpha\beta} + \omega_{\beta\alpha} - dG_{\alpha\beta} =: -DG_{\alpha\beta}, \quad (2.5)$$

where D is the covariant exterior derivative. This is *Cartan's zeroth structural equation*. For an orthonormal frame, $G_{\alpha\beta} = \delta_{\alpha\beta}$ and hence $\mathcal{Q}_{\alpha\beta} = \omega_{\alpha\beta} + \omega_{\beta\alpha}$. The Weyl 1-form is defined as $Q = (1/n)\mathcal{Q}_{\alpha\beta}G^{\alpha\beta}$. Hence, $\mathcal{Q}_{\alpha\beta} = \hat{Q}_{\alpha\beta} + QG_{\alpha\beta}$, where \hat{Q} is the traceless part of non-metricity. Here, we restrict our attention to manifolds with $\hat{Q} = \mathbf{0}$; in that case $(\mathcal{B}, \nabla, \mathbf{G})$ is called a Weyl–Cartan manifold. (At this time, we do not know what defect(s) \hat{Q} may represent. This remains to be investigated in the future.) In addition, if ∇ is torsion-free, then $(\mathcal{B}, \nabla, \mathbf{G})$ is called a Weyl manifold. One can show that [32]

$$\omega^\alpha{}_\alpha = \frac{n}{2}Q + \frac{1}{2}G^{\alpha\beta}dG_{\alpha\beta} = \frac{n}{2}Q + d \ln \sqrt{\det \mathbf{G}}. \quad (2.6)$$

And it follows that

$$D\sqrt{\det \mathbf{G}} = d\sqrt{\det \mathbf{G}} - \omega^\alpha{}_\alpha \sqrt{\det \mathbf{G}} = -\frac{n}{2}Q\sqrt{\det \mathbf{G}}, \quad (2.7)$$

i.e. the connection ∇ is not volume-preserving.

Similarly, we can define the torsion and curvature 2-forms with respect to the connection 1-forms as

$$T^\alpha = d\vartheta^\alpha + \omega^\alpha{}_\beta \wedge \vartheta^\beta \quad \text{and} \quad \mathcal{R}^\alpha{}_\beta = d\omega^\alpha{}_\beta + \omega^\alpha{}_\gamma \wedge \omega^\gamma{}_\beta. \quad (2.8)$$

These are *Cartan's first and second structural equations*. Figure 1 schematically shows special cases of metric-affine manifolds. In the presence of combined line and point defects, the material manifold is a Weyl–Cartan manifold.

The Bianchi identities read

$$D\mathcal{Q}_{\alpha\beta} := d\mathcal{Q}_{\alpha\beta} - \omega^\gamma{}_\alpha \wedge \mathcal{Q}_{\gamma\beta} - \omega^\gamma{}_\beta \wedge \mathcal{Q}_{\alpha\gamma} = \mathcal{R}^\alpha{}_\beta + \mathcal{R}^\beta{}_\alpha, \quad (2.9)$$

$$DT^\alpha := dT^\alpha + \omega^\alpha{}_\beta \wedge T^\beta = \mathcal{R}^\alpha{}_\beta \wedge \vartheta^\beta \quad (2.10)$$

and
$$D\mathcal{R}^\alpha{}_\beta := d\mathcal{R}^\alpha{}_\beta + \omega^\alpha{}_\gamma \wedge \mathcal{R}^\gamma{}_\beta - \omega^\gamma{}_\beta \wedge \mathcal{R}^\alpha{}_\gamma = 0. \quad (2.11)$$

Equations (2.10) and (2.11) are the geometrical analogues of Anthony's [33] compatibility equations (11) and (12) relating the dislocation and disclination density tensors.

(c) The compatible volume element on a Weyl manifold

In the presence of point defects, we need to relate non-metricity to the volume density of point defects. This is done using the notion of the compatible volume element [23,24]. A volume form on an n -manifold is a nowhere vanishing n -form. In the orthonormal coframe field $\{\vartheta^\alpha\}$, a volume

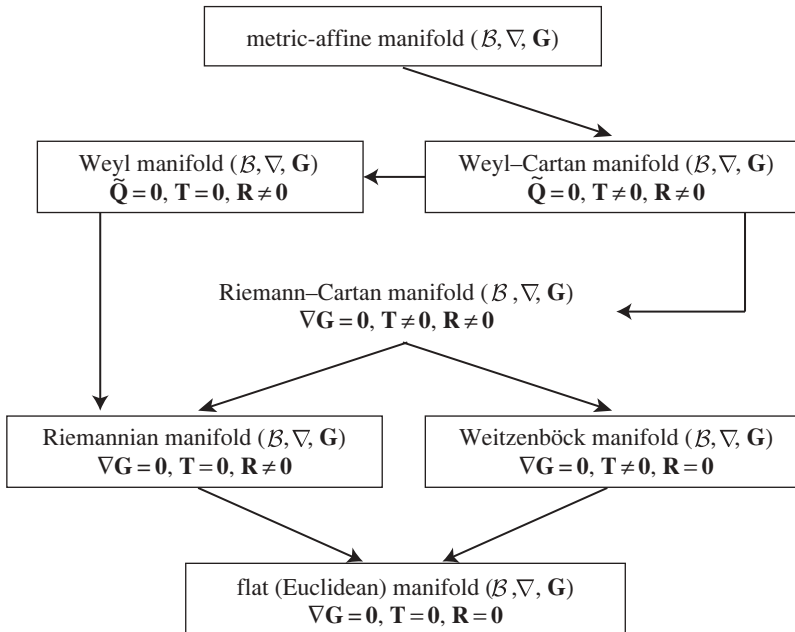


Figure 1. Special cases of metric-affine manifolds.

form can be written as $\mu = h\vartheta^1 \wedge \cdots \wedge \vartheta^n$, for some positive function h to be determined. In a coordinate chart $\{X^A\}$, the volume form is written as

$$\mu = h\sqrt{\det \mathbf{G}} dX^1 \wedge \cdots \wedge dX^n. \quad (2.12)$$

When $h = 1$, we recover the classical Riemannian volume element. The divergence of an arbitrary vector field \mathbf{W} on \mathcal{B} can be defined using the Lie derivative as $(\text{Div } \mathbf{W})\mu = \mathcal{L}_{\mathbf{W}}\mu$ [34]. For a given connection, the divergence of a vector field is defined as $\text{Div}_{\nabla}\mathbf{W} = W^A{}_{|A} = W^A{}_{,A} + \Gamma^A{}_{AB}W^B$. The connection μ is compatible with ∇ if $\mathcal{L}_{\mathbf{W}}\mu = (W^A{}_{|A})\mu$ [35]. Thus, $dh/h = d \ln h = (n/2)Q$. In coordinate form, this reads

$$\frac{\partial h}{\partial X^A} - \frac{n}{2}hQ_A = 0. \quad (2.13)$$

Note that the existence of a compatible volume element implies that the Weyl 1-form Q is closed, i.e. $dQ = (2/n)d \circ d \ln h = 0$.

(d) Geometric elasticity and anelasticity

So far, we have established the kinematic framework for the geometry of a body with defects. Next, we briefly review aspects of the theory of geometric nonlinear elasticity. A body \mathcal{B} is identified with a Riemannian manifold \mathcal{B} , and a configuration of \mathcal{B} is a mapping $\varphi: \mathcal{B} \rightarrow \mathcal{S}$, where \mathcal{S} is another Riemannian manifold. We assume that the body is stress free in the material manifold. The material velocity is the map $\mathbf{V}_t: \mathcal{B} \rightarrow T_{\varphi_t(\mathbf{X})}\mathcal{S}$ given by $\mathbf{V}_t(\mathbf{X}) = \mathbf{V}(\mathbf{X}, t) = \partial\varphi(\mathbf{X}, t)/\partial t$. The deformation gradient is the tangent map of φ and is denoted by $\mathbf{F} = T\varphi$. Therefore, at each point $\mathbf{X} \in \mathcal{B}$, it is a linear map $\mathbf{F}(\mathbf{X}): T_{\mathbf{X}}\mathcal{B} \rightarrow T_{\varphi(\mathbf{X})}\mathcal{S}$. If $\{x^a\}$ and $\{X^A\}$ are local coordinate charts on \mathcal{S} and \mathcal{B} , respectively, then the components of \mathbf{F} read $F^a{}_A(\mathbf{X}) = (\partial\varphi^a/\partial X^A)(\mathbf{X})$. The transpose of \mathbf{F} is defined by $\mathbf{F}^\top: T_{\mathbf{X}}\mathcal{S} \rightarrow T_{\mathbf{X}}\mathcal{B}$, $\langle\langle \mathbf{F}\mathbf{v}, \mathbf{v} \rangle\rangle_{\mathbf{g}} = \langle\langle \mathbf{V}, \mathbf{F}^\top\mathbf{v} \rangle\rangle_{\mathbf{G}}$, for all $\mathbf{V} \in T_{\mathbf{X}}\mathcal{B}$, $\mathbf{v} \in T_{\mathbf{X}}\mathcal{S}$. In components $(\mathbf{F}^\top(\mathbf{X}))^A{}_a = g_{ab}(\mathbf{x})F^b{}_B(\mathbf{X})G^{AB}(\mathbf{X})$, where \mathbf{g} and \mathbf{G} are metric tensors on \mathcal{S} and \mathcal{B} , respectively. \mathbf{F} has the following local representation: $\mathbf{F} = F^a{}_A(\partial/\partial x^a) \otimes dX^A$. The right Cauchy–Green deformation tensor $\mathbf{C}(\mathbf{X}): T_{\mathbf{X}}\mathcal{B} \rightarrow T_{\mathbf{X}}\mathcal{B}$ is defined by $\mathbf{C}(\mathbf{X}) = \mathbf{F}(\mathbf{X})^\top\mathbf{F}(\mathbf{X})$. In components, $C^A{}_B = (\mathbf{F}^\top)^A{}_a F^a{}_B$. One can

show that $\mathbf{C}^b = \varphi^*(\mathbf{g})$, i.e. $C_{AB} = (g_{ab} \circ \varphi)F^a_A F^b_B$. The following are the governing equations of nonlinear elasticity in material coordinates [36]:

$$\frac{\partial \rho_0}{\partial t} = 0, \quad \text{Div } \mathbf{P} + \rho_0 \mathbf{B} = \rho_0 \mathbf{A}, \quad \boldsymbol{\tau}^\top = \boldsymbol{\tau}, \quad (2.14)$$

where \mathbf{P} is the first Piola–Kirchhoff stress and $\boldsymbol{\tau} = \mathbf{J}\boldsymbol{\sigma}$ is the Kirchhoff stress, $\boldsymbol{\sigma}$ is the Cauchy stress, $\mathbf{J} = \sqrt{\det \mathbf{g} / \det \mathbf{G} \det \mathbf{F}}$ is the Jacobian, and $\sigma^{ab} = (1/\mathbf{J})P^a_A F^b_B$.

As usual, one can use different measures of strain. The left Cauchy–Green deformation tensor is defined as $\mathbf{B}^\sharp = \varphi^*(\mathbf{g}^\sharp)$ and has components $B^{AB} = (F^{-1})^A_a (F^{-1})^B_b g^{ab}$. The spatial analogues of \mathbf{C}^b and \mathbf{B}^\sharp are

$$\mathbf{c}^b = \varphi_*(\mathbf{G}), \quad c_{ab} = (F^{-1})^A_a (F^{-1})^B_b G_{AB} \quad (2.15)$$

and

$$\mathbf{b}^\sharp = \varphi_*(\mathbf{G}^\sharp), \quad b^{ab} = F^a_A F^b_B G^{AB}, \quad (2.16)$$

where \mathbf{b}^\sharp is the Finger deformation tensor. \mathbf{C} and \mathbf{b} have the same principal invariants usually denoted by I_1 , I_2 and I_3 [37]. For an isotropic material, the strain-energy function W depends only on the principal invariants of \mathbf{b} . It is standard to show that for a compressible and isotropic material the Cauchy stress has the following representation [38]:

$$\boldsymbol{\sigma} = 2 \left(\frac{I_2}{I_3} \frac{\partial W}{\partial I_2} + \frac{\partial W}{\partial I_3} \right) \mathbf{g}^\sharp + 2 \frac{\partial W}{\partial I_1} \mathbf{b}^\sharp - 2 \frac{\partial W}{\partial I_2} \mathbf{b}^{-1}. \quad (2.17)$$

Similarly, for an incompressible and isotropic material, the Cauchy stress has the following representation [38]:

$$\boldsymbol{\sigma} = \left(-p + 2I_2 \frac{\partial W}{\partial I_2} \right) \mathbf{g}^\sharp + 2 \frac{\partial W}{\partial I_1} \mathbf{b}^\sharp - 2 \frac{\partial W}{\partial I_2} \mathbf{b}^{-1}. \quad (2.18)$$

(e) Continuum mechanics of solids with distributed defects

In the presence of defects, a solid body may become residually stressed. In classical nonlinear elasticity, one assumes that the reference (natural) configuration is stress free. Stresses caused by external forces are then due to a deviation from the natural configuration. Such deviations are quantified using different measures of strain. Classically, residual stresses are computed by using a multiplicative decomposition, that is, by decomposing the deformation gradient into elastic and inelastic parts. In the present geometrical framework, such steps are not necessary as the effect of non-elastic components is directly contained in the geometry of the material manifold. Therefore, the first step in computing the residual stress for a given configuration of defects is to identify a material manifold in which the defective body is stress free. This manifold has a non-trivial geometry that explicitly depends on the geometrical nature of defects and their distributions. Once the material manifold is known, we look for an embedding of the underlying Riemannian material manifold into the Euclidean ambient space. Any measure of strain must be defined with respect to the material manifold.

In the following, we assume a fixed distribution of defects, find the corresponding material manifold and then compute the residual stress field by mapping the body into the ambient space. We assume a hyperelastic material with energy density W , which explicitly depends on the deformation gradient \mathbf{F} . Because the deformation gradient is a two-point tensor, the energy function explicitly depends on the metrics of both the material and ambient space manifolds, i.e.

$$W = W(\mathbf{F}, \mathbf{G}, \mathbf{g}). \quad (2.19)$$

The first Piola–Kirchhoff stress is calculated as

$$\mathbf{P} = \mathbf{g}^\sharp \frac{\partial W}{\partial \mathbf{F}}. \quad (2.20)$$

The Riemannian manifold $(\mathcal{B}, \mathbf{G})$ being the underlying Riemannian material manifold implies that

$$\left. \frac{\partial W}{\partial \mathbf{F}} \right|_{\mathbf{F}=\mathbf{id}, \mathbf{g}=\mathbf{G}} = \mathbf{0}. \quad (2.21)$$

Remark 2.1. In the present geometrical framework, it is assumed that the defect-free body is stress free in Euclidean space in the absence of external loads. The body may be composed of a material with multiple stress-free configurations, e.g. a strain-energy density with multiple wells. However, it is assumed that every material point is in the same energy well. In other words, we are not considering phase transformations. It is then assumed that some distribution of defects appears in the body that induces residual stresses. It should be emphasized that we are not considering nucleation or the work associated with the creation of defects. The stress-free configuration of the defective body—the material manifold—explicitly depends on the distribution of defects and their types but not on the constitutive equations of the material. However, residual stresses explicitly depend on the constitutive equations.

3. Examples of defects with cylindrical symmetry

Before we carry out the full computation of stress in the presence of discombinations, it is instructive to consider two simpler settings. We first look at a combination of a single dislocation and a single disclination and construct the corresponding material manifold using Volterra's cut-and-weld process [39]. In the second example, we solve the problem of an infinite circular cylindrical bar with a cylindrically symmetric distribution of point defects and find the non-metricity 1-forms corresponding to an isotropic distribution of point defects. This result will be needed later on when we calculate the residual stress field of a cylindrically symmetric distribution of discombinations.

(a) Combination of a single screw dislocation and a single wedge disclination along the same line

We look at a combination of a single screw dislocation and a single wedge disclination lying on the same line as a motivation for studying more complex combinations of defects for which Volterra's cut-and-weld approach cannot be used. We denote the Euclidean 3-space by \mathcal{B}_0 with flat metric in cylindrical coordinates (R_0, θ_0, Z_0) given by

$$dS^2 = dR_0^2 + R_0^2 d\theta_0^2 + dZ_0^2. \quad (3.1)$$

We cut \mathcal{B}_0 along the closed half-planes $\theta_0 = 0$ and $\theta_0 = \alpha (0 < \alpha < 2\pi)$, remove the line $R = 0$ and the region $0 < \theta_0 < \alpha$, translate the two closed half-planes by b in the Z_0 -direction and then identify the two closed half-planes. This is Volterra's cut-and-weld construction of a combined screw dislocation–wedge disclination (dispiration) with the Z -axis as its defect line. The coordinates

$$R = R_0, \quad \Theta = \beta(\theta_0 - \alpha) \quad \text{and} \quad Z = Z_0 - \frac{b}{2\pi}\theta_0, \quad (3.2)$$

where $\beta = 2\pi/(2\pi - \alpha)$ are smooth on \mathcal{B} [39]. Note that $\beta > 1$ if we remove a wedge region (positive disclination), but $\beta < 1$ corresponds to the insertion of a wedge ($\alpha < 0$, negative disclination). In the new coordinate system, the flat metric (3.1) has the following representation in cylindrical coordinates:

$$\begin{aligned} dS^2 &= dR^2 + R^2 \left(\frac{1}{\beta} d\Theta \right)^2 + \left(dZ + \frac{b}{2\pi\beta} d\Theta \right)^2 \\ &= dR^2 + \left(\frac{R^2}{\beta^2} + \frac{b^2}{4\pi^2\beta^2} \right) d\Theta^2 + dZ^2 + \frac{b}{\pi\beta} d\Theta dZ. \end{aligned} \quad (3.3)$$

Therefore, the material metric for the defective body has the following form:

$$\mathbf{G} = \begin{pmatrix} 1 & 0 & 0 \\ 0 & \frac{R^2}{\beta^2} + \frac{b^2}{4\pi^2\beta^2} & \frac{b}{2\pi\beta} \\ 0 & \frac{b}{2\pi\beta} & 1 \end{pmatrix}. \quad (3.4)$$

In the absence of external forces, we embed the body into the ambient space (S, \mathbf{g}) , which is the flat Euclidean 3-space, and look for solutions of the form $(r, \theta, z) = (r(R), \Theta, Z)$. Having the defective body in the material manifold, the anelasticity problem is transformed to an elasticity problem mapping a material manifold with a non-trivial geometry to the Euclidean ambient space. The deformation gradient is $\mathbf{F} = \text{diag}(r'(R), 1, 1)$, for which the incompressibility condition reads

$$J = \sqrt{\frac{\det \mathbf{g}}{\det \mathbf{G}}} \det \mathbf{F} = \frac{r'(R)r(R)}{R/\beta} = 1. \quad (3.5)$$

Assuming that $r(0) = 0$ to fix the rigid translations, we obtain $r = (1/\sqrt{\beta})R$. In order to easily compare the stress field with the linear solution, we consider a neo-Hookean solid for which we have [40] $P^{aA} = \mu F^a_B G^{AB} - p(F^{-1})_b^A g^{ab}$, where $p = p(R)$ is the unknown pressure field. The non-zero first Piola–Kirchhoff stress components read

$$\left. \begin{aligned} P^{rR} &= \frac{\mu}{\sqrt{\beta}} - \sqrt{\beta}p(R), & P^{\theta\Theta} &= \frac{\mu\beta^2}{R^2} - \frac{\beta}{R^2}p(R), \\ P^{zZ} &= \mu - p(R) + \frac{\mu b^2}{4\pi^2 R^2}, & P^{\theta Z} &= P^{z\Theta} = -\frac{\mu b\beta}{2\pi R^2}. \end{aligned} \right\} \quad (3.6)$$

The corresponding Cauchy stresses are

$$\left. \begin{aligned} \sigma^{rr} &= \frac{\mu}{\beta} - p(R), & \sigma^{\phi\phi} &= \frac{\mu\beta^2}{R^2} - \frac{\beta}{R^2}p(R), \\ \sigma^{zZ} &= \mu - p(R) + \frac{\mu b^2}{4\pi^2 R^2}, & \sigma^{\theta z} &= \sigma^{z\theta} = -\frac{\mu b\beta}{2\pi R^2}. \end{aligned} \right\} \quad (3.7)$$

In the absence of body forces, the only non-trivial equilibrium equation is $\sigma^{ra}_{|a} = 0$ ($p = p(R)$ is the consequence of the other two equilibrium equations), which is simplified to read

$$\sigma^{rr}_{,r} + \frac{1}{r}\sigma^{rr} - r\sigma^{\theta\theta} = 0. \quad (3.8)$$

Or

$$\sigma^{rr}_{,R} + \frac{1}{\sqrt{\beta}} \left(\frac{1}{r}\sigma^{rr} - r\sigma^{\theta\theta} \right) = 0. \quad (3.9)$$

This then gives us

$$p'(R) = \mu \left(\frac{1}{\beta} - \beta \right) \frac{1}{R}. \quad (3.10)$$

Assuming that the traction at $R = R_0$ is $-p_\infty$, i.e. $\sigma^{rr}(R_0) = -p_\infty$, we have

$$p(R) = \frac{\mu}{\beta} + p_\infty - \mu \left(\beta - \frac{1}{\beta} \right) \ln \frac{R}{R_0}. \quad (3.11)$$

The Cauchy stress is written as

$$\boldsymbol{\sigma} = \begin{pmatrix} \mu \left(\beta - \frac{1}{\beta} \right) \ln \frac{R}{R_0} & 0 & 0 \\ 0 & -\frac{p_\infty\beta}{R^2} + \frac{\mu(\beta^2 - 1)}{R^2} \left(1 + \ln \frac{R}{R_0} \right) & -\frac{\mu b\beta}{2\pi R^2} \\ 0 & -\frac{\mu b\beta}{2\pi R^2} & \frac{p_\infty}{\sqrt{\beta}} + \mu \left(1 - \frac{1}{\beta} \right) + \mu \left(\beta - \frac{1}{\beta} \right) \ln \frac{R}{R_0} + \frac{\mu b^2}{4\pi^2 R^2} \end{pmatrix}. \quad (3.12)$$

Note that the spatial metric in cylindrical coordinates has the form $\mathbf{g} = \text{diag}(1, r^2, 1)$. The non-zero physical components of the Cauchy stress read

$$\bar{\sigma}^{rr} = \sigma^{rr}, \quad \bar{\sigma}^{\theta\theta} = r^2 \sigma^{\theta\theta} = \frac{R^2}{\beta} \sigma^{\theta\theta} = -p_\infty + \mu \left(\beta - \frac{1}{\beta} \right) \left(\ln \frac{R}{R_0} + 1 \right) \quad (3.13)$$

and

$$\bar{\sigma}^{zz} = \sigma^{zz}, \quad \bar{\sigma}^{\theta z} = \bar{\sigma}^{z\theta} = r \sigma^{\theta z} = -\frac{\mu b \sqrt{\beta}}{2\pi R}. \quad (3.14)$$

Note that the coupling effect is seen only in shear stresses and obviously superposition breaks down.

Remark 3.1. For $p_\infty = 0, \alpha, b \ll 1$ and $\beta \approx 1$, we obtain

$$\left. \begin{aligned} \bar{\sigma}^{rr} &\approx \frac{\mu\alpha}{\pi} \ln \frac{R}{R_0}, & \bar{\sigma}^{\theta\theta} &\approx \frac{\mu\alpha}{\pi} \left(\ln \frac{R}{R_0} + 1 \right), \\ \bar{\sigma}^{zz} &\approx \frac{\mu\alpha}{\pi} \left(\ln \frac{R}{R_0} + \frac{1}{2} \right), & \bar{\sigma}^{\theta z} &\approx \bar{\sigma}^{z\theta} \approx -\frac{\mu b}{2\pi R}. \end{aligned} \right\} \quad (3.15)$$

This is exactly the classical solution obtained in linearized elasticity for the superposition of disclinations [41,42] and dislocations (with $\nu = 1/2$).

Remark 3.2. Note that, in general, in the presence of disclinations Burger's vector is not well defined as the rotations created by the disclinations also induce translations [43–45]. However, if the plane of rotation is perpendicular to the direction of translations at all points, Burger's vector is well defined.

(b) A cylindrically symmetric distribution of point defects

In [23,24], we built the material manifold of a spherically symmetric distribution of point defects in a ball of radius R_0 . Here, we consider the equivalent problem for a cylindrically symmetric distribution of point defects in an infinite circular cylindrical bar of radius R_0 and construct its material manifold and then calculate its residual stress field assuming that the defective body is an arbitrary incompressible isotropic body.

The key to model point defects is to relate the volume form to the density of point defects. Here, we assume a volume density of point defects $\eta(R)$. Denoting the volume form of the Weyl manifold by μ , for a sub-body $\mathcal{U} \subset \mathcal{B}$, the volumes of the point defect-free and the defective sub-body are

$$\hat{V}(\mathcal{U}) = \int_{\mathcal{U}} \hat{\mu}, \quad V(\mathcal{U}) = \int_{\mathcal{U}} \mu, \quad (3.16)$$

where $\hat{\mu}$ is the volume form in the material manifold in the absence of point defects. The volume of the point defects in \mathcal{U} is calculated as

$$V_d(\mathcal{U}) = \int_{\mathcal{U}} \hat{\mu} - \int_{\mathcal{U}} \mu = \int_{\mathcal{U}} (\hat{\mu} - \mu) = \int_{\mathcal{U}} \eta \hat{\mu}. \quad (3.17)$$

To explicitly relate this volume of point defects to the geometry of the material manifold, we look for a coframe field in the cylindrical coordinates (R, Θ, Z) , $R \geq 0, 0 \leq \Theta \leq \pi, Z \in \mathbb{R}$ of the following form:

$$\vartheta^1 = f(R)dR, \quad \vartheta^2 = Rd\Theta \quad \text{and} \quad \vartheta^3 = dZ, \quad (3.18)$$

for some unknown function f to be determined. With this coframe, we can compute explicitly the two volume forms, that is,

$$\hat{\mu} = RdR \wedge d\Theta \wedge dZ, \quad \mu = h(R)\vartheta^1 \wedge \vartheta^2 \wedge \vartheta^3 = Rf(R)h(R)dR \wedge d\Theta \wedge dZ, \quad (3.19)$$

for some positive function h satisfying (2.13). Therefore, $\hat{\mu} - \mu = [1 - f(R)h(R)]RdR \wedge d\theta \wedge dZ$, and $n(R) = 1 - f(R)h(R)$. We can now compute the non-metricity. We assume the following connection 1-form matrix:

$$\omega = [\omega^\alpha_\beta] = \begin{pmatrix} q(R)\vartheta^1 & \omega^1_2 & -\omega^3_1 \\ -\omega^1_2 & q(R)\vartheta^1 & \omega^2_3 \\ \omega^3_1 & -\omega^2_3 & 0 \end{pmatrix}, \quad (3.20)$$

where q is a function to be determined. Note that this choice of diagonal connection forms corresponds to $\mathcal{Q}_{11} = \mathcal{Q}_{22} = 2q(R)\vartheta^1$, $\mathcal{Q}_{33} = 0$. We first need to enforce $T^\alpha = 0$, for $\alpha = 1, 2, 3$. Note that

$$d\vartheta^1 = 0, \quad d\vartheta^2 = \frac{1}{Rf(R)}\vartheta^1 \wedge \vartheta^2, \quad d\vartheta^3 = 0. \quad (3.21)$$

From Cartan's first structural equations, we obtain the following connection 1-forms:

$$\omega^1_2 = -\left[\frac{1}{Rf(R)} + q(R)\right]\vartheta^2, \quad \omega^2_3 = \omega^3_1 = 0. \quad (3.22)$$

From the second structural equations, we can easily check that $\mathcal{R}^2_3 = \mathcal{R}^3_1 = 0$ are trivially satisfied and

$$\mathcal{R}^1_2 = -\frac{1}{f(R)}\left[q'(R) + \frac{q(R)}{R} - \frac{f'(R)}{Rf^2(R)}\right]\vartheta^1 \wedge \vartheta^2. \quad (3.23)$$

$\mathcal{R}^1_2 = 0$ gives us $(Rq(R))' = -(1/f(R))'$ and hence $Rq(R) = -1/f(R) + C$. When $q(R) = 0$, we know that $f(R) = 1$ and hence $C = 1$. Thus

$$q(R) = \frac{1}{R}\left[1 - \frac{1}{f(R)}\right]. \quad (3.24)$$

The Weyl 1-form is calculated as

$$\begin{aligned} Q &= \frac{1}{3}Q_{\alpha\beta}\delta^{\alpha\beta} = \frac{1}{3}(Q_{11} + Q_{22} + Q_{33}) = \frac{4}{3}q(R)\vartheta^1 \\ &= \frac{4}{3R}\left[1 - \frac{1}{f(R)}\right]\vartheta^1 = \frac{4(f(R) - 1)}{3R}dR. \end{aligned} \quad (3.25)$$

For our cylindrically symmetric point defect distribution, the relationship (2.13) is simplified to read

$$\frac{d}{dR} \ln h(R) = \frac{h'(R)}{h(R)} = \frac{3}{2} \frac{4(f(R) - 1)}{3R} = \frac{2(f(R) - 1)}{R}. \quad (3.26)$$

Therefore, $Rh'(R) + 2h(R) = 2(1 - n(R))$ and hence

$$h(R) = 1 - \frac{1}{R^2} \int_0^R 2yn(y) dy. \quad (3.27)$$

Thus

$$f(R) = \frac{1 - n(R)}{1 - (1/R^2) \int_0^R 2yn(y) dy}. \quad (3.28)$$

Remark 3.3. We conclude that, given an isotropic distribution of point defects with volume density $n = n(R)$, the corresponding non-metricity 1-forms are

$$Q_{11} = Q_{22} = \frac{1}{R} \left[\frac{1 - n(R)}{1 - (1/R^2) \int_0^R 2yn(y) dy} - 1 \right] dR, \quad Q_{33} = 0, \quad Q_{\alpha\beta} = 0, \quad \alpha \neq \beta. \quad (3.29)$$

The material metric in cylindrical coordinates (R, Θ, Z) has the following form:

$$\mathbf{G} = \begin{pmatrix} f^2(R) & 0 & 0 \\ 0 & R^2 & 0 \\ 0 & 0 & 1 \end{pmatrix}. \quad (3.30)$$

We use the cylindrical coordinates (r, θ, z) for the Euclidean ambient space with the following metric: $\mathbf{g} = \text{diag}(1, r^2, 1)$. To calculate the residual stress field, we embed the material manifold into the Euclidean ambient space and look for solutions of the form $(r, \theta, z) = (r(R), \Theta, Z)$. In the following, we consider incompressible solids.

For an incompressible solid, we have

$$J = \sqrt{\frac{\det \mathbf{g}}{\det \mathbf{G}}} \det \mathbf{F} = \frac{r(R)}{Rf(R)} r'(R) = 1. \quad (3.31)$$

Assuming that $r(0) = 0$ we obtain

$$r(R) = \left(\int_0^R 2xf(x) dx \right)^{1/2}. \quad (3.32)$$

The physical components of the deformation gradient are given by

$$\hat{F}^a_A = \sqrt{g_{aa}} \sqrt{G^{AA}} F^a_A \quad \text{no summation on } a \text{ or } A. \quad (3.33)$$

Therefore

$$\hat{\mathbf{F}} = \begin{pmatrix} \frac{R}{r(R)} & 0 & 0 \\ 0 & \frac{r(R)}{R} & 0 \\ 0 & 0 & 1 \end{pmatrix}. \quad (3.34)$$

Thus, the principal stretches (eigenvalues of $\mathbf{U} = \sqrt{\mathbf{C}}$) are

$$\lambda_1 = \frac{R}{r(R)}, \quad \lambda_2 = \frac{r(R)}{R} \quad \text{and} \quad \lambda_3 = 1. \quad (3.35)$$

Because for an isotropic material strain-energy function depends only on the principal stretches, i.e. $W = W(\lambda_1, \lambda_2, \lambda_3)$ [37], and the Cauchy stress is diagonal in the cylindrical coordinates (r, θ, z) , we have

$$\sigma^{rr} = \lambda_1 g^{11} \frac{\partial W}{\partial \lambda_1} - p(R) g^{11} = \frac{R}{r(R)} \frac{\partial W}{\partial \lambda_1} - p(R), \quad (3.36)$$

$$\sigma^{\theta\theta} = \lambda_2 g^{22} \frac{\partial W}{\partial \lambda_2} - p(R) g^{22} = \frac{1}{Rr(R)} \frac{\partial W}{\partial \lambda_2} - \frac{p(R)}{r^2(R)} \quad (3.37)$$

and

$$\sigma^{\phi\phi} = \lambda_3 g^{33} \frac{\partial W}{\partial \lambda_3} - p(R) g^{33} = \frac{\partial W}{\partial \lambda_3} - p(R). \quad (3.38)$$

In the absence of body forces, the only non-trivial equilibrium equation is $\sigma^{ra}_{|a} = 0$, which is simplified to read

$$\sigma^{rr}_{,r} + \frac{1}{r} \sigma^{rr} - r \sigma^{\theta\theta} = 0. \quad (3.39)$$

Or

$$\sigma^{rr}_{,R} + \frac{Rf}{r} \left(\frac{2}{r} \sigma^{rr} - 2r \sigma^{\theta\theta} \right) = 0. \quad (3.40)$$

This then gives us $p'(R) = k(R)$, where

$$k(R) = \frac{1}{r(R)} \left(\frac{\partial W}{\partial \lambda_1} - f(R) \frac{\partial W}{\partial \lambda_2} \right) + \frac{R}{r^2(R)} \left(1 - \frac{R^2 f(R)}{r^2(R)} \right) \left(\frac{\partial^2 W}{\partial \lambda_1^2} - \frac{r^2(R)}{R^2} \frac{\partial^2 W}{\partial \lambda_1 \partial \lambda_2} \right). \quad (3.41)$$

Suppose that at the boundary $\sigma^{rr}(R_0) = -p_\infty$. Thus

$$p(R) = p_\infty + \frac{R_0}{r(R_0)} \frac{\partial W}{\partial \lambda_1} \Big|_{R=R_0} + \int_R^{R_0} k(x) dx. \quad (3.42)$$

Having the pressure field, all the stress components are easily calculated.

4. An algorithm for semi-inverse problems with discombinations

The two previous examples demonstrated how to obtain the stress field for defects by building the corresponding material manifold. The first example depended on the cut-and-weld process to build the material metric. The second example demonstrated how to obtain the non-metricity for point defects. We are now interested in computing the stress field for a body with discombinations (with and without external loads). Before considering particular problems, we obtain the general equations that fully define the geometry of systems with given discombinations (assuming a traceless non-metricity). In three dimensions, this leads to a system of 22 nonlinear PDEs for the connection 1-forms and associated geometrical quantities. Obviously, this problem cannot be solved in general, but for semi-inverse problems for which the deformation is prescribed, an explicit computation can be performed. The basic idea is to start from a known geometry (for instance, a cylinder, a sphere, a rectangular block) and consider a family of known geometric deformations parametrized by a number of arbitrary parameters or functions. Then, the problem reduces to computing these unknowns based on the conditions of mechanical equilibrium. In the case of a material with defects, the body is characterized by its geometry, its local material properties (the strain-energy density function, mass density), but also its distribution of defects.

The step-by-step process to obtain the general equations that define the material manifold is as follows:

- Step 1: *The physical inputs.* We start naturally with the description of the physical defects. Traditionally, these are given by Burger's density vector for dislocations, Frank's density vector for disclinations, and the volume density of point defects. Each of these quantities has a natural geometrical equivalent in a continuum representation. Burger's density vector is associated with the torsion 2-form (as detailed in [7,46]). Frank's density vector is associated with the curvature 2-form (as detailed in [22]), and from the volume density of point defects, one can calculate the non-metricity 1-forms (see [23,24]) through equation (2.13).
- Step 2: *Geometry.* In a given coordinate chart $\{X^A\}$ whose geometry is closely related to the given physical fields, we define the coframe field as $\vartheta^a = F^a_A dX^A$. Further, we introduce the material connection 1-forms ω^α_β and compute the torsion and curvature 2-forms given by equations (2.8) with respect to the coframe field.

Counting the number of variables and unknowns. In n dimensions, \mathbf{F} has n^2 unknown elements. The connection 1-forms ω^α_β are also unknowns. We assume that $\omega^\alpha_\beta = -\omega^\beta_\alpha$ ($\alpha \neq \beta$) and $\omega^\alpha_\alpha = (n/2)Q$ (no summation) for some unknown Weyl 1-form Q . Note that, in the presence of symmetry, some of the ω^α_β s may vanish identically. Therefore, there are $1/2(n^2 - n) + 1$ unknown 1-forms or $(n/2)(n^2 - n) + n$ unknown scalars. In the compatible volume element, the function h is an unknown, i.e. 1 unknown. Therefore, the total number of unknowns is

$$N_u = n^2 + \left(\frac{n(n^2 - n)}{2} + n \right) + 1 = \frac{n^3}{2} + \frac{n^2}{2} + n + 1. \quad (4.1)$$

- Step 3: *Cartan's structural equations.* From steps 1 and 2, we have on the one hand a description of the defects in terms of curvature, torsion and non-metricity, and, on the other hand, a characterization of the same objects in terms of the coframe fields. Therefore, we

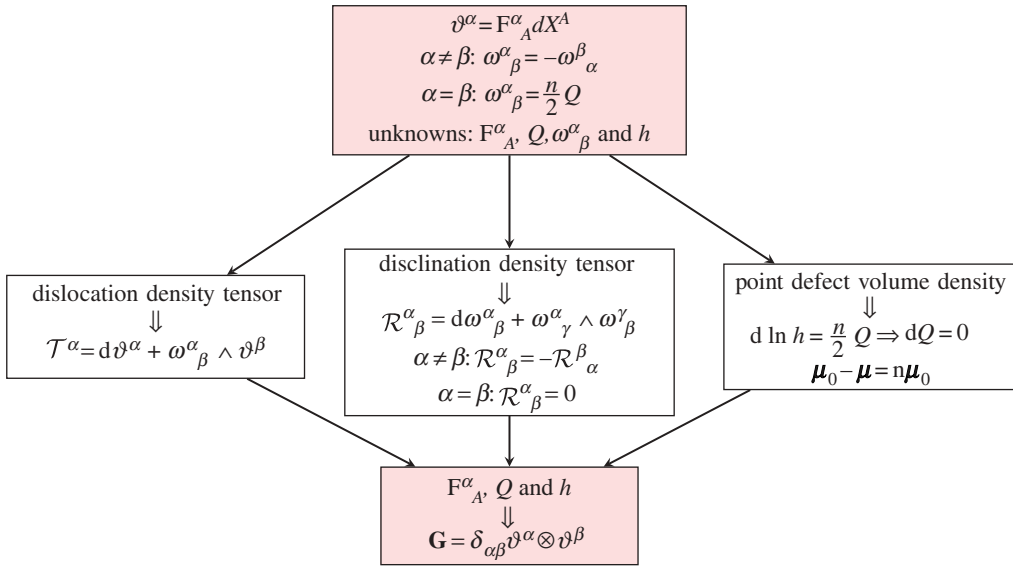


Figure 2. Construction of the material manifold for a defective body. Top: step 1, define the coframe field, the connection 1-forms and the volume functions. Middle: steps 2 and 3, from the physical inputs, solve for the unknown functions appearing in step 1. Bottom: step 4, obtain the material metric. (Online version in colour.)

can identify the dislocation density tensor, disclination density tensor and point defect volume density with their geometrical counterparts and the structural equations provide a number of equations for the unknowns (the functions $F^{\alpha A}$, the connection 1-forms ω^α_β , the Weyl 1-form Q and the volume function h).

Counting the number of equations. The first structural equations $\mathcal{T}^\alpha = d\vartheta^\alpha + \omega^\alpha_\beta \wedge \vartheta^\beta$ give us n , 1-form equations or n^2 scalar equations. The compatibility of the volume element $d \ln h = (n/2)Q$ (and hence $dQ = 0$) is a 1-form equation or n scalar equations. The relation $\hat{\mu} - \mu = n\mu_0$ is an n -form equation or 1 scalar equation. Note that $\hat{\mu}$ is the volume form of the point defect-free configuration. Finally, the second structural equations $\mathcal{R}^\alpha_\beta = d\omega^\alpha_\beta + \omega^\alpha_\gamma \wedge \omega^\gamma_\beta$ imply that, for $\alpha = \beta$, $\mathcal{R}^\alpha_\alpha = (n/2)dQ = 0$ (no summation) are trivially satisfied. For $\alpha \neq \beta$, $\mathcal{R}^\alpha_\beta = -\mathcal{R}^\beta_\alpha$, i.e. the second structural equations give us $1/2(n^2 - n)$, 1-form equations or $(n/2)(n^2 - n)$ scalar equations. Therefore, the number of governing equations is

$$N_e = n^2 + n + 1 + \frac{n(n^2 - n)}{2} = \frac{n^3}{2} + \frac{n^2}{2} + n + 1. \quad (4.2)$$

Note that, as expected but nevertheless reassuring, $N_u = N_e$.

Step 4: Material metric. Assuming that there exists a solution at step 3, we know the coframe field and hence the material metric $\mathbf{G} = \delta_{\alpha\beta} \vartheta^\alpha \otimes \vartheta^\beta$ can be computed. In a semi-inverse problem, the metric is known up to a number of undetermined functions to be specified by the elastic problem.

Step 5: Elasticity. Once the material metric is known, the standard equations of elasticity from a Riemannian manifold to the ambient space (a flat Riemannian manifold) given by (2.14) can be solved for the remaining unknown parameters. For given boundary conditions, the elastic computation gives the deformation gradient and the stress field (the residual stress in the case of free-traction boundary conditions).

Figure 2 summarizes our approach for constructing the material manifold of a defective solid.

Remark 4.1. Given a torsion 2-form distribution and starting with a coframe field the connection 1-forms are uniquely determined. This is a simple consequence of Cartan's lemma and a simple generalization of a similar result proved in [7]. Let us assume that $Q_{\alpha\beta}$ and T^α are given. In particular, we have Cartan's first structural equations $T^\alpha = d\vartheta^\alpha + \omega^\alpha_\beta \wedge \vartheta^\beta$. Suppose that there is another set of connection 1-forms $\tilde{\omega}^\alpha_\beta$ satisfying the same structural equations. Now, defining $\kappa^\alpha_\beta = \tilde{\omega}^\alpha_\beta - \omega^\alpha_\beta$, we have

$$\kappa^\alpha_\beta \wedge \vartheta^\beta = 0. \quad (4.3)$$

Using the zeroth structural equations and assuming that non-metricity is given we know that $\kappa^\alpha_\alpha = 0$ (no summation) and $\kappa^\alpha_\beta = -\kappa^\beta_\alpha$ ($\alpha \neq \beta$) and hence from Cartan's lemma we conclude that $\kappa^\alpha_\beta = 0$ and hence the connection 1-forms are uniquely calculated.

Remark 4.2. In general, the number of unknowns and equations for step 3 are equal. For $n = 3$, we have 22 equations for 22 unknowns. This is a large set of nonlinear coupled PDEs for which no analytical progress seems possible. However, in problems with some symmetry, one can use a semi-inverse approach, which means that most of F^α_A 's are assumed to be zero and the non-zero ones are assumed to be functions of only a small number of $\{X^A\}$ coordinates. This judicious ansatz will significantly simplify the construction of the material manifold and allows for the explicit computation of systems with a combination of defects.

5. A detailed example of discombinations

We combine the two examples of §3 and consider a combination of cylindrically symmetric distributions of screw dislocations, wedge disclinations and point defects in an infinite incompressible isotropic circular cylindrical bar allowed to only deform radially, that is, $(r, \theta, z) = (r(R), \Theta, Z)$. We present the construction of solutions with discombinations by following the step-by-step algorithm given in the previous section by first constructing the material manifold and then calculating the stress field under uniform hydrostatic pressure.

(a) Step 1: physical inputs

(i) Screw dislocations

We assume a radial density of screw dislocations $b(R)$. Written in terms of the torsion 2-forms, it reads simply

$$T^1 = T^2 = 0, \quad T^3 = \frac{b(R)}{2\pi} dR \wedge Rd\Theta. \quad (5.1)$$

(ii) Wedge disclinations

Similarly, a radial density of wedge disclinations $w(R)$ is related to the curvature 2-forms,

$$\mathcal{R}^1_2 = \frac{w(R)}{2\pi} dR \wedge Rd\Theta, \quad \mathcal{R}^2_3 = \mathcal{R}^3_1 = 0. \quad (5.2)$$

We define the auxiliary radial wedge disclination function as

$$W(R) = \frac{1}{2\pi} \int_0^R \rho w(\rho) d\rho. \quad (5.3)$$

(iii) Point defects

We assume again a volume density of point defects $n(R)$. Following the construction of §3*b*, the volume of point defects in \mathcal{U} is calculated as

$$V_d(\mathcal{U}) = \int_{\mathcal{U}} (\hat{\mu} - \mu) = \int_{\mathcal{U}} n\hat{\mu}. \quad (5.4)$$

Importantly, because the non-metricity is solely owing to the presence of point defects and not the other defects, we can directly use the result of remark 3.3 and set the non-metricity 1-forms to

$$Q_{11} = Q_{22} = \frac{1}{R} \left[\frac{1 - n(R)}{1 - (1/R^2) \int_0^R 2yn(y) dy} - 1 \right] dR, \quad Q_{33} = 0, \quad Q_{\alpha\beta} = 0, \quad \alpha \neq \beta. \quad (5.5)$$

(b) Step 2: geometry

We assume that the wedge disclinations and the screw dislocations are parallel to the Z-axis. Therefore, based on this geometry (and following remark 4.2 above), we expect the coframe field to be a function of R only and we use the following ansatz:

$$\vartheta^1 = f(R)dR, \quad \vartheta^2 = \xi(R)d\Theta \quad \text{and} \quad \vartheta^3 = dZ + \eta(R)d\Theta, \quad (5.6)$$

for some unknown functions f, ξ and η to be determined. A simple calculation gives

$$d\vartheta^1 = 0, \quad d\vartheta^2 = \frac{\xi'}{f\xi} \vartheta^1 \wedge \vartheta^2 \quad \text{and} \quad d\vartheta^3 = \frac{\eta'}{f\xi} \vartheta^1 \wedge \vartheta^2. \quad (5.7)$$

Note that, because the traceless part of non-metricity vanishes, $\omega^\alpha_\beta = -\omega^\beta_\alpha$ for $\alpha \neq \beta$. Moreover, the diagonal elements are related to the non-metricity given by (5.5) as explained in §3*b*. Therefore, the matrix of connection 1-forms is assumed to have the following form:

$$\omega = [\omega^\alpha_\beta] = \begin{pmatrix} F(R)\vartheta^1 & \omega^1_2 & -\omega^3_1 \\ -\omega^1_2 & F(R)\vartheta^1 & \omega^2_3 \\ \omega^3_1 & -\omega^2_3 & 0 \end{pmatrix}, \quad (5.8)$$

where

$$F(R) = \frac{f_0(R) - 1}{Rf(R)}, \quad f_0(R) = \frac{1 - n(R)}{1 - (1/R^2) \int_0^R 2yn(y) dy}. \quad (5.9)$$

(i) The torsion 2-forms

The first structural equations $T^\alpha = d\vartheta^\alpha + \omega^\alpha_\beta \wedge \vartheta^\beta$ can be used to compute the torsion 2-forms in terms of the connection 1-forms and the coframe field. Explicitly for $\alpha = 1$, it reads

$$\begin{aligned} T^1 &= d\vartheta^1 + \omega^1_1 \wedge \vartheta^1 + \omega^1_2 \wedge \vartheta^2 + \omega^1_3 \wedge \vartheta^3 \\ &= \omega^1_2 \wedge \vartheta^2 - \omega^3_1 \wedge \vartheta^3 \\ &= \omega^1_{12} \vartheta^1 \wedge \vartheta^2 - (\omega^1_{32} + \omega^3_{21}) \vartheta^2 \wedge \vartheta^3 + \omega^3_{11} \vartheta^3 \wedge \vartheta^1. \end{aligned} \quad (5.10)$$

Similarly, we have

$$T^2 = \left(\frac{\xi'}{f\xi} + F + \omega^1_{22} \right) \vartheta^1 \wedge \vartheta^2 + \omega^2_{23} \vartheta^2 \wedge \vartheta^3 - (\omega^1_{32} + \omega^2_{13}) \vartheta^3 \wedge \vartheta^1 \quad (5.11)$$

and

$$T^3 = \left(\frac{\eta'}{f\xi} - \omega^3_{21} - \omega^2_{13} \right) \vartheta^1 \wedge \vartheta^2 + \omega^2_{33} \vartheta^2 \wedge \vartheta^3 + \omega^3_{31} \vartheta^3 \wedge \vartheta^1. \quad (5.12)$$

(ii) The curvature 2-forms

Next, we compute the curvature 2-forms through the second Cartan's structural equations $\mathcal{R}^\alpha_\beta = d\omega^\alpha_\beta + \omega^\alpha_\gamma \wedge \omega^\gamma_\beta$ (trivially satisfied for $\alpha = \beta$). For instance for $\alpha = 1, \beta = 2$, we have

$$\begin{aligned}\mathcal{R}^1_2 &= d\omega^1_2 + \omega^1_1 \wedge \omega^1_2 + \omega^1_2 \wedge \omega^2_2 + \omega^1_3 \wedge \omega^3_2 \\ &= d\omega^1_2 + F\vartheta^1 \wedge \omega^1_2 + \omega^1_2 \wedge F\vartheta^1 + \omega^3_1 \wedge \omega^2_3 \\ &= d\omega^1_2 + \omega^3_1 \wedge \omega^2_3.\end{aligned}\quad (5.13)$$

Similarly, we have

$$\mathcal{R}^2_3 = d\omega^2_3 + \omega^1_2 \wedge \omega^3_1 + F\vartheta^1 \wedge \omega^2_3 \quad (5.14)$$

and

$$\mathcal{R}^3_1 = d\omega^3_1 + \omega^2_3 \wedge \omega^1_2. \quad (5.15)$$

(iii) The compatible volume element

Finally, we consider the Weyl 1-form Q . Because we assume that the only source of non-metricity is given by point defects, it is identical to that of a cylindrical bar with only point defects. Indeed, let h_0 denote the volume function in the case where the only defects are point defects and, similarly, define h to be the volume function for the discombination case. Then, we have

$$d \ln h_0 = d \ln h = \frac{3}{2}Q. \quad (5.16)$$

Thus, $\ln h = \ln h_0 + C_1$ or $h = Ch_0$. In the absence of dislocations and disclinations, we have $h = h_0$. Therefore, we conclude that $C = 1$, i.e. $h = h_0$ even in the case of discombinations. We define the volume density of point defects with respect to the no point defect configuration, which has the Riemannian volume form $\hat{\mu}$, and note that

$$\left. \begin{aligned}\hat{\mu} = \mu|_{f=h=1} &= \frac{\xi(R)}{R} \mu_0, & \mu = h\vartheta^1 \wedge \vartheta^2 \wedge \vartheta^3 &= \frac{f(R)h_0(R)\xi(R)}{R} \mu_0, \\ \mu_0 &= R dR \wedge d\Theta \wedge dZ.\end{aligned}\right\} \quad (5.17)$$

The volume density of point defects n is defined as $\hat{\mu} - \mu = n\hat{\mu}$. Thus, $1 - h_0(R)f(R) = n(R)$. Noting that $1 - h_0(R)f_0(R) = n(R)$, we conclude that $f(R) = f_0(R)$.

We have now set up the geometry of our problem by providing an ansatz for the coframe field and $\xi(R)$ and $\eta(R)$ are 2 unknown functions to be determined as functions of the physical fields.

(c) Step 3: Cartan's structural equations

We have defined the torsion 2-forms in terms of both the coframe field and the physical inputs. We can now solve the structural equations for the unknowns in terms of the given physical fields. We start again with the torsion 2-forms.

(i) The torsion 2-forms

We start with the first component of the vector-valued torsion 2-form (5.10), which according to (5.1) vanishes identically. In turn, this implies

$$\omega^1_{12} = \omega^3_{11} = 0, \quad \omega^1_{32} = -\omega^3_{21}. \quad (5.18)$$

Similarly, the vanishing of the second component of the torsion leads to

$$\omega^2_{23} = 0, \quad \omega^1_{22} = -\frac{\xi'}{f\xi} - F \quad \text{and} \quad \omega^1_{32} = -\omega^2_{13}. \quad (5.19)$$

Finally, by writing $\mathcal{T}^3 = (b(R)/2\pi)dR \wedge Rd\Theta = (b(R)/2\pi f_0 \xi) \vartheta^1 \wedge \vartheta^2$, we obtain

$$\omega^3_{31} = \omega^2_{33} = 0 \quad \text{and} \quad \omega^1_{32} = -\frac{1}{2f_0 \xi} \left[\eta' - \frac{Rb}{2\pi} \right]. \quad (5.20)$$

Therefore, the connection 1-forms can be written as

$$\omega^1_2 = -\left[\frac{\xi'}{f_0 \xi} + F \right] \vartheta^2 - \frac{1}{2f_0 \xi} \left[\eta' - \frac{Rb}{2\pi} \right] \vartheta^3, \quad (5.21)$$

$$\omega^2_3 = \frac{1}{2f_0 \xi} \left[\eta' - \frac{Rb}{2\pi} \right] \vartheta^1 \quad (5.22)$$

and

$$\omega^3_1 = \frac{1}{2f_0 \xi} \left[\eta' - \frac{Rb}{2\pi} \right] \vartheta^2. \quad (5.23)$$

(ii) The curvature 2-forms

The second Cartan's structural equations are trivially satisfied for $\alpha = \beta$. The only non-trivial ones are \mathcal{R}^1_2 and \mathcal{R}^2_3 . First consider, $\mathcal{R}^2_3 = 0$, using the identities (5.21)–(5.23), we have $d\omega^2_3 = 0$, $F\vartheta^1 \wedge \omega^2_3 = 0$, and hence

$$\mathcal{R}^2_3 = \omega^1_2 \wedge \omega^3_1 = \frac{1}{4f_0^2 \xi^2} \left(\eta' - \frac{Rb}{2\pi} \right)^2 \vartheta^2 \wedge \vartheta^3 = 0. \quad (5.24)$$

Therefore, we conclude that

$$\eta' = \frac{Rb}{2\pi} \Rightarrow \eta(R) = \frac{1}{2\pi} \int_0^R \rho b(\rho) d\rho + C. \quad (5.25)$$

In the absence of dislocations $\eta(R) = 0$ and thus $C = 0$. Hence, we have

$$\omega^1_2 = -\left[\frac{\xi'}{f_0 \xi} + F \right] \vartheta^2, \quad \omega^2_3 = \omega^3_1 = 0. \quad (5.26)$$

Next, consider

$$\mathcal{R}^1_2 = d\omega^1_2 = -\frac{1}{\xi f_0} \frac{d}{dR} \left[\frac{\xi'}{f_0} + F\xi \right] \vartheta^1 \wedge \vartheta^2 = \frac{Rw}{2\pi f_0 \xi} \vartheta^1 \wedge \vartheta^2.$$

Therefore

$$\frac{d}{dR} \left[\frac{\xi'}{f_0} + F\xi \right] = -\frac{Rw}{2\pi} \Rightarrow \frac{\xi'}{f_0} + F\xi = C - W(R). \quad (5.27)$$

Or

$$\frac{\xi'}{f_0} + \frac{(f_0 - 1)\xi}{Rf_0} = C - W(R). \quad (5.28)$$

When there are no defects $f_0 = 1$, $\xi = R$, $W = 0$, and hence $C = 1$. Therefore

$$\xi' + \frac{f_0 - 1}{R} \xi = f_0(1 - W). \quad (5.29)$$

The solution to this equation is

$$\xi(R) = \frac{C}{\gamma(R)} + \frac{1}{\gamma(R)} \int_0^R \gamma(x) f_0(x) (1 - W(x)) dx, \quad \gamma(R) = e^{\int_0^R ((f_0(x) - 1)/x) dx}. \quad (5.30)$$

Note that in the absence of defects $W = 0$, $f_0 = 1$, $\gamma = 1$, $\xi = R$, and hence $C = 0$. Thus

$$\xi(R) = \frac{1}{\gamma(R)} \int_0^R \gamma(x) f_0(x) (1 - W(x)) dx. \quad (5.31)$$

(d) Step 4: material metric

Having determined all our unknown functions $f(R)$, $\xi(R)$ and $\eta(R)$ in terms of the physical inputs, we can write the material metric. Note that $\mathbf{G} = \delta_{\alpha\beta} \vartheta^\alpha \otimes \vartheta^\beta = \vartheta^1 \otimes \vartheta^1 + \vartheta^2 \otimes \vartheta^2 + \vartheta^3 \otimes \vartheta^3$. Thus

$$\mathbf{G} = \begin{pmatrix} f^2 & 0 & 0 \\ 0 & \xi^2 + \eta^2 & \eta \\ 0 & \eta & 1 \end{pmatrix} \quad \text{and} \quad \mathbf{G}^\sharp = \begin{pmatrix} \frac{1}{f^2} & 0 & 0 \\ 0 & \frac{1}{\xi^2} & -\frac{\eta}{\xi^2} \\ 0 & -\frac{\eta}{\xi^2} & 1 + \frac{\eta^2}{\xi^2} \end{pmatrix}. \quad (5.32)$$

(e) Step 5: elasticity

From the material manifold, we obtain the stress field by embedding the body into the ambient space (S, \mathbf{g}) , which is the flat Euclidean 3-space, and look for solutions of the form $(r, \theta, z) = (r(R), \Theta, Z)$. Having the defective body in the material manifold the anelasticity problem is transformed to an elasticity problem from a material manifold with a non-trivial geometry to the Euclidean ambient space. The deformation gradient is $\mathbf{F} = \text{diag}(r'(R), 1, 1)$, which leads to the incompressibility condition

$$J = \sqrt{\frac{\det \mathbf{g}}{\det \mathbf{G}}} \det \mathbf{F} = \frac{r}{f_0 \xi} r' = 1. \quad (5.33)$$

Assuming that $r(0) = 0$ to fix the rigid translations, we obtain

$$r(R) = \left(\int_0^R 2f_0(x)\xi(x) dx \right)^{1/2}, \quad (5.34)$$

with the condition $\int_0^R f_0(x)\xi(x) dx > 0$.

The Finger tensor for our problem is given by

$$\mathbf{b}^\sharp = \begin{pmatrix} \frac{\xi^2}{r^2} & 0 & 0 \\ 0 & \frac{1}{\xi^2} & -\frac{\eta}{\xi^2} \\ 0 & -\frac{\eta}{\xi^2} & 1 + \frac{\eta^2}{\xi^2} \end{pmatrix}. \quad (5.35)$$

The principal invariants of \mathbf{b} are

$$I_1 = 1 + \frac{\xi^2}{r^2} + \frac{r^2}{\xi^2} + \frac{\eta^2}{\xi^2} \quad \text{and} \quad I_2 = 1 + \frac{\xi^2}{r^2} + \frac{r^2}{\xi^2} + \frac{\eta^2}{r^2}. \quad (5.36)$$

Because the material is assumed to be isotropic, we have in general that $\boldsymbol{\sigma} = (-p + I_2 B)\mathbf{g}^\sharp + A\mathbf{b}^\sharp - B\mathbf{b}^{-1}$, where $\mathbf{b}^\sharp = id_*(\mathbf{G}^\sharp)$ and $A(R) = 2(\partial W / \partial I_1)$, $B(R) = 2(\partial W / \partial I_2)$. Now, $(b^{-1})^{ab} = c^{ab} = g^{am} g^{bm} c_{mn}$ has the following representation:

$$\mathbf{b}^{-1} = \begin{pmatrix} \frac{r^2}{\xi^2} & 0 & 0 \\ 0 & \frac{\xi^2 + \eta^2}{r^4} & \frac{\eta}{r^2} \\ 0 & \frac{\eta}{r^2} & 1 \end{pmatrix}. \quad (5.37)$$

Therefore, the Cauchy stress can be written as

$$\sigma = \begin{pmatrix} -p + (A+B)\frac{\xi^2}{r^2} + B\left(1 + \frac{\eta^2}{R^2}\right) & 0 & 0 \\ 0 & \frac{-p+B}{r^2} + \frac{A+B}{\xi^2} & -\frac{A\eta}{\xi^2} - \frac{B\eta}{r^2} \\ 0 & -\frac{A\eta}{\xi^2} - \frac{B\eta}{r^2} & -p + A\left(1 + \frac{\eta^2}{\xi^2}\right) + B\left(\frac{r^2}{\xi^2} + \frac{\xi^2 + \eta^2}{r^2}\right) \end{pmatrix}. \quad (5.38)$$

The only remaining unknown, $p = p(R)$, is obtained from the only non-trivial equilibrium equation

$$\sigma^{rr},R + \frac{\xi}{r} \left(\frac{1}{r} \sigma^{rr} - r \sigma^{\theta\theta} \right) = 0, \quad (5.39)$$

which, following the classical case, simplifies to the ODE $p'(R) = k(R)$ with

$$\begin{aligned} k(R) &= (f_0 - 2)(A+B)\frac{\xi^3}{r^4} + B \left(\frac{Rb\eta}{\pi r^2} + (f_0 - 2)\frac{\xi\eta^2}{r^4} \right) \\ &\quad - f_0 \frac{A+\beta}{\xi} + (A'+B')\frac{\xi^2}{r^2} + B' \left(1 + \frac{\eta^2}{r^2} \right) + 2(A+B)\frac{\xi\xi'}{r^2}. \end{aligned} \quad (5.40)$$

For definition, we recall how the functions appearing in the Cauchy stress are related to the distribution of defects,

$$f_0(R) = \frac{1 - n(R)}{1 - (1/R^2) \int_0^R 2yn(y) dy}, \quad (5.41)$$

$$\eta(R) = \frac{1}{2\pi} \int_0^R \rho b(\rho) d\rho \quad (5.42)$$

$$\text{and} \quad \xi(R) = \frac{1}{\gamma(R)} \int_0^R \gamma(x) f_0(x) (1 - W(x)) dx, \quad \gamma(R) = e^{\int_0^R ((f_0(x)-1)/x) dx}. \quad (5.43)$$

Once the pressure $p(R)$ is known, the Cauchy stress is fully determined and the remaining calculations are identical to those of the previous sections. We note again that the presence of combined dislocation and disinclination induces shear stress and that the stress field cannot be calculated using superposition (in particular, it depends intimately on the point defect distribution through f_0 and γ).

6. Conclusion

We have presented a systematic method for constructing the material manifold of solids with distributed discombinations using Cartan's machinery of moving frames and structural equations. Given the physical fields (defect densities), we can compute the associated geometric quantities and write the general equations of equilibrium. In general, these equations are particularly difficult as they are a large number of nonlinear coupled PDEs. However, for semi-inverse problems where both deformation and defect distribution preserve elementary symmetries, a general method for computing the solution is achievable by first constructing the material manifold and second computing the conditions for mechanical equilibrium. As a model example, we constructed the material manifold of an infinite circular cylindrical bar with a cylindrically symmetric distribution of combined screw dislocations, wedge disinclinations and point defects (discombinations). We calculated the induced residual stress field for arbitrary incompressible isotropic solids and observed on that simple system the breakdown of the superposition principle. The algorithm presented in this paper offers a systematic and rigorous way to derive new solutions for semi-inverse problems for anelastic systems.

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