Weyl geometry and the nonlinear mechanics of distributed point defects

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The residual stress field of a nonlinear elastic solid with a spherically symmetric distribution of point defects is obtained explicitly using methods from differential geometry. The material manifold of a solid with distributed point defects—where the body is stress-free—is a flat Weyl manifold, i.e. a manifold with an affine connection that has non-metricity with vanishing traceless part, but both its torsion and curvature tensors vanish. Given a spherically symmetric point defect distribution, we construct its Weyl material manifold using the method of Cartan's moving frames. Having the material manifold, the anelasticity problem is transformed to a nonlinear elasticity problem and reduces the problem of computing the residual stresses to finding an embedding into the Euclidean ambient space. In the case of incompressible neo-Hookean solids, we calculate explicitly this residual stress field. We consider the example of a finite ball and a point defect distribution uniform in a smaller ball and vanishing elsewhere. We show that the residual stress field inside the smaller ball is uniform and hydrostatic. We also prove a nonlinear analogue of Eshelby's celebrated inclusion problem for a spherical inclusion in an isotropic incompressible nonlinear solid.

Keywords: geometric elasticity; point defects; residual stresses

1. Introduction

The stress field of a single point defect in an infinite linear elastic solid was obtained by Love (1927) almost 90 years ago. He observed a $1/r^3$ singularity. For distributed defects, Eshelby (1954) showed that for a body with a uniform distribution of point defects, in the framework of linearized elasticity, the body expands uniformly. In other words, a uniform distribution of point defects is stress-free (if the body is not constrained on its boundaries).[1] Such calculations for nonlinear solids have not been done to this date. In the linear elasticity setting, point defects are modelled as centres of expansion or contraction (Garikipati *et al.* 2006). In the nonlinear framework presented in this paper, we start with a distributed point defect and use non-metricity in the material manifold to model the effect of point defects.

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[1]We show in this paper that for an incompressible nonlinear solid, this result still holds.

It has been known for a long time that the mechanics of solids with distributed defects can be formulated using non-Riemannian geometries (Kondo 1955a,b; Bilby *et al.* 1955; Bilby & Smith 1956). In Yavari & Goriely (2012), we presented a comprehensive theory of the mechanics of distributed dislocations based on Riemann–Cartan geometry. We showed that in the geometric framework, several examples of residual stress field of solids with distributed dislocations can be solved analytically. We analytically calculated the residual stress field of several examples. Later, we (Yavari & Goriely in press) extended the geometric theory to the mechanics of solids with distributed disclinations. In the case of both dislocations and disclinations, there are exact solutions in the framework of nonlinear elasticity (Rosakis & Rosakis 1988; Zubov 1997; Acharya 2001).

While it has been noted that the geometric object relevant to point defects is non-metricity (Falk 1981; de Wit 1981; Grachev *et al.* 1989; Kröner 1990; Miri & Rivier 2002), there are no exact nonlinear solutions for point defects in the literature. In other words, the coupling between the geometry and the mechanics of point defects is missing. The purpose of this paper is to develop a fully geometric and exact (in the sense of elasticity) theory of distributed point defects. As an application of this geometric theory, we obtain the stress field of a spherically symmetric distribution of point defects in a neo-Hookean solid. We also prove a nonlinear analogue of Eshelby's celebrated inclusion problem for a spherical 'inclusion' in an isotropic incompressible nonlinear solid.

This paper is structured as follows. In §2, we briefly review some basic definitions and concepts from differential geometry and, in particular, Cartan's moving frames and Weyl geometry. Kinematics and equations of motion for nonlinear elasticity and anelasticity are discussed in §3. In §4, we look at the problem of a spherically symmetric distribution of point defects. Using Cartan's structural equations, we obtain an orthonormal coframe field and hence the material metric. We then make a connection between the material metric and the volume density of point defects using a compatible volume element in the Weyl material manifold. Having the material metric, we then calculate the residual stress field. Next, we study an example of a point defect distribution uniform in a small ball and vanishing outside the ball. We show that for any isotropic incompressible nonlinear solid, the residual stress field inside the small ball is uniform. This is a nonlinear analogue of Eshelby's celebrated inclusion problem. We then show that a uniform point defect distribution is the only spherically symmetric zero-stress point defect distribution. Finally, we compare the linear and nonlinear solutions for the radial stress distribution.

2. Non-Riemannian geometries and Cartan's moving frames

(*a*) *Riemann–Cartan manifolds*

We tersely review some elementary facts about affine connections on manifolds, and the geometry of Riemann–Cartan and Weyl manifolds. For more details, see Schouten (1954), Bochner & Yano (1952), Nakahara (2003), Nester (2010), Gilkey & Nikcevic (2011), Hehl *et al.* (1981) and Rosen (1982). A linear (affine) connection on a manifold $\mathcal{B}$ is an operation $\nabla : \mathcal{X}(\mathcal{B}) \times \mathcal{X}(\mathcal{B}) \to \mathcal{X}(\mathcal{B})$, where $\mathcal{X}(\mathcal{B})$

is the set of vector fields on $\mathcal{B}$, such that $\forall \, \mathbf{X}, \mathbf{Y}, \mathbf{X}_1, \mathbf{X}_2, \mathbf{Y}_1, \mathbf{Y}_2 \in \mathcal{X}(\mathcal{B}), \forall \, f, f_1, f_2 \in C^\infty(\mathcal{B}), \forall \, a_1, a_2 \in \mathbb{R}$:

$$\text{(i)} \quad \nabla_{f_1 \mathbf{X}_1 + f_2 \mathbf{X}_2} \mathbf{Y} = f_1 \nabla_{\mathbf{X}_1} \mathbf{Y} + f_2 \nabla_{\mathbf{X}_2} \mathbf{Y}, \tag{2.1}$$

$$\text{(ii)} \quad \nabla_{\mathbf{X}}(a_1 \mathbf{Y}_1 + a_2 \mathbf{Y}_2) = a_1 \nabla_{\mathbf{X}}(\mathbf{Y}_1) + a_2 \nabla_{\mathbf{X}}(\mathbf{Y}_2) \tag{2.2}$$

and $\quad$ $$\text{(iii)} \quad \nabla_{\mathbf{X}}(f\mathbf{Y}) = f\nabla_{\mathbf{X}}\mathbf{Y} + (\mathbf{X}f)\mathbf{Y}. \tag{2.3}$$

$\nabla_{\mathbf{X}}\mathbf{Y}$ is called 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 $\Gamma^C{}_{AB}$ are Christoffel symbols of the connection, and $\partial_A = \partial/\partial x^A$ are natural bases for the tangent space corresponding to a coordinate chart $\{x^A\}$. A linear connection is said to be compatible with a metric $\mathbf{G}$ of the manifold if

$$\nabla_{\mathbf{X}}\langle\!\langle \mathbf{Y}, \mathbf{Z} \rangle\!\rangle_{\mathbf{G}} = \langle\!\langle \nabla_{\mathbf{X}}\mathbf{Y}, \mathbf{Z} \rangle\!\rangle_{\mathbf{G}} + \langle\!\langle \mathbf{Y}, \nabla_{\mathbf{X}}\mathbf{Z} \rangle\!\rangle_{\mathbf{G}}, \tag{2.4}$$

where $\langle\!\langle .,. \rangle\!\rangle_{\mathbf{G}}$ is the inner product induced by the metric $\mathbf{G}$. It can be shown that ∇ is compatible with $\mathbf{G}$ if and only if $\nabla\mathbf{G} = \mathbf{0}$, or in components

$$G_{AB|C} = \frac{\partial G_{AB}}{\partial X^C} - \Gamma^S{}_{CA}G_{SB} - \Gamma^S{}_{CB}G_{AS} = 0. \tag{2.5}$$

An n-dimensional manifold $\mathcal{B}$ with a metric $\mathbf{G}$ and a $\mathbf{G}$-compatible connection ∇ is called a Riemann–Cartan manifold (Cartan 1924, 1955, 2001; Gordeeva *et al.* 2010).

The torsion of a connection is defined as

$$\boldsymbol{T}(\mathbf{X}, \mathbf{Y}) = \nabla_{\mathbf{X}}\mathbf{Y} - \nabla_{\mathbf{Y}}\mathbf{X} - [\mathbf{X}, \mathbf{Y}], \tag{2.6}$$

where

$$[\mathbf{X}, \mathbf{Y}](F) = \mathbf{X}(\mathbf{Y}(F)) - \mathbf{Y}(\mathbf{X}(F)) \quad \forall F \in C^\infty(\mathcal{S}) \tag{2.7}$$

is the commutator of $\mathbf{X}$ and $\mathbf{Y}$. In components in a local chart $\{X^A\}$, $T^A{}_{BC} = \Gamma^A{}_{BC} - \Gamma^A{}_{CB}$. ∇ 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 is a map $\boldsymbol{\mathcal{R}} : \mathcal{X}(\mathcal{B}) \times \mathcal{X}(\mathcal{B}) \times \mathcal{X}(\mathcal{B}) \to \mathcal{X}(\mathcal{B})$ defined by

$$\boldsymbol{\mathcal{R}}(\mathbf{X}, \mathbf{Y})\mathbf{Z} = \nabla_{\mathbf{X}}\nabla_{\mathbf{Y}}\mathbf{Z} - \nabla_{\mathbf{Y}}\nabla_{\mathbf{X}}\mathbf{Z} - \nabla_{[\mathbf{X}, \mathbf{Y}]}\mathbf{Z}, \tag{2.8}$$

or in components

$$\mathcal{R}^A{}_{BCD} = \frac{\partial \Gamma^A{}_{CD}}{\partial X^B} - \frac{\partial \Gamma^A{}_{BD}}{\partial X^C} + \Gamma^A{}_{BM}\Gamma^M{}_{CD} - \Gamma^A{}_{CM}\Gamma^M{}_{BD}. \tag{2.9}$$

(b) Cartan's moving frames

Consider a frame field $\{\mathbf{e}_\alpha\}_{\alpha=1}^N$ that at every point of a manifold $\mathcal{B}$ forms a basis for the tangent space. Assume that this frame is orthonormal, i.e. $\langle\!\langle \mathbf{e}_\alpha, \mathbf{e}_\beta \rangle\!\rangle_{\mathbf{G}} = \delta_{\alpha\beta}$. This is, in general, a non-coordinate basis for the tangent space. Given a coordinate basis $\{\partial_A\}$, an arbitrary frame field $\{\mathbf{e}_\alpha\}$ is obtained by a $GL(N, \mathbb{R})$-rotation of $\{\partial_A\}$ as $\mathbf{e}_\alpha = \mathsf{F}_\alpha{}^A\partial_A$ such that orientation is preserved, i.e. $\det \mathsf{F}_\alpha{}^A > 0$.

For the coordinate frame $[\partial_A, \partial_B] = 0$, but for the non-coordinate frame field, we have

$$[\mathbf{e}_\alpha, \mathbf{e}_\alpha] = -c^\gamma_{\alpha\beta}\mathbf{e}_\gamma, \tag{2.10}$$

where $c^\gamma_{\alpha\beta}$ are components of the object of anhonolomy. It can be shown that $c^\gamma_{\alpha\beta} = \mathsf{F}_\alpha^A \mathsf{F}_\beta^B (\partial_A \mathsf{F}^\gamma_B - \partial_B \mathsf{F}^\gamma_A)$, where F^γ_B is the inverse of F_γ^B. The frame field $\{\mathbf{e}_\alpha\}$ defines the co-frame field $\{\vartheta^\alpha\}_{\alpha=1}^N$ such that $\vartheta^\alpha(\mathbf{e}_\beta) = \delta^\alpha_\beta$. The object of anholonomy is defined as $c^\gamma = d\vartheta^\gamma$. Writing this in the coordinate basis, we have

$$c^\gamma = d(\mathsf{F}^\gamma_B dX^B) = \sum_{\alpha<\beta} c^\gamma_{\alpha\beta}\vartheta^\alpha \wedge \vartheta^\beta, \tag{2.11}$$

where $\wedge$ denotes wedge product of differential forms (Abraham *et al.* 1988).

Connection 1-forms are defined as

$$\nabla\mathbf{e}_\alpha = \mathbf{e}_\gamma \otimes \omega^\gamma_\alpha. \tag{2.12}$$

The corresponding connection coefficients are defined as $\nabla_{\mathbf{e}_\beta}\mathbf{e}_\alpha = \langle\omega^\gamma_\alpha, \mathbf{e}_\beta\rangle\mathbf{e}_\gamma = \omega^\gamma_{\beta\alpha}\mathbf{e}_\gamma$. In other words, $\omega^\gamma_\alpha = \omega^\gamma_{\beta\alpha}\vartheta^\beta$. Similarly, $\nabla\vartheta^\alpha = -\omega^\alpha_\gamma\vartheta^\gamma$, and $\nabla_{\mathbf{e}_\beta}\vartheta^\alpha = -\omega^\alpha_{\beta\gamma}\vartheta^\gamma$. In the non-coordinate basis, torsion has the following components:

$$T^\alpha_{\beta\gamma} = \omega^\alpha_{\beta\gamma} - \omega^\alpha_{\gamma\beta} + c^\alpha_{\beta\gamma}. \tag{2.13}$$

Similarly, the curvature tensor has the following components with respect to the frame field

$$\mathcal{R}^\alpha_{\beta\lambda\mu} = \partial_\beta\omega^\alpha_{\lambda\mu} - \partial_\lambda\omega^\alpha_{\beta\mu} + \omega^\alpha_{\beta\xi}\omega^\xi_{\lambda\mu} - \omega^\alpha_{\lambda\xi}\omega^\xi_{\beta\mu} + \omega^\alpha_{\xi\mu}c^\xi_{\beta\lambda}. \tag{2.14}$$

In the orthonormal frame, metric has the simple representation $\mathbf{G} = \delta_{\alpha\beta}\vartheta^\alpha \otimes \vartheta^\beta$.

(c) *Non-metricity and Weyl manifolds*

Given a manifold with a metric and an affine connection $(\mathcal{B}, \nabla, \mathbf{G})$, non-metricity is a map $\mathcal{Q} : \mathcal{X}(\mathcal{B}) \times \mathcal{X}(\mathcal{B}) \times \mathcal{X}(\mathcal{B}) \to \mathbb{R}$ defined as

$$\mathcal{Q}(\mathbf{U}, \mathbf{V}, \mathbf{W}) = \langle\!\langle\nabla_{\mathbf{U}}\mathbf{V}, \mathbf{W}\rangle\!\rangle_{\mathbf{G}} + \langle\!\langle\mathbf{V}, \nabla_{\mathbf{U}}\mathbf{W}\rangle\!\rangle_{\mathbf{G}} - \mathbf{U}[\langle\!\langle\mathbf{V}, \mathbf{W}\rangle\!\rangle_{\mathbf{G}}]. \tag{2.15}$$

In the frame $\{\mathbf{e}_\alpha\}$, $\mathcal{Q}_{\gamma\alpha\beta} = \mathcal{Q}(\mathbf{e}_\gamma, \mathbf{e}_\alpha, \mathbf{e}_\beta).$[2] Non-metricity 1-forms are defined as $\mathcal{Q}_{\alpha\beta} = \mathcal{Q}_{\gamma\alpha\beta}\vartheta^\gamma$. It is straightforward to show that

$$\mathcal{Q}_{\gamma\alpha\beta} = \omega^\xi_{\gamma\alpha}G_{\xi\beta} + \omega^\xi_{\gamma\beta}G_{\xi\alpha} - \langle dG_{\alpha\beta}, \mathbf{e}_\gamma\rangle = \omega_{\beta\gamma\alpha} + \omega_{\alpha\gamma\beta} - \langle dG_{\alpha\beta}, \mathbf{e}_\gamma\rangle, \tag{2.16}$$

where d is the exterior derivative. Thus

$$\mathcal{Q}_{\alpha\beta} = \omega_{\alpha\beta} + \omega_{\beta\alpha} - dG_{\alpha\beta} =: -DG_{\alpha\beta}, \tag{2.17}$$

where D is the covariant exterior derivative. This is called *Cartan's zeroth structural equation*. For an orthonormal frame $G_{\alpha\beta} = \delta_{\alpha\beta}$, and hence

$$\mathcal{Q}_{\alpha\beta} = \omega_{\alpha\beta} + \omega_{\beta\alpha}. \tag{2.18}$$

Weyl 1-form is defined as

$$Q = \frac{1}{n}\mathcal{Q}_{\alpha\beta}G^{\alpha\beta}. \tag{2.19}$$

[2]Here, we mainly follow the notation of Hehl & Obukhov (2003).

Thus

$$\mathcal{Q}_{\alpha\beta} = \tilde{\mathcal{Q}}_{\alpha\beta} + QG_{\alpha\beta}, \tag{2.20}$$

where $\tilde{\mathcal{Q}}$ is the traceless part of non-metricity. If $\tilde{\mathcal{Q}} = \mathbf{0}$, $(\mathcal{B}, \nabla, \mathbf{G})$ is called a Weyl–Cartan manifold. In addition, if ∇ is torsion-free, $(\mathcal{B}, \nabla, \mathbf{G})$ is called a Weyl manifold. It can be shown that

$$\mathcal{R}^{\alpha}{}_{\alpha} = \frac{n}{2}dQ. \tag{2.21}$$

This implies that for a flat Weyl manifold, $dQ = 0$. One can show that (Hehl *et al.* 1995)

$$\omega^{\alpha}{}_{\alpha} = \frac{n}{2}Q + \frac{1}{2}G^{\alpha\beta}dG_{\alpha\beta} = \frac{n}{2}Q + d\ln\sqrt{\det \mathbf{G}}. \tag{2.22}$$

Also

$$D\sqrt{\det \mathbf{G}} = d\sqrt{\det \mathbf{G}} - \omega^{\alpha}{}_{\alpha}\sqrt{\det \mathbf{G}} = -\frac{n}{2}Q\sqrt{\det \mathbf{G}}, \tag{2.23}$$

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

The torsion and curvature 2-forms are defined as

$$\mathcal{T}^{\alpha} = d\vartheta^{\alpha} + \omega^{\alpha}{}_{\beta} \wedge \vartheta^{\beta} \tag{2.24}$$

and

$$\mathcal{R}^{\alpha}{}_{\beta} = d\omega^{\alpha}{}_{\beta} + \omega^{\alpha}{}_{\gamma} \wedge \omega^{\gamma}{}_{\beta}. \tag{2.25}$$

These are called *Cartan's first and second structural equations.* In this framework, Bianchi identities then read:

$$D\mathcal{Q}_{\alpha\beta} := d\mathcal{Q}_{\alpha\beta} - \omega^{\gamma}{}_{\alpha} \wedge \mathcal{Q}_{\gamma\beta} - \omega^{\gamma}{}_{\beta} \wedge \mathcal{Q}_{\alpha\gamma} = \mathcal{R}_{\alpha\beta} + \mathcal{R}_{\beta\alpha}, \tag{2.26}$$

$$D\mathcal{T}^{\alpha} := d\mathcal{T}^{\alpha} + \omega^{\alpha}{}_{\beta} \wedge \mathcal{T}^{\beta} = \mathcal{R}^{\alpha}{}_{\beta} \wedge \vartheta^{\beta} \tag{2.27}$$

and
$$D\mathcal{R}^{\alpha}{}_{\beta} := d\mathcal{R}^{\alpha}{}_{\beta} + \omega^{\alpha}{}_{\gamma} \wedge \mathcal{R}^{\gamma}{}_{\beta} - \omega^{\gamma}{}_{\beta} \wedge \mathcal{R}^{\alpha}{}_{\gamma} = 0. \tag{2.28}$$

Note that for a flat manifold $D\mathcal{T}^{\alpha} = 0$ and $D\mathcal{Q}_{\alpha\beta} = 0$.

(d) The compatible volume element on a Weyl manifold

Given a Weyl manifold, one needs a volume element to be able to calculate volume of an arbitrary subset. Our motivation here is to have a natural way of measuring volumes in the material manifold and hence to be able to calculate the volume density of point defects using the geometry of the Weyl material manifold. Here, by compatible volume element, we mean a volume element that has vanishing covariant derivative. The volume element of the underlying Riemannian manifold is not appropriate; we need a natural volume element in the sense of Saa (1995) (see also Mosna & Saa 2005). A volume element on $\mathcal{B}$ is a non-vanishing n-form (Nakahara 2003). In the orthonormal coframe field $\{\vartheta^{\alpha}\}$,

the volume form can be written as

$$\boldsymbol{\mu} = h\vartheta^1 \wedge \cdots \wedge \vartheta^n, \tag{2.29}$$

for some positive function h to be determined. In a coordinate chart $\{X^A\}$, the volume form is written as

$$\boldsymbol{\mu} = h\sqrt{\det \mathbf{G}}\, dX^1 \wedge \cdots \wedge dX^n. \tag{2.30}$$

Divergence of an arbitrary vector field $\mathbf{W}$ on $\mathcal{B}$ can be defined using the Lie derivative as (Abraham *et al.* 1988)

$$(\mathrm{Div}\mathbf{W})\boldsymbol{\mu} = \mathfrak{L}_{\mathbf{W}}\boldsymbol{\mu}. \tag{2.31}$$

On the other hand, divergence is also defined using the connection as

$$\mathrm{Div}_{\boldsymbol{\nabla}}\mathbf{W} = W^A{}_{|A} = W^A{}_{,A} + \Gamma^A{}_{AB}W^B. \tag{2.32}$$

According to Saa (1995), $\boldsymbol{\mu}$ is compatible with $\boldsymbol{\nabla}$ if

$$\mathfrak{L}_{\mathbf{W}}\boldsymbol{\mu} = (W^A{}_{|A})\boldsymbol{\mu}, \tag{2.33}$$

which is equivalent to

$$D(h\sqrt{\det \mathbf{G}}) = 0. \tag{2.34}$$

Using (2.23), we can write

$$D(h\sqrt{\det \mathbf{G}}) = hD\sqrt{\det \mathbf{G}} + \sqrt{\det \mathbf{G}}\, dh = \left(dh - \frac{n}{2}hQ\right)\sqrt{\det \mathbf{G}} = 0. \tag{2.35}$$

Thus

$$\frac{dh}{h} = d\ln h = \frac{n}{2}Q. \tag{2.36}$$

In coordinate form, this reads

$$\frac{\partial \ln h}{\partial X^A} = \frac{n}{2}Q_A, \tag{2.37}$$

or

$$\frac{\partial h}{\partial X^A} - \frac{n}{2}hQ_A = 0. \tag{2.38}$$

Remark 2.1. Note that a Weylian metric on $\mathcal{B}$ is given by the pair $(\mathbf{G}, Q)$ with the equivalence relation $(\mathbf{G}, Q) \sim (e^A\mathbf{G}, Q - d\Lambda)$ for an arbitrary smooth function Λ on $\mathcal{B}$ (Folland 1970). Now if $Q = d\Omega$ for some smooth function Ω, then by choosing $\Lambda = \Omega$, we have

$$(\mathbf{G}, Q) \sim (e^\Omega\mathbf{G}, 0). \tag{2.39}$$

In other words, when the Weyl 1-form is exact, there exists an equivalent Riemannian manifold $(\mathcal{B}, e^\Omega\mathbf{G})$. In the equivalent Riemannian manifold, the volume form is $e^{n\Omega/2}\boldsymbol{\mu}_{\mathbf{G}}$, where $\boldsymbol{\mu}_{\mathbf{G}}$ is the standard Riemannian volume form of $\mathbf{G}$. The volume form $e^{n\Omega/2}\boldsymbol{\mu}_{\mathbf{G}}$ is identical to Saa's compatible volume element (Saa 1995). In this paper, we call $(\mathcal{B}, e^\Omega\mathbf{G})$ and $(\mathcal{B}, \mathbf{G})$, the equivalent, and the underlying Riemannian manifolds, respectively.
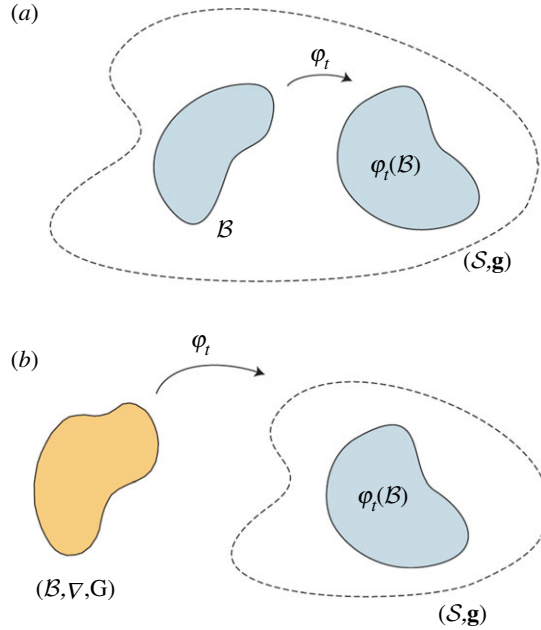
Figure 1. (*a*) Kinematics of nonlinear elasticity. Reference configuration is a submanifold of the ambient space manifold. The material metric is the induced submanifold metric. (*b*) Kinematics of nonlinear anelasticity. Material manifold is a metric-affine manifold $(\mathcal{B}, \nabla, \mathbf{G})$. Motion is a time-dependent mapping from the underlying Riemannian material manifold $(\mathcal{B}, \mathbf{G})$ into the Riemannian ambient space manifold $(\mathcal{S}, \mathbf{g})$. (Online version in colour.)

3. Geometric nonlinear elasticity and anelasticity

(*a*) *Kinematics of nonlinear elasticity*

Let us first review a few of the basic notions of geometric nonlinear elasticity. A body $\mathcal{B}$ is identified with a Riemannian manifold $\mathcal{B}^3$ and a configuration of $\mathcal{B}$ is a mapping $\varphi : \mathcal{B} \to \mathcal{S}$, where $\mathcal{S}$ is another Riemannian manifold (Marsden & Hughes 1983; Yavari *et al.* 2006), where the elastic body lives (figure 1*a*). The set of all configurations of $\mathcal{B}$ is denoted by $\mathcal{C}$. A motion is a curve $c : \mathbb{R} \to \mathcal{C}; t \mapsto \varphi_t$ in $\mathcal{C}$. A fundamental assumption is that the body is stress-free in the material manifold. It is the geometry of these two manifolds that describes any possible residual stresses.

For a fixed t, $\varphi_t(\mathbf{X}) = \varphi(\mathbf{X}, t)$ and for a fixed $\mathbf{X}$, $\varphi_\mathbf{X}(t) = \varphi(\mathbf{X}, t)$, where $\mathbf{X}$ is the position of material points in the reference configuration $\mathcal{B}$. The material velocity is given by

$$\mathbf{V}_t(\mathbf{X}) = \mathbf{V}(\mathbf{X}, t) = \frac{\partial \varphi(\mathbf{X}, t)}{\partial t} = \frac{\mathrm{d}}{\mathrm{d}t} \varphi_\mathbf{X}(t). \tag{3.1}$$

Similarly, the material acceleration is defined by

$$\mathbf{A}_t(\mathbf{X}) = \mathbf{A}(\mathbf{X}, t) = \frac{\partial \mathbf{V}(\mathbf{X}, t)}{\partial t} = \frac{\mathrm{d}}{\mathrm{d}t} \mathbf{V}_\mathbf{X}(t). \tag{3.2}$$

[3]This is, in general, the underlying Riemannian manifold of the material manifold.

In components, $A^a = \partial V^a/\partial t + \gamma^a{}_{bc} V^b V^c$, where $\gamma^a{}_{bc}$ is the Christoffel symbol of the local coordinate chart $\{x^a\}$. Note that $\mathbf{A}$ does not depend on the connection coefficients of the material manifold. Here, it is assumed that φ_t is invertible and regular. The spatial velocity of a regular motion φ_t is defined as $\mathbf{v}_t = \mathbf{V}_t \circ \varphi_t^{-1}$, and the spatial acceleration $\mathbf{a}_t$ is defined as $\mathbf{a} = \dot{\mathbf{v}} = \partial \mathbf{v}/\partial t + \nabla_{\mathbf{v}}\mathbf{v}$. In components, $a^a = \partial v^a/\partial t + (\partial v^a/\partial x^b)v^b + \gamma^a{}_{bc}v^b v^c$.

Geometrically, deformation gradient—a central object describing deformation—is the tangent map of φ and is denoted by $\mathbf{F} = T\varphi$. Thus, at each point $\mathbf{X} \in \mathcal{B}$, it is a linear map

$$\mathbf{F}(\mathbf{X}): T_{\mathbf{X}}\mathcal{B} \to T_{\varphi(\mathbf{X})}\mathcal{S}. \tag{3.3}$$

If $\{x^a\}$ and $\{X^A\}$ are local coordinate charts on $\mathcal{S}$ and $\mathcal{B}$, respectively, the components of $\mathbf{F}$ are

$$F^a{}_A(\mathbf{X}) = \frac{\partial \varphi^a}{\partial X^A}(\mathbf{X}). \tag{3.4}$$

$\mathbf{F}$ has the following local representation:

$$\mathbf{F} = F^a{}_A\, \partial_a \otimes \mathrm{d}X^A. \tag{3.5}$$

Transpose of $\mathbf{F}$ is defined by

$$\mathbf{F}^\mathsf{T}: T_{\mathbf{x}}\mathcal{S} \to T_{\mathbf{X}}\mathcal{B} \quad \text{and} \quad \langle\!\langle \mathbf{F}\mathbf{V}, \mathbf{v}\rangle\!\rangle_{\mathbf{g}} = \langle\!\langle \mathbf{V}, \mathbf{F}^\mathsf{T}\mathbf{v}\rangle\!\rangle_{\mathbf{G}}, \tag{3.6}$$

for all $\mathbf{V} \in T_{\mathbf{X}}\mathcal{B}$, $\mathbf{v} \in T_{\mathbf{x}}\mathcal{S}$. In components, $(F^\mathsf{T}(\mathbf{X}))^A{}_a = g_{ab}(\mathbf{x})F^b{}_B(\mathbf{X})G^{AB}(\mathbf{X})$, where $\mathbf{g}$ and $\mathbf{G}$ are metric tensors on $\mathcal{S}$ and $\mathcal{B}$, respectively. The right Cauchy–Green deformation tensor is defined by

$$\mathbf{C}(X): T_{\mathbf{X}}\mathcal{B} \to T_{\mathbf{X}}\mathcal{B} \quad \text{and} \quad \mathbf{C}(\mathbf{X}) = \mathbf{F}^\mathsf{T}(\mathbf{X})\mathbf{F}(\mathbf{X}). \tag{3.7}$$

In components, $C^A_B = (F^\mathsf{T})^A{}_a F^a{}_B$. It is straightforward to show that $\mathbf{C}^\flat$ is the pull-back of the spatial metric, i.e.

$$\mathbf{C}^\flat = \varphi^*\mathbf{g} = \mathbf{F}^*\mathbf{g}\mathbf{F}, \quad \text{i.e.} \quad C_{AB} = (g_{ab} \circ \varphi)F^a{}_A F^b{}_B. \tag{3.8}$$

(b) Material manifold and anelasticity

In classical elasticity, one starts with a stress-free configuration embedded in the ambient space and then makes this embedding time-dependent (a motion; figure 1a). In anelastic problems (anelastic in the sense of Eckart (1948)), the stress-free configuration is another manifold with a geometry explicitly depending on the anelasticity source(s) (figure 1b). In other words, in our geometric approach, one by-passes the notion of local intermediate configuration by using an appropriate geometry in the material manifold that automatically makes the body with distributed defects stress-free. The ambient space being a Riemannian manifold $(\mathcal{S}, \mathbf{g})$, the computation of stresses requires a Riemannian material manifold $(\mathcal{B}, \mathbf{G})$ (the underlying Riemannian material manifold) and a map $\varphi: \mathcal{B} \to \mathcal{S}$. For example, in the case of non-uniform temperature changes and bulk growth (Ozakin & Yavari 2010; Yavari 2010), one starts with a material metric $\mathbf{G}$ that specifies the relaxed distances of the material points. However, the material metric cannot always be obtained directly.
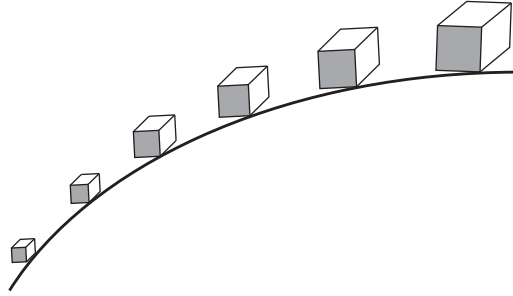
Figure 2. In a Weyl manifold, the Riemannian volume element varies from point to point.

It turns out that for defects in solids, a metric-affine manifold can describe the stress-free configuration of the body. In the case of dislocations, the material connection is flat, metric-compatible and has a non-vanishing torsion, which is identified with the dislocation density tensor—i.e. the material manifold is a Weitzenböck manifold (Weitzenböck 1923; Yavari & Goriely 2012). Given a dislocation density tensor, one can obtain the torsion of the affine connection. Then, using Cartan's moving frames and structural equations, one can find an orthonormal frame compatible with the torsion tensor. This, in turn, provides the material metric. Then, the computation of stress amounts to finding a mapping from the underlying Riemannian material manifold to the ambient space manifold. In the case of disclinations, the physically relevant object is the curvature of a torsion-free and metric-compatible connection, and one can again find the metric using Cartan's structural equations (Yavari & Goriely in press).

For a solid with distributed point defects, the material manifold is a Weyl manifold. Point defects affect the volume of the stress-free configuration and this can be described using non-metricity with a vanishing traceless part, as will be shown shortly. The metric is obtained using Cartan's structural equations and the compatible volume element of the Weyl material manifold. We conclude that all the anelastic effects can be embedded in the appropriate geometric characterization of the material manifold on which the computation of stresses reduces to a classical elasticity problem. This means that, in particular, the deformation gradient by construction is purely elastic.

Remark 3.1. In a body with distributed point defects, we expect the natural volume element to change from point to point (figure 2), and this change of volume element is, in general, anisotropic. Weyl 1-form can model such an anisotropic change in the volume element. This is why the traceless part of non-metricity is not needed in modelling distributed point defects. See Lazar & Maugin (2007) for a similar discussion.

(c) Equations of motion

The internal energy density E (or free energy density Ψ) of a solid depends on the deformation gradient **F**. Because a scalar function of a two-point tensor must

explicitly depend on both $\mathbf{G}$ and $\mathbf{g}$, we have

$$E = E(\mathbf{X}, \mathsf{N}, \mathbf{F}, \mathbf{G}, \mathbf{g}) \quad \text{and} \quad \Psi = \Psi(\mathbf{X}, \Theta, \mathbf{F}, \mathbf{G}, \mathbf{g}), \tag{3.9}$$

where N and Θ are the specific entropy and absolute temperature, respectively.

One can derive the equations of motion by either using an action principle or using covariance of energy balance (Marsden & Hughes 1983; Yavari & Marsden in press). For a motion $\varphi : \mathcal{B} \to \mathcal{S}$, where $(\mathcal{B}, \mathbf{G})$ and $(\mathcal{S}, \mathbf{g})$ are, respectively, the (underlying) Riemannian material and ambient space manifolds, the governing equations obtained as a consequence of the conservation of mass and balance of linear and angular momenta, in material form read

$$\frac{\partial \rho_0}{\partial t} = 0, \quad \text{Div}\mathbf{P} + \rho_0 \mathbf{B} = \rho_0 \mathbf{A}, \quad \mathbf{P}\mathbf{F}^\mathsf{T} = \mathbf{F}\mathbf{P}^\mathsf{T}, \tag{3.10}$$

where ρ_0, $\mathbf{P}, \mathbf{B}$ and $\mathbf{A}$ are the material mass density, the first Piola–Kirchhoff stress, the body force per unit undeformed volume (calculated using the Riemannian volume form) and the material acceleration, respectively. In components, the Cauchy equation $(3.10)_2$ reads

$$\frac{\partial P^{aA}}{\partial X^A} + \Gamma^A{}_{AB} P^{aB} + \gamma^a{}_{bc} F^b{}_A P^{cA} + \rho_0 B^a = \rho_0 A^a, \tag{3.11}$$

where $\Gamma^A{}_{BC}$ are the Christoffel symbols of the material metric. Equivalently, in spatial coordinates

$$\mathbf{L_v}\rho = 0, \quad \text{div}\boldsymbol{\sigma} + \rho \mathbf{b} = \rho \mathbf{a}, \quad \boldsymbol{\sigma}^\mathsf{T} = \boldsymbol{\sigma}, \tag{3.12}$$

where ρ, $\boldsymbol{\sigma}, \mathbf{b}$ and $\mathbf{a}$ are the spatial mass density, Cauchy stress, body force per unit deformed volume and spatial acceleration, respectively. $\mathbf{L_v}\rho$ is the Lie derivative of the mass density with respect to the (time-dependent) spatial velocity. Note that $\sigma^{ab} = (1/J) P^{aA} F^b{}_A$, where $J = \sqrt{\det \mathbf{g}/\det \mathbf{G}} \det \mathbf{F}$ is the Jacobian.

4. Residual stress field of a spherically symmetric distribution of point defects

As an application of the geometric theory, we revisit a classical problem of linear elasticity in the general framework of exact nonlinear elasticity. Namely, we construct the material manifold of a spherically symmetric distribution of point defects in a ball of radius R_o, which is traction-free (or is under uniform pressure) on its boundary sphere. The Weyl material manifold is then used to calculate the residual stress field.

(a) The Weyl material manifold

In order to find a solution, we follow the procedure in (Adak & Sert 2005; Yavari & Goriely 2012) and start by an ansatz for the material coframe field. We then find a flat connection, which is torsion-free but has a non-vanishing non-metricity compatible with the given point defect distribution. We do this using Cartan's structural equations and the compatible volume form of the Weyl

material manifold. In the spherical coordinates (R, Θ, Φ), $R \geq 0$, $0 \leq \Theta \leq \pi$, $0 \leq \Phi < 2\pi$, let us look for a coframe field of the following form:[4]

$$\vartheta^1 = f(R)\, \mathrm{d}R, \quad \vartheta^2 = R\, \mathrm{d}\Theta \quad \text{and} \quad \vartheta^3 = R\sin\Theta\, \mathrm{d}\Phi, \tag{4.1}$$

for some unknown function f to be determined. We choose the following connection 1-forms:

$$\boldsymbol{\omega} = [\omega^\alpha{}_\beta] = \begin{pmatrix} \omega^1{}_1 & \omega^1{}_2 & -\omega^3{}_1 \\ -\omega^1{}_2 & \omega^2{}_2 & \omega^2{}_3 \\ \omega^3{}_1 & -\omega^2{}_3 & \omega^3{}_3 \end{pmatrix}, \tag{4.2}$$

where

$$\omega^1{}_2 = -\frac{1}{R}\vartheta^2, \quad \omega^2{}_3 = -\frac{\cot\Theta}{R}\vartheta^3, \quad \omega^3{}_1 = \frac{1}{R}\vartheta^3, \quad \omega^1{}_1 = \omega^2{}_2 = \omega^3{}_3 = q(R)\vartheta^1, \tag{4.3}$$

for a function q to be determined. This means that

$$\mathcal{Q}_{\alpha\beta} = 2\delta_{\alpha\beta} q(R)\vartheta^1. \tag{4.4}$$

We now need to enforce $\mathcal{T}^\alpha = 0$. Note that

$$\mathrm{d}\vartheta^1 = 0, \quad \mathrm{d}\vartheta^2 = \frac{1}{Rf(R)}\vartheta^1 \wedge \vartheta^2, \quad \mathrm{d}\vartheta^3 = -\frac{1}{Rf(R)}\vartheta^3 \wedge \vartheta^1 + \frac{\cot\Theta}{R}\vartheta^2 \wedge \vartheta^3. \tag{4.5}$$

From Cartan's first structural equations, we obtain

$$\left. \begin{aligned} \mathcal{T}^1 &= 0, \quad \mathcal{T}^2 = \left[\frac{1}{Rf(R)} - \frac{1}{R} + q(R)\right]\vartheta^1 \wedge \vartheta^2 \\ \mathcal{T}^3 &= \left[\frac{1}{Rf(R)} - \frac{1}{R} + q(R)\right]\vartheta^3 \wedge \vartheta^1. \end{aligned} \right\} \tag{4.6}$$

and

Therefore,

$$q(R) = \frac{1}{R}\left[1 - \frac{1}{f(R)}\right]. \tag{4.7}$$

It can be checked that for these connection 1-forms $\mathcal{R}^\alpha{}_\beta = 0$ are trivially satisfied. In this example, the Weyl 1-form is written as

$$Q = 2q(R)\vartheta^1 = \frac{2}{R}\left[1 - \frac{1}{f(R)}\right]\vartheta^1 = \frac{2(f(R) - 1)}{R}\mathrm{d}R. \tag{4.8}$$

It is seen that $\mathrm{d}Q = 0$, as is expected for a flat Weyl manifold.

---

[4]This construction is similar to that of Adak & Sert (2005). Note that the Riemannian volume element is $\boldsymbol{\mu_G} = \vartheta^1 \wedge \vartheta^2 \wedge \vartheta^3 = R^2 f(R)\sin\Theta\, \mathrm{d}R \wedge \mathrm{d}\Theta \wedge \mathrm{d}\Phi$, and hence $f(R) > 0$.

(b) Volume density of point defects

Consider a spherical shell of radius R and thickness ΔR. In the absence of point defects (Euclidean material manifold), the volume of this shell is

$$\Delta V_0 = 2\pi \int_0^\pi \sin\Theta\, d\Theta \int_R^{R+\Delta R} \xi^2\, d\xi = 4\pi \int_R^{R+\Delta R} \xi^2\, d\xi. \qquad (4.9)$$

Now in the underlying Riemannian material manifold, the volume of the same spherical shell with point defects is

$$\Delta V_{\text{Riemannian}} = 2\pi \int_0^\pi \sin\Theta\, d\Theta \int_R^{R+\Delta R} \xi^2 f(\xi)\, d\xi = 4\pi \int_R^{R+\Delta R} \xi^2 f(\xi)\, d\xi. \qquad (4.10)$$

If there are only vacancies in this spherical shell (and no interstitials), we expect the volume of the Riemannian material manifold to be smaller than ΔV_0. In other words, for a distribution of vacancies, we expect $0 < f(R) < 1$.

In the presence of point defects, the compatible volume element in the Weyl material manifold is written as

$$\boldsymbol{\mu} = h(R)\vartheta^1 \wedge \vartheta^2 \wedge \vartheta^3 = R^2 f(R) h(R) \sin\Phi\, dR \wedge d\Theta \wedge d\Phi, \qquad (4.11)$$

for some positive function h satisfying (2.37). In the Weyl material manifold, the volume of the spherical shell of radius R and thickness ΔR is[5]

$$\Delta V = 2\pi \int_0^\pi \sin\Theta\, d\Theta \int_R^{R+\Delta R} \xi^2 f(\xi) h(\xi)\, d\xi = 4\pi \int_R^{R+\Delta R} \xi^2 f(\xi) h(\xi)\, d\xi. \qquad (4.12)$$

Total volume of defects in the spherical shell is $\Delta V_d = \Delta V_0 - \Delta V$. Thus

$$\Delta V_d = 4\pi \int_R^{R+\Delta R} \xi^2 [1 - f(\xi) h(\xi)]\, d\xi. \qquad (4.13)$$

The volume density of point defects is defined as[6]

$$\mathsf{n}(R) = \lim_{\Delta R \to 0} \frac{\Delta V_d}{\Delta V_0} = \lim_{\Delta R \to 0} \frac{4\pi \int_R^{R+\Delta R} \xi^2 [1 - f(\xi) h(\xi)]\, d\xi}{4\pi R^2 \Delta R} = 1 - f(R) h(R). \qquad (4.14)$$

Therefore,

$$f(R) = \frac{1 - \mathsf{n}(R)}{h(R)}. \qquad (4.15)$$

Note that $f(R) > 0$ and $h(R) > 0$ imply that

$$\mathsf{n}(R) < 1. \qquad (4.16)$$

For our spherically symmetric point defect distribution, the relationship (2.37) is simplified to read

$$\frac{d}{dR} \ln h(R) = \frac{h'(R)}{h(R)} = \frac{3(f(R) - 1)}{R}. \qquad (4.17)$$

---

[5]Note that for the case of a spherically symmetric point defect distribution as a consequence of the Poincaré Lemma, $Q = d\Omega$ (remark 2.1). In other words, we are calculating the volume of the equivalent Riemannian manifold of the Weyl material manifold.
[6]For a distribution of vacancies, $\mathsf{n}(R) < 0$, and for a distribution of interstitials, $\mathsf{n}(R) > 0$.

From (4.15) and (4.17), we obtain

$$Rh'(R) + 3h(R) = 3(1 - \mathsf{n}(R)). \tag{4.18}$$

Hence

$$h(R) = 1 - \frac{1}{R^3} \int_0^R 3y^2 \mathsf{n}(y) \, \mathrm{d}y. \tag{4.19}$$

Therefore,

$$f(R) = \frac{1 - \mathsf{n}(R)}{1 - (1/R^3) \int_0^R 3y^2 \mathsf{n}(y) \, \mathrm{d}y}. \tag{4.20}$$

To check for consistency, let us consider a spherically symmetric distribution of vacancies in a ball of radius R_o such that $\mathsf{n}(R) < 0$ ($h(R) > 1$) and $\mathsf{n}'(R) > 0$. For a distributed vacancy, we expect a smaller relaxed volume, i.e. $\boldsymbol{\mu}_0 > \boldsymbol{\mu_G}$ and hence $f(R) < 1$, where $\boldsymbol{\mu}_0$ and $\boldsymbol{\mu_G}$ are the volume forms of the flat Euclidean manifold and the underlying Riemannian manifold, respectively. This can easily be verified using (4.20).

Example 4.1. If $\mathsf{n}(R) = \mathsf{n}_0$, then $f(R) = 1$.

Remark 4.2. For an arbitrary distribution of point defects, the defective solid is stress-free in a Weyl manifold $(\mathcal{B}, \mathbf{G}, Q)$. Let us denote the volume form of the Weyl manifold by $\boldsymbol{\mu}$. For a subbody $\mathcal{U} \subset \mathcal{B}$, the volume of the virgin (defect-free) and the defective subbody are

$$V_0(\mathcal{U}) = \int_{\mathcal{U}} \boldsymbol{\mu}_0 \quad \text{and} \quad V(\mathcal{U}) = \int_{\mathcal{U}} \boldsymbol{\mu}. \tag{4.21}$$

The volume of the point defects in $\mathcal{U}$ is calculated as

$$V_d(\mathcal{U}) = \int_{\mathcal{U}} \boldsymbol{\mu}_0 - \int_{\mathcal{U}} \boldsymbol{\mu} = \int_{\mathcal{U}} (\boldsymbol{\mu}_0 - \boldsymbol{\mu}) = \int_{\mathcal{U}} \mathsf{n} \boldsymbol{\mu}_0. \tag{4.22}$$

This implies that n is the volume density of the point defects. Note that for vacancies $V_d < 0$.

(c) Residual stress calculation

The material metric in spherical coordinates (R, Θ, Φ) has the following form:

$$\mathbf{G} = \begin{pmatrix} f^2(R) & 0 & 0 \\ 0 & R^2 & 0 \\ 0 & 0 & R^2 \sin^2 \Theta \end{pmatrix}. \tag{4.23}$$

We use the spherical coordinates (r, θ, ϕ) for the Euclidean ambient space with the following metric:

$$\mathbf{g} = \begin{pmatrix} 1 & 0 & 0 \\ 0 & r^2 & 0 \\ 0 & 0 & r^2 \sin^2 \theta \end{pmatrix}. \tag{4.24}$$

In order to obtain the residual stress field, we embed the material manifold into the ambient space. We look for solutions of the form $(r, \theta, \phi) = (r(R), \Theta, \Phi)$, and

hence $\det \mathbf{F} = r'(R)$. Assuming an incompressible solid, we have

$$J = \sqrt{\frac{\det \mathbf{g}}{\det \mathbf{G}}} \det \mathbf{F} = \frac{r^2(R)}{R^2 f(R)} r'(R) = 1. \tag{4.25}$$

Assuming that $r(0) = 0$, this gives us

$$r(R) = \left(\int_0^R 3\xi^2 f(\xi) \, d\xi \right)^{1/3}. \tag{4.26}$$

For a neo-Hookean material, we have $P^{aA} = \mu F^a{}_B G^{AB} - p(F^{-1})_b{}^A g^{ab}$, where $p = p(R)$ is the pressure field. Thus

$$\mathbf{P} = \begin{pmatrix} \dfrac{\mu R^2}{f(R) r^2(R)} - \dfrac{p(R) r^2(R)}{f(R) R^2} & 0 & 0 \\[2ex] 0 & \dfrac{\mu}{R^2} - \dfrac{p(R)}{r^2(R)} & 0 \\[2ex] 0 & 0 & \dfrac{\mu}{R^2 \sin^2 \Theta} - \dfrac{p(R)}{r(R)^2 \sin^2 \Theta} \end{pmatrix}. \tag{4.27}$$

Hence

$$\boldsymbol{\sigma} = \begin{pmatrix} \dfrac{\mu R^4}{r^4(R)} - p(R) & 0 & 0 \\[2ex] 0 & \dfrac{\mu}{R^2} - \dfrac{p(R)}{r^2(R)} & 0 \\[2ex] 0 & 0 & \dfrac{1}{\sin^2 \Theta} \left[\dfrac{\mu}{R^2} - \dfrac{p(R)}{r^2(R)} \right] \end{pmatrix}. \tag{4.28}$$

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

$$\sigma^{rr}{}_{,r} + \frac{2}{r} \sigma^{rr} - r\sigma^{\theta\theta} - r \sin^2 \theta \, \sigma^{\phi\phi} = 0. \tag{4.29}$$

Or

$$\frac{r^2}{R^2 f} \sigma^{rr}{}_{,R} + \frac{2}{r} \sigma^{rr} - 2r\sigma^{\theta\theta} = 0. \tag{4.30}$$

This then gives us

$$p'(R) = -\frac{2\mu}{r(R)} \left[f(R) \left(\frac{R}{r(R)} \right)^6 - 2 \left(\frac{R}{r(R)} \right)^3 + f(R) \right]. \tag{4.31}$$

Let us assume that the defective body is a ball of radius R_o. Assuming that the boundary of the ball is traction-free ($\sigma^{rr}(R_o) = 0$), we obtain

$$p(R_o) = \mu \frac{R_o^4}{r^4(R_o)}. \tag{4.32}$$

Therefore, the pressure at all points inside the ball is

$$p(R) = \mu \frac{R_o^4}{r^4(R_o)} + 2\mu \int_R^{R_o} \left[f(\xi) \frac{\xi^6}{r^7(\xi)} - 2\frac{\xi^3}{r^4(\xi)} + \frac{f(\xi)}{r(\xi)} \right] d\xi, \tag{4.33}$$

and the radial stress is

$$\sigma^{rr}(R) = -2\mu \int_R^{R_o} \left[f(\xi) \frac{\xi^6}{r^7(\xi)} - 2\frac{\xi^3}{r^4(\xi)} + \frac{f(\xi)}{r(\xi)} \right] d\xi + \mu \left[\frac{R^4}{r^4(R)} - \frac{R_o^4}{r^4(R_o)} \right]. \tag{4.34}$$

For a given point defect distribution $n(R)$, $f(R)$ is obtained using (4.20). Pressure and stress are then calculated by substituting $f(R)$ into (4.33) and (4.34), respectively.

Remark 4.3. When $n(R) = n_0$, we saw that $f(R) = 1$. This then implies that $r(R) = R$ and $p(R) = \mu$, i.e. this point defect distribution is stress-free. Eshelby (1954) showed this in the linearized setting. We will show in §4d that this is the only zero-stress spherically symmetric point defect distribution.

Remark 4.4. We can calculate the stress field for the case when on the boundary of the body tractions are non-zero. Assuming that $P^{rR}(R_o) = -p_\infty$, we have

$$\sigma^{rr}(R) = -2\mu \int_R^{R_o} \left[f(\xi) \frac{\xi^6}{r^7(\xi)} - 2\frac{\xi^3}{r^4(\xi)} + \frac{f(\xi)}{r(\xi)} \right] d\xi$$

$$+ \mu \left[\frac{R^4}{r^4(R)} - \frac{R_o^4}{r^4(R_o)} \right] - p_\infty \frac{f(R_o) R_o^2}{r^2(R_o)}. \tag{4.35}$$

Example 4.5. Let us consider the following point defect distribution:[7]

$$n(R) = \begin{cases} n_0 & 0 \le R \le R_i, \\ 0 & R > R_i, \end{cases} \tag{4.36}$$

where $R_i < R_o$. Thus

$$0 \le R \le R_i : \ f(R) = 1 \tag{4.37}$$

and

$$R > R_i : \ f(R) = \frac{1}{1 - n_0(R_i/R)^3}. \tag{4.38}$$

Also

$$0 \le R \le R_i : \ r(R) = R \tag{4.39}$$

and

$$R > R_i : \ r(R) = \left[R^3 + n_0 R_i^3 \ln \left(\frac{(R/R_i)^3 - n_0}{1 - n_0} \right) \right]^{1/3}. \tag{4.40}$$

Note that for $0 \le R \le R_i$:

$$p(R) = \mu \frac{R_o^4}{r^4(R_o)} + 2\mu \int_{R_i}^{R_o} \left[f(\xi) \frac{\xi^6}{r^7(\xi)} - 2\frac{\xi^3}{r^4(\xi)} + \frac{f(\xi)}{r(\xi)} \right] d\xi = p_i, \tag{4.41}$$

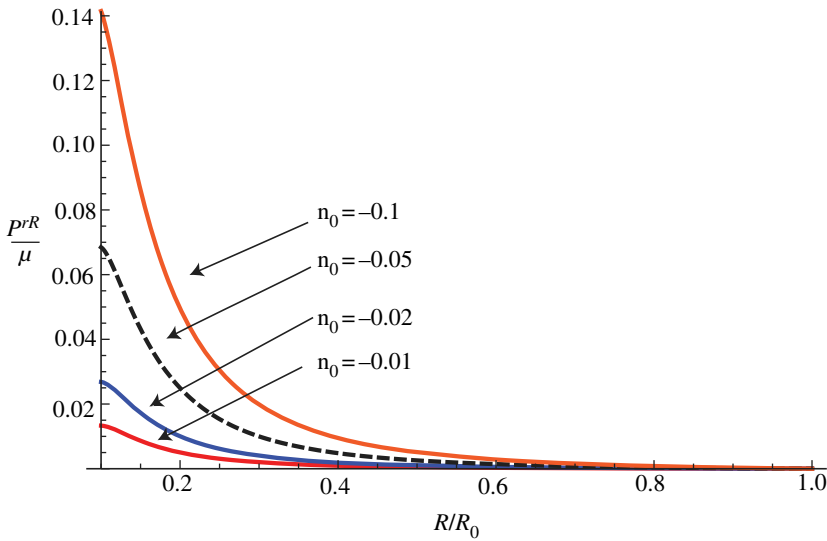[7]Note that the total volume of point defects is $((4\pi/3)R_i^3)n_0$.

Figure 3. P^{rR} distributions for $R_i = R_o/10$ and different values of n_0. (Online version in colour.)

i.e. pressure is uniform and consequently, $\sigma^{rr} = \mu - p_i$ is uniform. Figure 3 shows the distribution of P^{rR} in the interval $[R_i, R_o]$ for different vacancy distributions and when $R_o = 10R_i$.

Remark 4.6. The other two stress components are also equal to $\mu - p_i$ in the ball $R \leq R_i$. To see this, note that in curvilinear coordinates, the components of a tensor may not have the same physical dimensions. The following relation holds between the Cauchy stress components (unbarred) and its physical components (barred) (Truesdell 1953):

$$\bar{\sigma}^{ab} = \sigma^{ab}\sqrt{g_{aa}g_{bb}} \quad \text{no summation on } a \text{ or } b. \tag{4.42}$$

The spatial metric in spherical coordinates has the form $\text{diag}(1, r^2, r^2 \sin^2 \theta)$, and this means that the non-zero Cauchy stress components are

$$\bar{\sigma}^{rr} = \sigma^{rr} = \mu \frac{R^4}{r^4(R)} - p(R), \quad \bar{\sigma}^{\theta\theta} = r^2 \sigma^{\theta\theta} = \mu \frac{r^2(R)}{R^2} - p(R) \Bigg\}$$

$$\text{and} \quad \bar{\sigma}^{\phi\phi} = r^2 \sin^2 \theta \sigma^{\phi\phi} = \mu \frac{r^2(R)}{R^2} - p(R). \tag{4.43}$$

It follows that inside the sphere of radius R_i both $\bar{\sigma}^{\theta\theta}$ and $\bar{\sigma}^{\phi\phi}$ are equal to $\mu - p_i$. Thinking of the ball $R \leq R_i$ as an inclusion, this is a nonlinear analogue of Eshelby's celebrated inclusion problem (Eshelby 1957). This result also holds for an arbitrary nonlinear isotropic incompressible solid as shown next.

Now let us assume that the body is isotropic and incompressible (not necessarily neo-Hookean). The second Piola–Kirchhoff stress tensor has the following representation (Marsden & Hughes 1983):

$$S_{AB} = \alpha_0 G_{AB} + \alpha_1 C_{AB} + \alpha_2 C_A{}^D C_{DB}, \tag{4.44}$$

where α_0, α_1 and α_2 are functions of position and invariants of $\mathbf{C}$. For $R \le R_i$, $C_{AB} = \delta_{AB}$ and hence $S_{AB} = \alpha \delta_{AB}$, where $\alpha = \alpha_0 + \alpha_1 + \alpha_2$ is a constant for a homogeneous solid. This means that similar to the neo-Hookean solid, $P^{aA} = (\alpha - p(R))\delta^{aA}$. Equilibrium equations dictate $p(R) = \alpha$, and hence we have proved the following proposition.

Proposition 4.7. *For a homogeneous spherical ball of radius R_o made of an isotropic and incompressible solid, traction-free on its boundary sphere, and with the following point defect distribution:*

$$\mathsf{n}(R) = \begin{cases} \mathsf{n}_0 & 0 \le R \le R_i, \\ 0 & R_i < R \le R_o, \end{cases} \tag{4.45}$$

in the ball $R \le R_i$, the stress is uniform and hydrostatic.

Remark 4.8. This proposition still holds when $P^{rR}(R_o) = -p_\infty$. In this case, the uniform value of the hydrostatic pressure inside the sphere of radius R_i is

$$p_i = 2\mu \int_{R_i}^{R_o} \left[f(\xi) \frac{\xi^6}{r^7(\xi)} - 2\frac{\xi^3}{r^4(\xi)} + \frac{f(\xi)}{r(\xi)} \right] \mathrm{d}\xi + \mu \frac{R_o^4}{r^4(R_o)} - p_\infty. \tag{4.46}$$

(d) Zero-stress spherically symmetric point defect distributions

Next, we identify all those spherically symmetric point defect distributions that are zero-stress. This is equivalent to the underlying Riemannian material manifold being flat (in the case of simply connected material manifolds). Given the coframe field (4.1) using Cartan's first structural equations, its Levi–Civita connections are obtained as

$$\bar{\omega}^1{}_2 = -\frac{1}{Rf(R)}\vartheta^2, \quad \bar{\omega}^2{}_3 = -\frac{\cot \Theta}{R}\vartheta^3 \quad \text{and} \quad \bar{\omega}^3{}_1 = \frac{1}{Rf(R)}\vartheta^3. \tag{4.47}$$

Using Cartan's second structural equations, we obtain the following Levi–Civita curvature 2-forms:

$$\left. \begin{aligned} \bar{\mathcal{R}}^1{}_2 &= \frac{f'(R)}{Rf^3(R)}\vartheta^1 \wedge \vartheta^2, \quad \bar{\mathcal{R}}^2{}_3 = -\frac{1}{R^2}\left(1 - \frac{1}{f^2(R)}\right)\vartheta^2 \wedge \vartheta^3 \\ \text{and} \qquad \bar{\mathcal{R}}^3{}_1 &= \frac{f'(R)}{Rf^3(R)}\vartheta^3 \wedge \vartheta^1. \end{aligned} \right\} \tag{4.48}$$

The Riemannian material manifold is flat if and only if $f'(R) = 0$ and $f^2(R) = 1$. This means that $f(R) = 1$ is the only possibility. From (4.20), we see that the zero-stress point defect distributions must satisfy the following integral equation:

$$R^3\mathsf{n}(R) = \int_0^R 3y^2\mathsf{n}(y)\,\mathrm{d}y \quad \forall \ R \ge 0. \tag{4.49}$$

Taking derivatives of both sides, we obtain $\mathsf{n}'(R) = 0$ or $\mathsf{n}(R) = \mathsf{n}_0$.

(e) Comparison with the classical linear solution

Here, we compare our nonlinear solution with the classical linearized elasticity solution. For a sphere of radius R_o made of an incompressible linear elastic solid
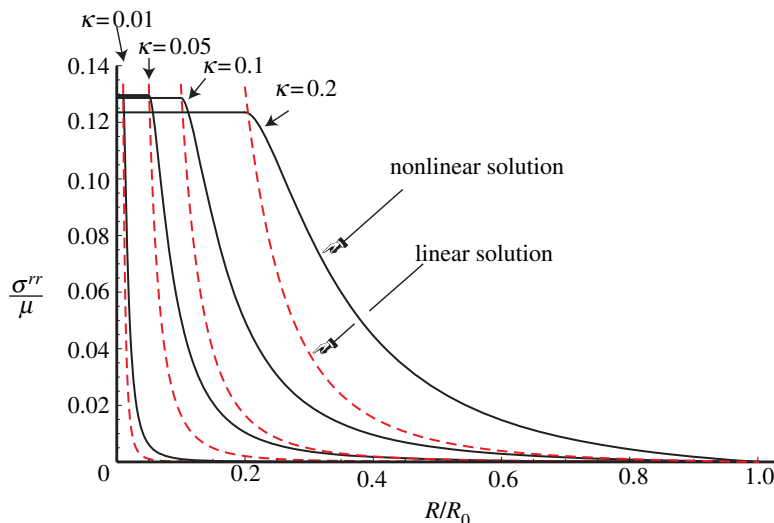
Figure 4. Comparison of the linear (dashed) and nonlinear (solid) solutions for the radial stress distribution for $\mathsf{n}_0 = -0.1$ and different values of $\kappa = R_i/R_o$. (Online version in colour.)

with a single point defect at the origin, recall that (Teodosiu 1982)

$$\sigma^{rr} = -\frac{4\mu\,C}{R^3}\left(1 - \frac{R^3}{R_o^3}\right) \quad \text{and} \quad \sigma^{\theta\theta} = \sigma^{\phi\phi} = \frac{2\mu\,C}{R^3}\left(1 + \frac{2R^3}{R_o^3}\right), \tag{4.50}$$

where

$$C = \frac{\delta v}{4\pi}, \tag{4.51}$$

and δv being the volume change due to the point defect. To compare our nonlinear solution with this classical solution, we note that

$$\delta v = \frac{4\pi}{3}R_i^3\mathsf{n}_0. \tag{4.52}$$

Therefore,

$$C = \frac{1}{3}R_i^3\mathsf{n}_0. \tag{4.53}$$

While an explicit exact analytic solution is not available, an asymptotic expansion for R_i small gives

$$\sigma^{rr} = -\frac{4\mu\,C}{R^3}\left\{\left(1 - \frac{R^3}{R_o^3}\right)\left[1 + \log\left(\frac{R_o^3}{R_i^3(1 - \mathsf{n}_0)}\right)\right] + \log\left(\frac{R^3}{R_o^3}\right)\right\} + \mathrm{O}(R_i^6), \tag{4.54}$$

valid for $R_i \leq R \leq R_o$. We see that the linear solution is modified by a geometric factor $\log(R_o^3/(R_i^3(1-\mathsf{n}_0)))$ and a nonlinear logarithmic correction. Note that (4.54) diverges in the limit $R_i \to 0$, holding δv fixed. The latter is the strength of the centre of contraction/expansion, and is the quantity held fixed in continuum treatment of point defects. As can be seen in figure 4, the two solutions are very close, and the classical linear solution captures most of the features of the nonlinear solution but it diverges at the origin and systematically underestimates

the stress outside the core of the defect. By comparison, the nonlinear solution is regular over the entire domain. The nonlinear analysis of a continuous distribution of point defects in a small core provides an effective way of regularizing the solution for the stress. This is particularly important in deriving estimates for fracture and plastic yielding.

5. Conclusions

In this paper, we constructed the material manifold of a spherically symmetric distribution of point defects, which is a flat Weyl manifold, i.e. a manifold equipped with a metric and a flat and symmetric affine connection, which has a non-vanishing traceless non-metricity. Using Cartan's moving frames and Cartan's structural equations, we constructed an orthonormal coframe field that describes the material manifold. We then embedded the material manifold in the Euclidean three-space. In the case of neo-Hookean materials, we were able to calculate the residual stress field. As particular examples, we showed that a uniform distribution of point defects is zero-stress. We also showed that for a point defect distribution uniform in a sphere of radius R_i and vanishing outside this sphere, the residual stress field in the sphere of radius R_i is uniform (in any isotropic and incompressible solid). This is a nonlinear analogue of Eshelby's celebrated result for spherical inclusions in linear elasticity. We also compared our nonlinear solution with the classical linear elasticity solution of a single point defect. We observed that as expected for a small volume of point defects, the two solutions are close.

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