A Weyl geometric model for thermo-mechanics of solids with metrical defects

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Abstract

This work seeks a rational route to large-deformation, thermo-mechanical modeling of solid continua with metrical defects. It assumes the geometries of reference and deformed configurations to be of the Weyl type and introduces the Weyl one-form – an additional set of geometrically transparent degrees of freedom that determine ratios of lengths in different tangent spaces. The Weyl one-form prevents the metric from being compatible with the connection and enables exploitation of the incompatibility for characterizing metrical defects in the body. When such a body undergoes temperature changes, additional incompatibilities appear and interact with the defects. This interaction is modeled using the Weyl transform, which keeps the Weyl connection invariant whilst changing the non-metricity of the configuration. An immediate consequence of the Weyl connection is that the critical points of the stored energy are shifted. We exploit this feature to represent the residual stresses. In order to relate stress and strain in our non-Euclidean setting, use is made of the Doyle-Ericksen formula, which is interpreted as a relation between the intrinsic geometry of the body and the stresses developed. Thus the Cauchy stress is conjugate to the Weyl transformed metric tensor of the deformed configuration. The evolution equation for the Weyl one-form is consistent with the two laws of thermodynamics. Our temperature evolution equation, which couples temperature, deformation and Weyl one-form, follows from the first law of thermodynamics. Using the model, the self-stress generated by a point defect is calculated and compared with the linear elastic solutions. We also obtain conditions on the defect distribution (Weyl one-form) that render a thermo-mechanical deformation stress-free. Using this condition, we compute specific stress-free deformation profiles for a class of prescribed temperature changes.

1 Introduction

The inelastic response of a material body is brought about by anomalies in their internal structure – what is loosely referred to as 'geometric frustration'. In materials with structural order (crystalline materials, to wit), these anomalies are identified with dislocations and disinclinations. Anomalies

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in structured solids have been studied using tools from differential geometry over a long time. The work by Bilby et al. [2] is a classical example where geometric tools were employed to study dislocations in a crystalline solid. They addressed the technologically important problem of describing dislocations using a continuous field and constructed a geometric space with an asymmetric affine connection whose torsion was related to the density of dislocations; see [13] for a differential geometric description. To generalize such a description of defects, Wang [24] introduced the notion of a material connection, which was characterized using the material uniformity field. The parallel transport of vectors between different tangent spaces was aided by this material uniformity field. Invariants of the material connection describing the intrinsic geometry of the material body (torsion, curvature etc.) were related to the density of defects.

Inelasticity at the continuum scale, on the other hand, is often modelled with internal variables. Phenomena such as thermo-elasticity, visco-elasticity, visco-plasticity, growth, damage etc. fall within the scope of such a description; a brief introduction to a class of these theories may be found in Gurtin et al. [12]. These theories introduce scalar, vector or tensor internal variables, with little or no geometric (kinematic) interpretation. As a consequence, the deformation field is often coupled with these internal variables somewhat arbitrarily. Moreover, the idea of an intermediate configuration, frequently used with these theories, is hard to appreciate from both physical and mathematical standpoints. The elasto-plastic decomposition, used in finite deformation plasticity, is an example that exploits the notion of an intermediate configuration via a multiplicative decomposition of the deformation gradient; see [20] for a brief historical review. As the geometry of the intermediate configuration is opaque, its introduction also corrupts notions of differentiation for vector and tensor fields. On the whole, the clarity offered by geometrically motivated micro-mechanical theories of Kondo, Bilby and others is often lost in such a description of inelasticity at the continuum scale.

The assumption of a fixed relaxed configuration has been questioned before by Eckart [7]. He used an anelasticity tensor to characterize the anelastically deformed solid; this tensor was determined based on an evolution equation for the metric tensor. More recently Rajagopal and Srinivasa [18] used a notion of evolving natural configurations to describe inelastic response of a variety of materials. On similar lines, a geometrically founded continuum thermo-mechanical theory was proposed by Stojanovitch and co-workers [22]. It was based on the decomposition of the deformation gradient into elastic and thermal parts. The individual parts were assumed to be non-integrable, even as the total deformation gradient remained integrable. A frame field having non-zero anholonomy was defined using the thermal part of the deformation gradient. The Weitzenbok connection was constructed by demanding the frame fields to be parallel. It should be mentioned that the connection utilized by Stojanovitch and co-workers was the same used by Bilby and others to describe a dislocated solid. This modeling approach does not affect the metric on the body manifold. This implies that the distance between material points do not change as the temperature of the body is varied from the reference temperature; hence no strains are introduced. Because of this property, the Weitzenbok connection does not appear to offer an attractive route for modelling thermo-elasticity. Ozakin and Yavari [17] have proposed an alternate geometric framework for thermo-elastic deformations. Their work is based on a hypothesized material or relaxed manifold whose geometry is non-Euclidean. In such a configuration, a thermally strained body is stress free. They implement this hypothesis by allowing the metric tensor of the material manifold temperature dependent. Deformation now becomes a map between the material and spatial configurations. The difference in the geometry of spatial and material manifolds leads to stresses in the former. Using this setting, they obtain deformation and temperature fields which do not produce stresses. The condition for a temperature change to be stress free is worked out as the vanishing of the curvature tensor of the material manifold. However, the free energy is not a
function of the curvature of the material manifold. A major problem with the worldview of Ozakin and Yavari is posed by the material manifold – the premise that the material manifold is stress-free cannot be verified since the notion of stress for the material manifold is undefined. Moreover, having a configuration which is virtual (i.e. physically unrealizable) only increases the opacity of the theory. The geometric description of thermo-elastic bodies discussed in [17] has been extended to include time evolution by Sadik and Yavari [21].

Considerable effort has gone in the modelling of point defects, biological growth and thermal strains through an internal variable perspective. Models belonging to this genre try to capture the local zones of expansion or contraction using internal variables. Cowin and Nunziato [5] introduced the void volume fraction as an additional kinematic variable which followed a second order evolution rule. Based on this, they demonstrated that a porous material could support two kinds of waves: one determined by its elastic properties and the other by properties related to porosity. Similarly, Garikipati et al. [9] developed a continuum formulation for point defects within the framework of linear elasticity. Point defects were understood as centers of expansion or contraction. A formation volumetric tensor was introduced to characterize point defects; the dipole tensor conjugate to the formation volumetric tensor described the forces required to keep the point defect in mechanical equilibrium. The linear nature of the theory permitted the use of Green’s functions to determine the stresses due to the point defects. In a more recent work, Moshe et al. [16] has developed a metric description for defects in amorphous solids. Here, the absence of long range order in the material makes it impossible to define Burgers’ vector in terms of the torsion tensor. However, using the Levi-Civita parallel transport, the authors arrive at a notion for Burgers’ vector. They also show that, in a two dimensional setting, a conformal change of the metric tensor is sufficient to represent dislocation- and disinclination-like defects in amorphous solids. The question of restructurability of geometrically frustrated solids is addressed by Zurlo and Truskinovsky [29]. They develop a surface deposition protocol to additively manufacture these residually stressed bodies. Yavari and Goriely [28] formulate a geometric theory for point defects. They postulate that the stress-free configuration of a body with point defects may be identified with a Weyl manifold. The density of defects in the body is defined as the deviation of the volume form of the material manifold from the Euclidean volume form. Using this, they compute the stresses generated by a shrink-fit in the finite deformation setting. To represent the shrink fit, the volume form is assumed to be discontinuous across the shrink fit surface; this is however not in conformity with the structure of a differentiable manifold. They also employ the usual equilibrium equations without explicating on its variational structure, even though the divergence of stress depends on the Weyl connection. Moreover, with the focus being only on analytical solutions, the constitutive framework adopted by Yavari and Goriely remains somewhat simplistic. For instance, no information on distant curvature was made use of in the model.

Though an important problem, the modelling of the mechanical response of solids with metrical defects and temperature change is inadequately addressed in the literature. By metrical defects we mean the anomalies in the material body, which modify the local notion of length. Point defects and growth are examples of metric anomalies. A key component in building such a theory is a geometric space that consistently incorporates the modified notion of length due to defects and temperature change. This is what we set out to pursue, using a Weyl geometric setting. Weyl manifolds are geometric spaces where the metric is incompatible with the connection. This incompatibility has previously been exploited to describe point defects [28, 19]; however there are considerable differences in our present worldview. The Weyl transform which keeps the connection invariant but alters the metric by a positive factor is now thought of as a modification introduced in the configuration of the body due to temperature change. Identifying the reference and deformed configurations as Weyl manifolds make it possible to represent defects and temperature changes in
a consistent manner. This modeling perspective also has an important advantage: it completely avoids the mysterious intermediate configuration. The inelastic response of the body arising out of the defect distribution is buried within the connection associated with the configuration. An important consequence of having a connection different form the flat Levi-Civita is that the critical points of the stored energy function are non-trivially modified. This modification may be exploited to represent configurations which are residually stressed. This fact, to the best of our knowledge, remains unexplored in the literature on defect mechanics. The description has a parallel with the idea of 'pseudo-'forces encountered in particle mechanics; these forces arise only when the components of the connection are non-trivial. This approach is used to predict the stresses created by a diffused shrink fit. The prediction of the radial stress by our methodology is found to be in line with that of the linear elastic solution; however the hoop stress is found to be quite different. The deviation in the hoop stress is essentially due to the diffused representation of the shrink fit. Further, the model is applied to arrive at a condition for a body to be in a state of zero stress under a prescribed temperature change. Using this condition we also recover a well know stress free configurations known from linear elasticity.

This article is organized into eight sections and an appendix. Section 2 gives a brief introduction to a Weyl manifold and discusses its key invariants. Kinematics of a body with metrical defects are discussed in section 3. Kinetics required to describe the dynamics of the defective body are considered in section 4; an important aspect being the adaptation of the classical Doyle-Ericksen formula within the Weylian setting. The equilibrium equation of the Weyl one-form is also derived in this section. In section 5, restrictions imposed by the laws of thermodynamics on the constitutive relations are discussed. Restricting the theory only to local equilibrium considerations, self stresses generated due to a point defect are discussed in section 6. Conditions for a configuration to be stress free state is discussed in section 7. Section 8 concludes the article with a few observations and comments on further possible applications of the present model. The appendix briefly discusses the numerical procedure used to solve the diffused shrink fit problem.

2 Weyl geometry

The defining hypothesis of a Riemannian manifold is that the positive definite metric is preserved under parallel transport. H Weyl [26, 25], in an effort to include electromagnetism within the framework of general relativity, made the following hypothesis: the parallel transport of the metric along a curve is proportional to the metric itself. In other words, the ratios of length between different tangent spaces also need to be parallel transported. This hypothesis introduces an additional degree of freedom which generalizes the Riemannian geometry by an independent scale at each tangent space of the manifold. Even though Weyl’s relativity did not succeed in unifying general relativity and electro-magnetism, the resulting mathematical tool was used to describe other physical phenomena (for recent developments in Weyl relativity, see [1]). We now briefly review the construction of the Weyl geometry. Let \( \mathcal{M} \) be an \( n \) dimensional differentiable manifold with a Riemannian metric \( g \) and \( \gamma \) be a curve in \( \mathcal{M} \) given by, \( \gamma : (0, 1) \to \mathcal{M} \). Using coordinates, the curve may be given by \( (x^1(t), \ldots, x^n(t)) \in \mathcal{M}, \ t \in (0, 1) \). The infinitesimal version of Weyl’s hypothesis may be written as,

\[
\frac{d}{dt} g(V, W) = \phi(\gamma'(t))g(V, W)
\]

where \( \phi \) is a one-form introduced to describe the scale degrees of freedom at each tangent space. Note that as \( \phi \) is set to zero, Eq. 1 reduces to the defining hypothesis.
of Riemannian geometry. We now formally define a Weylian manifold to be the triplet \((M, g, \phi)\), consisting of a differential manifold \(M\), a Riemannian metric \(g\) and a one-form \(\phi\). On integrating Eq. 1 along the curve \(\gamma\), we arrive at a relation between inner-products at \(T_{x(\gamma(0))}M\) and \(T_{x(\gamma(t_1))}M\) given by,

\[
g(V(t), W(t)) = g(V(0), W(0))e^{\int_0^t \phi(\gamma'(t))dt}.
\]

We denote the length of a vector \(V\) by \(l = g(V, V)\). To obtain the variation of \(l\) along \(C\), we set \(V \equiv W\) in Eq. 2, leading to the following relationship,

\[
l(s) = l(0)e^{\int_0^s \phi(\gamma'(t))dt}
\]

If we choose the curve to be closed, i.e. \(\gamma(0) = \gamma(1)\), the transport of the inner-product given in Eq. 2 becomes,

\[
g(V(1), W(1)) = g(V(0), W(0))e^{\int \phi(\gamma'(t))dt}
\]

Using Stokes’ theorem for the line integral, the equation above may be written as,

\[
\int_\Omega d\phi = \oint_\gamma \phi
\]

where, \(\Omega\) is the area enclosed by the closed curve \(\gamma\). If the line integral in Eq. 3 vanishes for any closed curve \(\gamma\), then we have \(d\phi = 0\). Now using Poincaré’s lemma, we have an exact Weyl one-form \(\phi\):

\[
\oint \phi(\gamma'(t))dt = 0 \implies \phi = df
\]

where \(f\) is a scalar valued function and \(df\) denotes the differential of \(f\). Thus integrability of the Weyl one-form ensures that the parallel transport of the inner-product is path independent.

2.1 Weyl connection

An affine connection is an additional structure defined on a smooth manifold, using which one can differentiate vector and tensor fields. It also defines a notion of parallel transport on a tangent bundle. On a differentiable manifold, one can define infinitely many connections. However, we consider the unique torsion free connection which is natural to Weyl’s hypothesis. In terms of covariant derivatives, Weyl's hypothesis may be written as,

\[
\nabla g = \phi g
\]

where, \(\nabla(\cdot)\) is the covariant derivative relative to the Weyl connection. In component form, the equation may be written as,

\[
g_{ij;k} = \phi_k g_{ij}
\]

We introduce a new tensor field \(Q := \phi \otimes g\), called the non-metricity tensor, which describes the incompatibility of the Weyl connection with the metric. In the equation above, \(g_{ij;k}\) denotes the covariant derivative of the metric tensor. With respect to an arbitrary connection, \(g_{ij;k}\) may be written as,

\[
g_{ij;k} = \partial_k g_{ij} - \Gamma^l_{ki}g_{lj} - \Gamma^l_{kj}g_{li}
\]
Here $\Gamma^k_{ij}$ denotes the Christoffel symbol of the second kind. The assumption that the connection is torsion free implies a symmetry condition on the lower two indices of the Christoffel symbol, $\Gamma^k_{ij} = \Gamma^k_{ji}$. Using Eq. 8 in Eq. 9 along with the torsion free assumption leads to the following expression for the coefficients of the Weyl connection.

$$\Gamma^l_{mi} = \frac{1}{2} g^{kl} (\partial_m g_{ik} + \partial_i g_{km} - \partial_k g_{mi}) - \frac{1}{2} (\phi_m \delta^l_i + \phi_i \delta^l_m - \phi_j g_{mi} g^{jl})$$ (10)

If the Weyl one-form is integrable then we have,

$$\Gamma^l_{mi} = \frac{1}{2} g^{kl} (\partial_m g_{ik} + \partial_i g_{km} - \partial_k g_{mi}) - \frac{1}{2} (\partial_m f \delta^l_i + \partial_i f \delta^l_m - \partial_j g_{mi} g^{jl})$$ (11)

Note that for any Weyl manifold (integrable or non-integrable), the connection may be written as the sum of the Levi-Civita connection and a $(1,2)$ tensor. This $(1,2)$ tensor is determined by the metric and the Weyl one-form. Another important property of a Weyl connection is the invariance under Weyl transformation. A Weyl transformation is defined by,

$$g_{ij} \rightarrow e^s g_{ij}; \quad \phi \rightarrow \phi + ds$$ (12)

where, $s$ is a real valued function. One may immediately verify the invariance of the connection by substituting Eq. 12 in Eq. 10. However, if we define $\tilde{g}_{ij} := e^s g_{ij}, \tilde{\phi} := \phi + ds$ and substitute them in Eq. 9 we arrive at the following,

$$\tilde{g}_{ij;k} = \tilde{\phi}_k \tilde{g}_{ij}$$ (13)

The invariance of the Weyl connection under Weyl transformation is a cornerstone in our thermo-mechanical theory; section 3 discusses this aspect in detail.

### 2.2 Equivalence of an integrable Weyl manifold and Riemannian manifold

The notion of an integrable Weyl manifold was established at the beginning of this section. We now discuss its equivalence with a Riemannian manifold. This equivalence is established by showing that Weyl’s connection boils down to the Levi-Civita connection when the Weyl one-form is exact. For the sake of completeness we record the Levi-Civita connection induced on a Riemannian manifold by the metric $g$. The Christoffel symbols associated with the Levi-Civita connection are given by,

$$\Gamma^l_{mi} = \frac{1}{2} g^{kl} (\partial_m g_{ik} + \partial_i g_{km} - \partial_k g_{mi})$$ (14)

By setting the Riemannian metric as $e^f g$ and computing the Christoffel symbols of the associated Levi-Civita connection, we are led to the connection coefficients of an integrable Weyl connection given in Eq. 11. This result implies that an integrable Weyl manifold is a Riemannian manifold with a modified metric.

### 2.3 Invariants of a Weyl connection

On a Weyl manifold, the presence of a metric permits us to define the arc length for any curve on the manifold. This is similar to the case with Riemannian manifolds. Let $\gamma$ be a curve on $M$; the expression for the arc-length of $\gamma$ is given by,

$$l = \int_{\gamma} e^s \sqrt{\phi \left( \frac{d\gamma}{dt} \right)^2 g \left( \frac{d\gamma}{dt}, \frac{d\gamma}{dt} \right)} dt$$ (15)
\( g(\ldots) \) is the Riemannian metric associated with a Weyl manifold, \( \frac{dx}{dt} \) is the vector field tangent to \( \gamma \) and \( s \) is the variable of the Weyl transformation. Note that \( s \) weights the metric at each point on the curve. We choose the following three-form as the volume form,

\[ dV = e^{\frac{ns}{2}} \sqrt{g} dx^1 \wedge \ldots \wedge dx^n \]  

where \( n \) is the dimension of the manifold and \( g \) the determinant of the Riemannian metric. Note that the volume-form is not compatible with the Weyl connection. Apart from non-metricity, the Weyl connection may also have curvature. As with a Riemannian manifold, the curvature operator is defined as the non-commutativity of second covariant derivatives.

\[ R(X,Y)(Z) = \nabla_X \nabla_Y Z - \nabla_Y \nabla_X Z - \nabla_{[X,Y]} Z \]  

In the equation above, \( X, Y \) and \( Z \) are vector fields on \( \mathcal{M} \). The curvature operator is linear in all its input arguments; it is also anti-symmetric in \( X \) and \( Y \). If one writes the curvature operator in a coordinate (holonomic) basis, the last term in the above equation vanishes. The components of the curvature tensor are given by,

\[ R^i_{\; klj} = \partial_k \Gamma^l_{\; ji} - \partial_j \Gamma^l_{\; ki} + \Gamma^l_{\; ka} \Gamma^a_{\; ji} - \Gamma^l_{\; ja} \Gamma^a_{\; ki} \]  

The Ricci curvature is given by,

\[ R_{ij} = R^k_{\; ikj} \]  

In contrast to the Riemannian case, the Ricci tensor of a Weyl manifold is unsymmetric and thus may be decomposed into its symmetric and antisymmetric parts.

\[ R_{ij} = \hat{R}_{ij} + K_{ij} \]  

\( \hat{R}_{ij} \) and \( K_{ij} \) respectively denote the symmetric and antisymmetric parts of the Ricci tensor. The antisymmetric tensor \( K \) is sometimes called the distant curvature. It is given by the exterior derivative of the Weyl one-form.

\[ K = d\phi \]  

For an integrable Weyl manifold, the distant curvature vanishes making the Ricci tensor symmetric; this follows from the identity \( dd = 0 \). Using the symmetric part of the Ricci tensor, the following scalar curvature can be defined,

\[ R = g^{ij} R_{ij} \]  

Note that \( R \) does not depend on the distant curvature. The scalar measure extracted form the anti-symmetric distant curvature is

\[ K = g^{ik} g^{jl} K_{ij} K_{kl} \]  

Using the machinery of Weyl manifolds discussed so far, we now proceed to develop a thermo-mechanical theory for a solid body with metrical defects.

### 3 Kinematics

We assume the reference and deformed configurations to be Weylian manifolds. These configurations are respectively denoted by the triplets \( (B, G, \xi) \) and \( (S, g, \phi) \), where \( B \) and \( S \) are smooth three-manifolds. The metric tensors of the reference and deformed configurations are denoted by \( g \) and \( G \) and the associated Weyl one-forms by \( \eta \) and \( \phi \) respectively. We introduce an additional kinematic variable in the deformed configuration called the Weyl scaling, which is denoted by \( s \).
$s$ is identified as the variable of Weyl transformation discussed in the previous section. The Weyl transformation modifies the deformed metric by scaling it by a positive scalar and changing the one-form by an exact one-form $ds$. In this work, we assume that Weyl transformation models the thermal strain introduced in the body due to temperature change. Since the Weyl connection is invariant under Weyl transformation, the Weyl scaling does not modify the connection. However the metric and the non-metricity are modified due to temperature change. This modification represents the change in the strain field and defect distribution in the material body. The Weyl transformed metric and the one-form of the deformed configuration are denoted by $\bar{g} := e^s g$ and $\bar{\phi} = \phi + ds$ respectively. We relate $s$ to the temperature field of the deformed configuration through the following relationship,

$$s = \alpha(T - T_0).$$  \hspace{1cm} (24)

The equation above is a constitutive relation chosen for simplicity, although other relationships are possible. The variables $\alpha$, $T$ and $T_0$ respectively denote the co-efficient of thermal expansion, temperature field and reference temperature of the body. Throughout this work, we assume the metric tensors $G$ and $g$ as Euclidean. The deformation map relating the reference and deformed configurations is given by,

$$\varphi : B \to S.$$ \hspace{1cm} (25)

The derivative of the deformation map or the tangent map is denoted by $F$; it maps tangent vectors from the reference configuration to those of the deformed configuration. If we denote the co-ordinates of the reference and deformed configurations by $(X^1, ..., X^3)$ and $(x^1, ..., x^3)$, then the deformation gradient can be expressed as,

$$\frac{\partial}{\partial x^i} = F^i_l \frac{\partial}{\partial X^l}$$ \hspace{1cm} (26)

where $\frac{\partial}{\partial X^l}$ and $\frac{\partial}{\partial x^i}$ are the coordinate bases for $T_X B$ and $T_{\varphi(X)} S$ respectively. These basis vectors may be identified with vectors tangent to the coordinate lines at each point of the manifold. Whenever the deformed configuration has a metric tensor, the right Cauchy-Green deformation tensor $C : T_X B \times T_X B \to \mathbb{R}$ can be defined by pulling back the metric tensor of $S$ to $B$:

$$C = \varphi^* g.$$ \hspace{1cm} (27)

In this equation, $\varphi^*(\cdot)$ denotes the pull-back map. The covariant components of $C$ are thus given by,

$$C_{IJ} = F^i_l g_{ij} F^j_l$$ \hspace{1cm} (28)

As the temperature of the body changes from the reference, the metric and the Weyl one-form of the deformed configuration change via the Weyl transformation. In the presence of thermal strains, the Cauchy-Green deformation tensor denoted by $\tilde{C}$ is given by,

$$\tilde{C}_{IJ} = F^i_l \tilde{g}_{ij} F^j_l = e^s F^i_l g_{ij} F^j_l$$ \hspace{1cm} (29)

From now on, we will use the expression in Eq. 29 as the definition of the right Cauchy-Green deformation tensor. Note that Eq. 29 reduces to the usual definition of the right Cauchy-Green deformation tensor when $s$ is set to zero. This pertains to the case of no temperature change in the body. Components of the Green-Lagrangian strain in the presence of temperature change are given by,

$$E_{IJ} = \frac{1}{2}(\tilde{C}_{IJ} - G_{IJ})$$ \hspace{1cm} (30)

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As a consequence of Weyl transformation, the principal stretches are scaled by \( \exp \left( \frac{s}{2} \right) \). If \( \lambda_i \) are the principal stretches of \( \mathbf{C} \), it follows that,

\[
\bar{\lambda}_i^2 = \exp(s) \lambda_i^2
\]  

(31)

\( \bar{\lambda}_i \) are the principal stretches of \( \bar{\mathbf{C}} \). The invariants of \( \bar{\mathbf{C}} \) and \( \mathbf{C} \) are related in the following way,

\[
\bar{I}_1 = \exp(s) I_1; \quad \bar{I}_2 = \exp(2s) I_2; \quad \bar{I}_3 = \exp(3s) I_3,
\]

(32)

Here, \( I_i \) and \( \bar{I}_i \) are the principal invariants of \( \mathbf{C} \) and \( \bar{\mathbf{C}} \) respectively. In the literature, the Green-Lagrangian strain tensor is sometimes defined as half the difference between the deformed and the reference metrics (see [10], [8]). Although this definition might make sense in a small deformation setting, it is problematic since the addition of metric tensors is not well defined. To be more precise, the reference metric operates only on tangent vectors of the reference configuration, while the deformed metric operates on tangent vectors of the deformed configuration. In some cases, by the 'deformed metric', the pulled-back metric is implied. The distinction between the deformed metric and the pulled back metric is quite important in a geometrically motivated continuum theory, since the metric tensor may be construed as a separate dynamical field describing the intrinsic geometry of the body.

The Jacobian of deformation in the presence of temperature change is denoted by \( \bar{J} \) and is given by,

\[
\bar{J} = \exp \left( \frac{3s}{2} \right) \sqrt{\frac{g}{G}} \det \mathbf{F}
\]

(33)

where, \( g \) and \( G \) denote the determinants of the reference and deformed metric tensors. The non-metricity tensors of the reference and deformed configurations are denoted by \( \mathbf{H} \) and \( \mathbf{Q} \) respectively. These tensors are defined by,

\[
\mathbf{H} = \xi \otimes \mathbf{G}; \quad \mathbf{Q} = \phi \otimes \mathbf{g}
\]

(34)

In this work, the non-metricity tensor of the deformed configuration completely characterizes the residual stresses developed in the body due to inelastic effects. The initial configuration may also be trivially viewed as a deformed configuration with identity map as deformation. With this understanding, the tensor \( \mathbf{H} \) has significance well beyond what the metric tensor of the initial configuration offers. Specifically, as a conjugate to the kinematic variable \( \xi \), one may talk about residual stresses using just one configuration. This may be contrasted with elastic stresses (stresses due to deformation) whose description necessitates both the reference and deformed configurations.

The pull-back of the deformed configurations Weyl one-form, denoted as \( \phi' \in T^* \mathcal{B} \), is given by,

\[
\phi' = \varphi^* \phi
\]

(35)

Similarly, the pulled-back non-metricity tensor \( \mathbf{Q}' \) is defined by \( \mathbf{Q}' := \varphi^*(\mathbf{Q}) \), which leads to the following expression,

\[
\mathbf{Q}' = \phi' \otimes \bar{\mathbf{C}}
\]

(36)

This expression is obtained by applying the pull-back map to the Weyl one-form and the metric tensor. Similarly, the pull-back of the distant curvature is denoted by \( \mathbf{K}' := \varphi^*(\mathbf{K}) \). Since the pull-back map commutes with exterior derivative, we can write \( \mathbf{K}' \) as,

\[
\mathbf{K}' = \varphi^* d\phi \\
= d(\varphi^* \phi) \\
= d\phi'
\]

(37)
The spatial rate of deformation tensor \( \mathbf{d} \), characterizes the relative velocity of the material in a small neighbourhood around a point in the deformed configuration and is given by,

\[
\mathbf{d} = \frac{1}{2} \mathcal{L}_v \mathbf{g}
\]  

(38)

where, \( \mathcal{L}_v(.) \) denotes the Lie derivative. When the geometry of the material body is Riemannian, the formula above reduces to

\[
d_{ij} = \frac{1}{2} (v_{ij} + v_{ji})
\]

An index after a semicolon denotes the covariant derivative (given by the appropriate connection). The Lie derivative of the metric tensor is,

\[
\mathcal{L}_v \partial_c (g_{ab}) = v_c \partial_c g_{ab} + g_{cb} \partial_a v^c + g_{ca} \partial_b v^c
\]

(39)

By adding and subtracting \( \gamma^c_{da} v^d \) and \( \gamma^c_{db} v^d \) in the last equation and using the definition of covariant derivative, we arrive at,

\[
\mathcal{L}_v \partial_c (g_{ab}) = v_c \nabla_a v^c + g_{cb} \nabla_a v^c + g_{ca} \nabla_b v^c
\]

(40)

Now, using the properties of Weyl connection, the equation above may be rewritten as,

\[
\mathcal{L}_v \partial_c (g_{ab}) = \phi_c v^c g_{ab} + \nabla_a \phi_b + \nabla_b \phi_a - (\phi_a v_b + \phi_b v_a)
\]

(42)

where, \( v_a = g_{ab} v^b \) and the relation \( \nabla_a v_c = \nabla_a g_{cb} v^c + g_{cb} \nabla_a v^c \) have been used. Using Eq. 42, the rate of deformation tensor may now be computed. Substituting Eq. 42 in Eq. 38, we arrive at rate of deformation tensor of a body whose configurational geometry is Weylian.

\[
d_{ij} = \frac{1}{2} \left( v_{ij} + v_{ji} - (\phi_i v_j + v_i \phi_j) + \phi_k v^k g_{ij} \right)
\]

(43)

It should be noted that the rate of deformation tensor for a body with Weyl geometry has three additional terms compared with the Riemannian case. These additional terms are a consequence of the incompatibility of the connection with the metric.

### 3.1 Connections of reference and deformed configurations

The connection of the reference configuration is assumed to be time independent, while that of the deformed configuration evolves with time. The connection coefficients of reference and deformed configurations are denoted by \( \Gamma^c_{AB} \) and \( \gamma^c_{ab} \) respectively. If the reference configuration has a non-trivial connection (different from the flat Levi-Civita), then the body has a distribution of defects, which may require residual stresses for mechanical equilibrium to be maintained. The connection of the deformed configuration is determined by the evolution of the Weyl one-form, which in turn is coupled to the evolving temperature field. This evolution models the generation, motion and extinction of metrical defects due to externally applied thermo-mechanical stimuli.

### 4 Kinetics

The balance of linear momentum in the reference configuration is given by,

\[
\nabla \mathbf{P} + \mathbf{B} = \rho_0 \frac{d \mathbf{V}}{dt}
\]

Here, \( \mathbf{P} \) is the first Piola stress and \( \nabla(.) \) is the divergence operator determined by the Weyl connections of the reference and deformed configurations. The Piola stress \( \mathbf{P} \) is related to the
Cauchy stress $\sigma$ through the Piola transform (which is applied to the second index of the Cauchy stress). We define the symmetric Piola (second Piola) stress as the pull-back of the first index of the first Piola stress. The relation between the Cauchy stress and second Piola stress is thus given by,

$$ S = J \varphi^*(\sigma) \quad (45) $$

### 4.1 Evolution of Weyl one-form

The equilibrium condition for the Weyl one-form is obtained as a critical point of the free-energy with respect to the one-form $\phi$. In the reference configuration, this condition may be written as,

$$ \delta \hat{\psi}_0 = 0; \quad \delta \phi \hat{\psi}_0 := \delta \phi \int_B \psi_0 dV \quad (46) $$

where, $\hat{\psi}_0$ is the free energy of the body and $\delta \phi(\cdot)$ denotes the Gâteaux or the variational derivative. Assuming that the free energy depends on $F', Q', K'$ and $T$, its variation may be evaluated as,

$$ \delta \phi \psi_0 = \frac{\partial \psi_0}{\partial F'} : \delta \phi F + \frac{\partial \psi_0}{\partial Q'} : \delta \phi Q' + \frac{\partial \psi_0}{\partial K'} : \delta \phi K' \quad (47) $$

$\delta \phi(A)$ denotes the directional derivative of the tensor $A$ with respect to $\phi$. Since the deformation gradient does not depend on $\phi$, we have $\delta \phi F = 0$. We also have $\delta \phi K = d\delta \phi$ and hence $\delta \phi K' = d(\delta \phi)'$; here $(\delta \phi)' := \varphi^*(\delta \phi)$. Similarly, $\delta \phi Q' = (\delta \phi)' \otimes \mathbb{C}$. We also introduce the following definitions for a simpler exposition,

$$ M := \frac{\partial \psi_0}{\partial Q'}, \quad N := \frac{\partial \psi_0}{\partial K'} \quad (48) $$

Using these results and definitions, the variation of the free energy may be written as,

$$ \int_B \left( M^{JK} C_{JK}(\delta \phi)' + N^{IJ} \partial_{[I}(\delta \phi)'_{J]} \right) dV = 0 \quad (49) $$

Applying the relation between $(\delta \phi)'$ and $\delta \phi$ and using the divergence theorem on the second term, we arrive at,

$$ \nabla_J N^{JJ} - M^{JK} C_{JK} = 0 \quad (50) $$

### 4.2 Doyle-Ericksen formula

In continuum mechanics, the Doyle-Ericksen formula \cite{6, 15} is an important result, which relates stress (Cauchy stress) with the metric of the deformed configuration. Through the metric, this formula is thus able to relate the intrinsic geometry of the deformed configuration to the stresses developed. The Doyle-Ericksen formula is given by,

$$ \sigma^{ij} = 2 \rho \frac{\partial \psi}{\partial g_{ij}} \quad (51) $$

$\rho$ and $\psi$ are the mass density and free energy density of the deformed configuration. An interesting aspect of the formula is that it emphasizes length as a fundamental quantity. If the last statement is understood abstractly, then there is no reason to restrict length just to its Euclidean notion. To obtain a relationship between the Cauchy stress and the scaled metric $\bar{g}$, we replace $g$ in Eq. \ref{51} by $\bar{g}$, so the desired relation is given by,

$$ \sigma^{ij} = 2 \rho \frac{\partial \psi}{\partial \bar{g}_{ij}} \quad (52) $$
In the reference configuration, the equation above provides a relation between the second Piola stress and the right Cauchy-Green deformation tensor,

\[ S_{IJ} = 2\rho_0 \frac{\partial \psi_0}{\partial C_{IJ}} \]  

(53)

Note that this equation is related to Eq. 52. To prove the equivalence, one starts by noticing that,

\[ \varphi_* \frac{\partial \psi_0}{\partial C_{IJ}} = \frac{\partial \psi}{\partial \bar{g}_{ij}} \]  

(54)

Moreover, the second Piola stress is related to the Cauchy stress though the push-forward of its first index and an inverse Piola transform applied to the second index. Formally, these two operations may be written together as,

\[ \sigma^{ij} = \frac{1}{J} \varphi_*(S^{IJ}) \]  

(55)

Eqs. 54 and 55 together lead us to the required equivalence. In the present context, the notion of stress is understood in the sense of Eq. 51. The positive scalar factor introduced in the metric by the Weyl transformation does not create a new notion of stress, unlike what was conceived of by Gurtin. Gurtin in [11] postulated the existence of new stresses called micro-stresses and a new balance rule called the micro-force balance. These stresses were shown as energetically conjugate to the internal variables introduced to describe the inelastic deformation. Moreover, the divergence-type balance law for the internal variables was restrictive and a physical meaning for these micro-stresses remained elusive. Identifying thermal strains as a geometric object permits us to reinterpret the classical geometric results seamlessly. This is often impossible with internal variable theories, which require additional postulates for closure.

### 4.3 Comparison with Duhamel-Neuman relation

In linear thermo-elasticity, the Duhamel-Neuman hypothesis is commonly adopted to model the mechanical response of solids in the presence of temperature change. It postulates the existence of a new tensor-valued internal variable called the thermal strain whose evolution is directly proportional to the temperature change in the body. The total strain \( \varepsilon_{\text{Tot}} \), defined as the symmetric part of the displacement gradient, is recovered by an additive splitting,

\[ \varepsilon_{\text{Tot}} = \varepsilon_{\text{Mec}} + \varepsilon_{\text{The}} \]  

(56)

The mechanical and thermal parts of the strain are denoted by \( \varepsilon_{\text{Mec}} \) and \( \varepsilon_{\text{The}} \) respectively. For a body admitting isotropic thermal expansion, \( \varepsilon_{\text{The}} \) relates to the change in temperature \( (T - T_0) \) in the following way,

\[ \varepsilon_{\text{The}} = \alpha(T - T_0)I \]  

(57)

Several extensions of this additive splitting to finite deformation thermo-elasticity exist in the literature. Splitting of the deformation gradient in thermal and elastic parts comes in two forms: \( F = F_e F_T \) and \( F = F_T F_e \). Implicit in these settings is the notion of an intermediate configuration to describe the incompatibility created by thermal deformation. Yet another extension of the Duhamel-Neuman hypothesis to finite deformation is through an additive decomposition of the rate of deformation tensor into mechanical and thermal components \( d = d_e + d_T \) (for details see [15]), where,

\[ d = \frac{1}{2} \rho_0 \left[ \left( \frac{\partial^2 \chi}{\partial \tau^2} : L \nu \tau \right) + \frac{\partial^2 \chi}{\partial \tau \partial T} \right] T \]  

(58)
and \( \mathbf{d}_e \) and \( \mathbf{d}_T \) are given as,

\[
\mathbf{d}_e = \frac{\rho_0}{2} \left( \frac{\partial^2 \chi}{\partial \tau^2} : \mathbf{L}_\tau \mathbf{T} \right); \quad \mathbf{d}_T = \frac{\rho_0}{2} \frac{\partial^2 \chi}{\partial \tau \partial T} \mathbf{T}.
\]  (59)

Here, \( \chi \) denotes the complementary free energy and \( \mathbf{T} \) the Kirchhoff stress. The thermo-elastic splitting given in Eq. (58) is verifiable using Legendre transform; hence it is not a hypothesis. It only requires the existence of a temperature dependent free energy. In any case, the splitting of the rate of deformation tensor cannot account for the incompatibility due to thermal strain since the geometry of the body remains essentially Euclidean.

With our present formulation, we are able to avoid the notion of an intermediate configuration whilst incorporating the incompatibility due to thermal strains in a consistent manner. The rate of deformation tensor \( \mathbf{d} = \frac{1}{2} \mathbf{L}_\mathbf{g} \) may be written as,

\[
\mathbf{d} = \varepsilon \mathbf{d} + \frac{1}{2} \mathbf{v}[s] \mathbf{g}.
\]  (60)

The equation above follows from the properties of the Lie derivative, \( \mathbf{v}[,.] \) denotes the action of a vector field on a function, \( \mathbf{d} := \mathbf{L}_\mathbf{g} \) and \( \mathbf{d} := \mathbf{L}_\mathbf{g} \). The current geometric methodology has the added advantage that the rate of deformation tensor may be determined kinematically, without the use of inverse elastic relations. Neither complementary free energy nor Legendre transform is used to arrive at the equation. However, the decomposition given in Eq. (58) may also be adopted in the present setting.

5 Thermodynamics

We use a local equilibrium thermodynamics framework to determine the restrictions imposed on the constitutive functions by the laws of thermodynamics. In line with the standard hypothesis, we postulate the existence of state variables called the specific internal energy density and specific entropy, denoted by \( U \) and \( \eta \) respectively. \( U \) is assumed to depend on the right Cauchy-Green deformation tensor, non-metricity tensor, distant curvature and specific entropy. \( U \) may also depend on co-ordinates of the reference configuration; however we choose to work with an internal energy which is homogeneous, i.e. the explicit spatial dependence is ignored. The balance of energy, which is the statement of the first law of thermodynamics, may be written as,

\[
\frac{d}{dt} \int_B \rho_0 \left( U + \frac{1}{2} \mathbf{G}(\mathbf{V}, \mathbf{V}) \right) dV = \int_B \langle \mathbf{B}, \mathbf{V} \rangle dV + \int_{\partial B} \langle \mathbf{t}, \mathbf{V} \rangle dA - \int_{\partial B} \langle \mathbf{q}, \mathbf{n} \rangle dA
\]  (61)

In the above equation, \( \langle ., . \rangle \) denotes the natural pairing between cotangent and tangent vectors. The heat flux vector and the unit vector normal to the boundary \( \partial B \) are denoted by \( \mathbf{q} \) and \( \mathbf{n} \) respectively. Kanso et al. [13] have interpreted the stress tensor as a bundle valued two-form. Such a description has the advantage of having the integrals in the balance of energy consistent with the integration of differential forms. However, introducing such notions of stress do not affect the resulting equations; hence we do not dwell on such technical details here. The temperature gradient of the deformed configuration is given by \( \bar{g}^{ij} \partial_j T \). To determine the heat flux vector of the reference configuration, one may adopt one of the following two routes. In the first, one exploits the constitutive relation between temperature gradient and heat flux in the deformed configuration and use the Piola transform to bring the heat flux vector to the reference configuration. Alternatively, one may use the Piola transform on the temperature gradient of the deformed configuration and
use the referential version of the constitutive rule connecting heat flux and temperature gradient. The two routes are equivalent if the constitutive rule is transformed carefully.

The equilibrium equation for the one-form given in Eq. 51 does not account for time dependent relaxation experienced by defects. We model time dependent relaxation by adjoining the equilibrium equation for the Weyl one-form with an additional viscous term. Such a procedure to obtain the evolution rule for states that relax to equilibrium has been employed in arriving at the Cahn-Hillard and Ginsberg-Landau equations. Geometric evolutions like the Ricci flow and mean curvature flow equations also have a similar variational structure. The equilibrium equation for the one-form with relaxation may be written as,

$$\mathcal{L}_V(\phi^I) = \frac{1}{m} \delta_{\phi^I} \tilde{\psi}_0 \quad (62)$$

$\mathcal{L}_V(.)$ denotes the Lie derivative with respect to the velocity field, $m$ is a constant describing the time dependent relaxation experienced by defects. In addition to the balance of energy for the whole body, we also postulate that a local form of energy balance holds (the fields used in the integral statement of Eq. 51 are assumed sufficiently smooth so that localization theorem can be applied), which may be written as,

$$\rho_0 \dot{\psi} = \frac{1}{2} S^{IJ} \dot{C}_{IJ} + N^{IJ} \phi^I_{[I,J]} + M^{IJK} \dot{C}_{JK} \phi^I_I - \partial_I q^I + \rho_0 R - m \phi^I \phi^I_I \quad (63)$$

where, $R$ denotes the heat source and $(.)_{[I,J]}$ the anti-symmetrization with respect to the indices $I$ and $J$. The last equation is obtained from Eq. 51 through the use of the balance of linear momentum, divergence theorem and localization theorem. We impose the second law of thermodynamics through the Clausius-Duhem inequality; its local form is given by,

$$\rho_0 \dot{\eta} \geq \frac{R}{T} - \partial_I \left( \frac{q^I}{T} \right) \quad (64)$$

Applying the Legendre transform $\psi_0 = U - T \eta$ with respect to the conjugate variables $\eta$ and $T$, we arrive at,

$$\dot{\eta} = \frac{1}{T} (\dot{U} - \dot{\psi}_0 - \dot{\theta} \eta); \quad \eta = - \frac{\partial \psi_0}{\partial T} \quad (65)$$

The reference free energy density is assumed to be a function of the right Cauchy-Green deformation tensor, non-metricity tensor, distant curvature tensor and temperature. The rate of Helmholtz free energy density is calculated as,

$$\psi_0 = \frac{\partial \psi_0}{\partial C_{IJ}} \dot{C}_{IJ} + \frac{\partial \psi_0}{\partial Q'_{IJK}} \dot{C}_{JK} \phi^I_I + \frac{\partial \psi_0}{\partial Q''_{IJK}} \phi^I_I \dot{C}_{JK} + \frac{\partial \psi_0}{\partial K'_{IJ}} \phi^I_{[I,J]} + \frac{\partial \psi_0}{\partial T} \quad (66)$$

In arriving at the equation, use is made of the relation $\dot{Q}_{IJK} = \dot{\phi}^I_I \dot{C}_{KL} + \phi^I_I \dot{C}_{KL}$. Using the relationship between entropy, internal energy and free-energy density in Eq. 52, we have the following form of second law,

$$\rho_0 (\dot{U} - \dot{\psi}_0 - \dot{T} \eta) + \partial_I q^I - \frac{q^I}{T} \partial_I T - \rho_0 R \geq 0 \quad (67)$$

Now, substituting the rate of free energy and internal energy in Eq. 67 leads to,

$$\left( \frac{1}{2} S^{IJ} - \rho_0 \left( \frac{\partial \psi_0}{\partial C_{IJ}} + \frac{\partial \psi_0}{\partial Q'_{KIJ}} \phi^I_K \right) \right) \dot{C}_{IJ} + \left( M^{IJK} \rho_0 \frac{\partial \psi_0}{\partial Q''_{IJK}} \dot{C}_{JK} \right) \phi^I_I + \left( N^{IJ} - \rho_0 \frac{\partial \psi_0}{\partial K'_{IJ}} \right) \phi^I_{[I,J]} - \left( \frac{\partial \psi_0}{\partial T} + \eta \right) \dot{T} - m \phi^I \phi^I_I - \frac{q^I}{T} \partial_I T \geq 0 \quad (68)$$
Applying a Coleman-Noll type procedure to the last equation gives us the requisite constitutive relations. Thus the second Piola stress is given by,

\[ S^{IJ} = 2\rho_0 \left( \frac{\partial \psi_0}{\partial \bar{C}_{IJ}} + \frac{\partial \psi_0}{\partial Q'_{KIJ}} \phi'_K \right) \] (69)

Similarly, we also have,

\[ M^{IJK} = \frac{\partial \psi_0}{\partial Q'_{IJK}}; \quad N^{IJ} = \frac{\partial \psi_0}{\partial K'_{IJ}} \] (70)

The last two relations were established through a variational argument in the previous Section 4.1. Using these constitutive relations in the dissipation inequality leads to,

\[ -\left( m \dot{\psi}_I + q^I \dot{\phi}_I \right) \geq 0 \] (71)

From this, it follows that \( m < 0 \) and \( q^I = -L^{IJ} \partial \frac{\dot{J}}{\dot{T}} \), where \( L \) is the thermal conductivity which is positive definite.

### 5.1 Temperature evolution

The temperature evolution equation is obtained by substituting the constitutions for second Piola stress and entropy into the local form of energy balance. Using Eq. 65, the rate of entropy production \( \dot{\eta} \) is given by,

\[ \dot{\eta} = -\left( \frac{\partial^2 \psi_0}{\partial T^2} \frac{\partial^2 \psi_0}{\partial C \partial T} : \dot{C} + \frac{\partial^2 \psi_0}{\partial Q' \partial T} \dot{Q}' + \frac{\partial^2 \psi_0}{\partial K' \partial T} \dot{K}' \right) \] (72)

substituting Eqs. 72, 65 and 69 into the energy balance leads to the following evolution equation for temperature.

\[ -\rho_0 T \left( \frac{\partial^2 \psi_0}{\partial T^2} \frac{\partial^2 \psi_0}{\partial C \partial T} : \dot{C} + \frac{\partial^2 \psi_0}{\partial Q' \partial T} \dot{Q}' + \frac{\partial^2 \psi_0}{\partial K' \partial T} \dot{K}' \right) = -\nabla . q + \rho_0 R \] (73)

### 5.2 Residual stresses due to defects

An accurate prediction of residual stresses requires complete information on the distribution of defects. As assumed, the Weyl one-form of the deformed configuration encodes the metrical defects present in the body. This one-form may or may not evolve, depending on the thermo-mechanical processes the body is subjected to. Assume the initial configuration \( B \) as unloaded and without deformation, but with defects. The no-deformation assumption implies that \( F = I \), whereupon it follows that Cauchy, first and second Piola stresses are indistinguishable or, in other words, the Piola transform and pull-back operation are trivial (identities).

\[ P = S; \quad S = \sigma \] (74)

The condition of no external traction or displacement on \( B \) implies that the residual stresses have to be self equilibrating.

\[ \sigma^{IJ}_{;J} = 0 \] (75)

In addition, if we assume that residual stresses are obtainable from a stored energy function, then the stress tensor may be written as,

\[ \sigma^{IJ} = 2\rho_0 \frac{\partial \psi_R}{\partial G_{IJ}} \] (76)
where, $\psi^R$ is the free energy due to defects. The last equation is the Doyle-Ericksen formula discussed in the previous section. The metric tensor appearing in the formula is one on $\mathcal{B}$. The assumption that residual stresses are characterizable using a free energy, is grounded in the physical reality that a residually stressed body, on being cut, would deform. This implies that the energy stored in the body due to the presence of defects may be converted to strain energy through a deformation process. This property is often used in an experimental characterization of residual stresses through destructive testing. It should be noted that the free energy for the residual stress field need not be the same as the stored energy used to determine a deformation process. Distributions of the Weyl one-form and the stored energy $\psi^R$ together determine the residual stress distribution on $\mathcal{B}$.

When $\mathcal{B}$ is subjected to deformation, the defects present in the body evolve, which along with the deformation-induced stresses equilibrates the externally applied loads. Thus we postulate that the free energy of the body at a configuration has two components: one due to deformation and temperature, and the other due to defects. Using a referential description, the component of free energy due to defects is written as a function of the pulled back non-metricity tensor and the pulled back distant curvature; we denote this component by $\psi_0^R$. The deformation and temperature dependent component of free energy is denoted by $\psi_0^\phi$; it is assumed to be a function of the deformation gradient, metric tensor of the deformed configuration and temperature.

$$\psi_0 = \psi_0^\phi(F, g, T) + \psi_0^R(Q', K')$$ (77)

Assuming the Doyle-Ericksen formula to hold in the deformed configuration, the second Piola stress is now given by,

$$\mathbf{S} = \frac{\partial \psi_0^\phi}{\partial \bar{\mathbf{C}}} + \frac{\partial \psi_0^R}{\partial Q'} \frac{\partial Q'}{\partial \bar{\mathbf{C}}}$$ (78)

The first term on the right hand side is the second Piola stress caused by deformation, while the second term is due to the defects. Note that, when the Weyl one-form vanishes, so does the defect component of the free energy leading to the usual expression for the second Piola stress. Similarly, when deformation vanishes, $\mathbf{F} = \mathbf{I}$ and the right Cauchy-Green deformation tensor reduces to the metric of the deformed configuration leading to Eq. (76).

### 5.3 A specific constitutive rule

Having dwelt on the thermodynamic framework and the form of the constitutive rules in the previous subsections, we now make a specific choice for the constitutive relations. We assume the deformation part of the free energy to be of the compressible Neo-Hookian type. Indeed, any hyperelastic free energy function could be used in its place. The stored energy for a compressible neo-Hookian material is given by,

$$\psi_0^\phi = \frac{\mu}{2} (\bar{I}_1 - 3) - \mu \log(\bar{J}) + \frac{\lambda}{2} \log(\bar{J})^2$$ (79)

Note that the principal invariants used in the stored energy density are Weyl transformed. For the defect part of the free energy, we assume the following form,

$$\psi_0^R = \frac{1}{2} (k_1 \bar{Q}'_{IJK} G^{IL} G^{JM} G^{KN} Q_L^M K^I_K + k_2 G^{KM} G^{LN} K'_K L^M N)$$ (80)

In the last equation, $k_1$ and $k_2$ are material constants characterizing the defect-induced free energy. The defect free energy may be further simplified as,

$$\psi_0^R = \frac{1}{2} \left( k_1 \bar{C}_{IJ} \bar{C}'_{\phi I J K} \phi'^K + k_2 K'_{MN} K^I_M N \right)$$ (81)
In the above expression, the definitions $C_{IJ} = C_{KL}G^{IK}G^{JL}$ and $K'_{IJ} = G^{IK}G^{JL}K'_{KL}$ are used. The second Piola stress generated from such a free energy is given by,

$$S_{IJ} = \mu G_{IJ} + \frac{1}{2}(-\mu + \lambda \log(\bar{J}))\bar{C}^{-1} + k_1 C_{IJ} \phi'_{K} \phi'_{K} \tag{82}$$

Using Eq. 48, tensors $M$ and $N$ for the assumed free energy function are given by,

$$M^{IJK} = k_1 \bar{C}_{IJ} \phi'_{K}; \quad N^{IJ} = k_2 K'^{IJ} \tag{83}$$

6 Stresses due to a point defect

We present the calculation of self stresses due to a point defect using the geometric theory considered in the preceding sections. Presently, we ignore defect evolution and focus only on the mechanical equilibrium. This description exploits the fact that the equilibrium configuration of a body with a nontrivial Weyl connection is different from that with a flat Levi-Civita connection. For a body with a hyperelastic stored energy and flat Levi-Civita connection, the identity deformation is always a critical point under zero traction and zero boundary displacement. In other words, the reference configuration (identity deformation) is a natural state. In the present approach, the identity deformation is stress-free but not the only critical point of the stored energy function: we conjecture that this critical point is unstable when the body is defective. In the presence of point defects, the connection is modified locally and the Weyl one-form encodes this information.

In the linear elasticity setting, point defects are analogous to a spherical inclusion forced into a spherical cavity of slightly different diameter. The difference in the volume of the cavity and inclusion results in stresses in the inclusion and the matrix surrounding it. The infinitesimal version of the inclusion problem introduces the notion of a dipole tensor to characterize the pre-stress caused by the point defect. This description may be referred to as Eshelby’s method of eigenstrain in the infinitesimal setting. For a recent review on modelling point defects based on the elasticity theory, see [4]. The accuracy of linear elastic predictions for point defects depends on how closely the dipole tensor represents the point defect and the dependence of the dipole tensor on the energy functional.

Different approaches have been suggested for obtaining the dipole tensor from molecular dynamic simulations of point defects. These methods use the atomistic stress, displacement or the Kansaki force to deduce the elastic dipole tensor. A main disadvantage of the linear elastic approach to point defects is that it cannot be extended to include nonlinear interactions.

We now consider a spherical body with radius one and a point defect placed at the origin. As opposed to linear elasticity, the point defect is modelled by a one-form which is localized near the origin and reaches zero asymptotically away from the origin. This description is similar to a shrink-fit problem with a diffused shrink-fit surface. A spherical coordinate system is used for the reference and deformed configurations of the body; these coordinates are denoted by $(R, \Theta, \Xi)$ and $(r, \theta, \xi)$ respectively. We adopt the stored energy function given in Eq. 79 and set the coefficient $k_1$ to zero. The Weyl one-form is assumed to be integrable. The metric tensor in the spherical coordinate system is given by,

$$G_{IJ} = \begin{bmatrix} 1 & 0 & 0 \\ 0 & R^2 \sin^2 \Xi & 0 \\ 0 & 0 & R^2 \end{bmatrix}; \quad g_{ij} = \begin{bmatrix} 1 & 0 & 0 \\ 0 & r^2 \sin^2 \xi & 0 \\ 0 & 0 & r^2 \end{bmatrix}, \tag{84}$$

We choose $f$ to be of the form,

$$f = \frac{L}{1 + \exp(-kR)} \tag{85}$$
Here, $L$ and $k$ are parameters controlling the point defect distribution. We may mention that the equation above is a choice and other choices are possible permitting us to model different kinds of point defects like extra matter and vacancy. Note that Eq. 85 depends only on the radial coordinate.

We assume that no displacement or traction conditions are applied to the body. Because of the spherical symmetry, the equilibrium configuration is also assumed to be radially symmetric. This leads to the following expressions for the deformation gradient and right Cauchy-Green deformation tensor,

$$F_i^j = \begin{bmatrix} \frac{\partial r}{\partial R} & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 1 \end{bmatrix}; \quad C_{IJ} = \begin{bmatrix} \left(\frac{\partial r}{\partial R}\right)^2 & 0 & 0 \\ 0 & r^2 & 0 \\ 0 & 0 & r^2 \end{bmatrix}. \quad (86)$$

The trace of $C$, $C^{-1}$ and the Jacobian of deformation are given by,

$$G_{IJ}C_{IJ} = \left(\frac{\partial r}{\partial R}\right)^2 + 2\left(\frac{r}{R}\right)^2; \quad G_{IJ}(C^{-1})_{IJ} = \left(\frac{\partial r}{\partial R}\right)^{-2} + 2\left(\frac{r}{R}\right)^{-2}; \quad J = \frac{\partial r}{\partial R}\left(\frac{r}{R}\right)^2. \quad (87)$$

The equilibrium configuration for the assumed Weyl connection is obtained by solving the Euler-Lagrange equation for the stored energy; these equations are nothing but the equilibrium equations given in Eq. 44. We use a finite element based numerical procedure to minimize the stored energy which is discussed in Appendix A. The radial component of the Weyl one-form and the radial displacement at equilibrium are shown in Fig. 1. Fig. 2 compares the radial and hoop stresses computed using linear elasticity as well as the present methodology. The linear elastic solutions were obtained by Teodosiu [23]. The stresses in the linear elastic case was predicted by assuming the elastic constants of the inclusion and the matrix to be same; the values of $\lambda$ and $\mu$ were assumed to be 1 and 0.3 respectively. The difference in volume between the inclusion and the cavity was taken as -0.005. The same elastic constants are assumed for our model as well. The constant $L$ and $k$ were in Eq. 85 are assumed to be 1.35 and 17.5 respectively.

The radial and hoop stress distributions for the matrix and inclusion in the linear elastic case are given by [23],

$$\sigma_r = \begin{cases} \frac{-4\mu C}{r^2}; & 0 \leq r \leq r_0 \\ \frac{-4\mu C}{r^3}\left(1 + \frac{r^3}{R_0^3}\right); & r_0 \leq r \leq R_0 \end{cases} \quad \text{and} \quad \sigma_\theta = \begin{cases} \frac{-4\mu C}{r^2}; & 0 \leq r \leq r_0 \\ \frac{2\mu C}{r^2}\left(1 + 2\frac{r^3}{R_0^3}\right); & r_0 \leq r \leq R_0 \end{cases}. \quad (88)$$

where, $r_0$ is the radius of the cavity into which the inclusion is forced, $R_0$ the radius of the sphere, $C = \frac{\nu'}{4\pi(1+\frac{\nu'}{\nu})}$ and $\nu'$ the difference in volume between the inclusion and the cavity. From Fig 2 it is seen that the radial stress predicted by the present method compares well with the linear elastic approach, even though the former produces a milder gradient. This may be owing to a diffused representation of the interface between the inclusion and the matrix. The diffused representation manifests in the hoop stress as well; the unphysical discontinuity in the hoop stress via linear elasticity is absent in our predictions. Higher hoop stresses are predicted by our method, which is essentially due to the smoothness enforced by the diffused representation of the shrink-fit interface. The diffused representation has also the important advantage that interfaces need not be tracked explicitly.
Figure 1: Radial displacement at equilibrium for the assumed one-form $df$

Figure 2: Comparisons of radial and hoop stresses computed by the present method and linear elasticity. The linear elastic solution was obtained from [23]
We now discuss a framework to calculate non-trivial configurations which are in a stress-free state in the presence of metrical defects. This problem is technologically important, since a manufacturing process may, in principle, be tuned to optimize the defect distribution such that during operation it is close to a state of zero stress. Arteries are a good example of systems which are known to optimize their stress levels by accumulating extra-matter in the form of growth. In the context of zero stress configurations, we ask if, for a given deformation, it is possible to put the body in a state of zero stress by a distribution of metrical defects. Using our thermo-mechanical theory, we obtain a condition for the one-form such that body is in a state of zero stress. Applying this condition, we compute non-trivial configurations which are in a state of zero stress for a given temperature change. For the sake of analytical tractability, we assume the body to be in a state of thermal equilibrium. The relaxation experienced by the defects to reach the equilibrium state is also ignored. For the calculations performed in this section, we adopt the constitutive rule discussed in Section 5.3.

We now deduce the constraint imposed on the one-form by the condition of zero stress; this condition is obtained by setting the second Piola stress to zero. Even though any stress measure may be utilized to obtain the zero stress condition, expressing it in terms of the second Piola stress is more convenient as the free energy is postulated in the reference configuration. For the assumed free energy, the zero stress condition is given by,

\[
\frac{\mu}{2} G^{IJ} + \frac{1}{2} (-\mu + \lambda \ln(\bar{J})) (\bar{C}^{-1})^{IJ} + k_1\bar{C}^{IJ} \phi^I \phi^J = 0.
\]  

(90)

It should be noted that defects influence the stresses only through \(\phi^I \phi^J\), which is nothing but the magnitude of the one-form given by \(G^{-1}(\phi^I, \phi^J)\). Contracting the last equation with the reference metric tensor, we arrive at the following equation relating \(\phi^I \phi^J\) and the components of the right Cauchy-Green deformation tensor,

\[
\phi^I \phi^J = \frac{k_1}{C^{IJ}G_{IJ}} \left[ \frac{3\mu}{2} + \frac{1}{2} (-\mu + \lambda \ln(\bar{J})) (\bar{C}^{-1})^{IJ} \bar{G}_{IJ} \right].
\]  

(91)

If the deformation is assumed to be known, then the equation above may be thought of as a constraint on the Weyl one-form. The equilibrium distribution of the Weyl one-form may then be arrived at based on the minimization problem for \(\phi\) given in Eq. 46 with the last equation acting as a constraint.

On the other hand, if one assumes the defect density to be given and ask if there exists a deformation which renders the body stress free, Eq. 90 becomes a condition on the deformation gradient. However, the deformation gradient computed from the Eq. 90 need not be integrable, i.e. there may not exist a deformation map whose derivative is the \(F\) computed from Eq. 90. Integrability of \(F\) is guaranteed, if the anholonomy associated with the tangent vector in the range of \(F\) vanishes. If we denote the tangent vector in the range of \(F\) by \(\{e_1, e_2, e_3\}\), then

\[
e_i = F_i^J \frac{\partial}{\partial x^J}.
\]  

(92)

We are asking for the condition under which \(e_i = \frac{\partial}{\partial x^i}\) for some coordinates \(x^i\). The anholonomy associated with the vector fields \(e_i\) is given by,

\[
[e_i, e_j] = A_{ij} e_k
\]  

(93)
[...] denotes the Lie bracket between the vector fields. If all the Lie brackets vanish, then one can find a coordinate system such that the each vector of the frame field can be described as a tangent to some coordinate line. In terms of the deformation gradient, the components of anholonomy may be found as,

\[ A_{ij}^k = \left( F_i^j \frac{\partial F_k^i}{\partial X^j} - F_j^i \frac{\partial F_k^i}{\partial X^j} \right). \]  

The condition for integrability of \( F \) may now be written as,

\[ A_{ij}^k = 0 \]  

For multiply connected bodies, additional conditions are required depending on the multi-connectedness of the domain. For the integrability of the deformation gradient in such a domain, see [27]. In the following, we explore simple distributions of defects which keep the body in a stress free state.

7.1 Stress free configuration under temperature change

We specialize the zero stress equations obtained in the previous sub-section to incompatible strains caused by temperature change. Assuming the temperature field to be given, the variable of Weyl transformation is determined using Eq. 24. It is well established that not all temperature distributions can be made stress-free by applying deformation [3]. The necessary condition for a body with temperature change to be stress free is Eq. 90 with the one-form given by \( \phi = ds \).

Substituting the condition above into Eq. 90 leads to,

\[ \frac{\mu}{2} G_{IJ} + \frac{1}{2} \left( -\mu + \lambda \log(\bar{J}) \right)(\bar{C}^{-1})^{IJ} + k_1 \bar{C}^{IJ} G^{KL} s_L s_K = 0. \]  

The last equation is an implicit relation for the deformation gradient. In addition, the integrability of \( F \) discussed in Eq. 95 also needs to be imposed.

Now, we compute the deformed shape of the body with a constant temperature field imposed, i.e. \( s \) is a constant in Eq. 90. Assuming a Cartesian coordinate system for the reference and deformed configurations, the metric tensors in these configurations may be written as \( \delta_{ij} \) and \( e^s \delta_{ij} \) respectively. From Eq. 96, we arrive at the following relation for the deformation gradient,

\[ F^T F = \frac{1}{\mu e^{2s}} \left( \mu - \frac{3}{2} \lambda s - \lambda \log(\det(F)) \right) I. \]  

We assume a solution of the form \( F = c \Lambda, \Lambda \in SO(3) \) and \( c \in \mathbb{R} \). Substituting these in Eq. 90 we arrive at the following equation for \( c \),

\[ c^2 = \frac{1}{\mu e^{2s}} \left( \mu - \frac{3}{2} \lambda s - 3\lambda \log c \right) \]  

The SO(3) part is irrelevant since we are looking at a body with no displacement and traction conditions applied. If we set \( s = 0 \) in the above equation, it reduces to \( c^2 + \frac{3}{\mu} \lambda \log c = 1 \). The solution to this equation is \( c = 1 \). This solution recovers the reference configuration of the body.

Non-trivial stress-free configurations for different values of \( s \) may be computed through a numerical root finding technique, applied to Eq. 98. The values of \( c \) computed for different values \( s \) are shown in Fig. 3. The curve shown in Fig. 3 is slightly nonlinear; this is because of the nonlinear constitutive rule assumed for stress. Having computed the deformation gradient, one needs to establish that \( F \) is compatible. For the present scenario, compatibility is not an issue as the
The deformation gradient is constant. The above calculation also establishes the classical result that, for an isotropic body subjected to constant temperature field and free-free boundary conditions, the deformation is volumetric and without stress. The constitutive relation for stress also plays a major role in determining stress free configurations. It may so happen that certain constitutive rules would not permit any solution for a stress free configuration and constructing such constitutive rules should be an interesting exercise. The role played by constitutive inequalities is also worth exploration.

8 Conclusion

We have reported a geometric theory for thermo-mechanical deformation of bodies with metrical defects. We have exploited the geometric setting initially proposed by Weyl in the context of general relativity to represent bodies with metrical defects. These defects are identified with the incompatibility of the connection and the metric. Our proposal on the thermo-mechanics of defect-mediated deformation has completely dispensed with the notion of an intermediate configuration. The defect equilibrium, described by the Weyl one-form, is obtained as a critical point of the free energy. The Weyl transformation is used to model the interaction of incompatibilities introduced by temperature change. To include dissipation in the defect evolution, we introduced a viscous term in the defect equilibrium equation, which made the evolution of one-form a gradient flow. Using the laws of thermodynamics, restrictions have been obtained on the constitutive rules. The important problem of relating stress and strains in a non-Euclidean setting is resolved via the Doyle-Ericksen formula.

We have applied our theory to a diffused version of the shrink-fit problem which represents point defects. With the equilibrium configurations computed using a minimization procedure, we have shown that the shifted critical point of the stored energy in the presence of a Weyl connection results in residual stresses. This solution could also recover aspects of the linear elastic shrink-fit problem. Other than mathematical expedience, a diffused representation is also practically meaningful, say in the context of additive manufacturing processes that materials in the form of thin layers. In addition, we have derived conditions for a defective body to be in a state of zero stress. Using this condition, we have been able to recover zero stress configurations resulting from simple temperature distribution. Also recovered in the process are the well known linear elastic
results, albeit in a nonlinear setting.

We have focused mostly on the geometric aspects in the model and addressed only a few simple boundary value problems. We have left unaddressed the characterization of the Weyl one-form to a particular kind of point defect. This characterization can be done using molecular dynamic calculations or from density function theory calculations. Such characterizations do exist for the dipole tensor used in the linear elastic case. A more interesting problem would be to study the interaction of dislocations and point defects within a similarly geometric framework. This would require the connection to have torsion. The numerical solution procedure presently adopted is somewhat simplistic and does not respect all the geometric features of the model. Geometrically motivated discretization schemes based on finite element exterior calculus might be a very good approach to arrive at efficient and accurate numerical solution schemes.

A Numerical solution procedure

This section discusses the numerical procedure used to obtain the solution of the minimization problem discussed in Section 6. We formulate the (mechanical) equilibrium of a body with a point defect as a minimization problem over a Weyl manifold, with the Weyl connection specified. As discussed earlier, the connection on the manifold modifies the critical points of the stored energy function. These configurations are computed using a finite element based discretization procedure. Since we are looking at a radially symmetric problem, only the radial displacement is discretized using a three noded quadratic Lagrange finite element. The minima of the discretized stored energy function is computed using Newton’s method which requires the first and the second derivatives of the discrete stored energy. The first derivative of the stored energy is often called the residual force, we denote it by \( R \). The condition \( R = 0 \) represent the equilibrium of forces at the node. The discrete equilibrium is analogous to the linear momentum equation given in Eq. [44]. Since the body has non-trivial connection, we use following equation to compute an incremental change in the deformation.

\[
F^a_A = H^a_A + \left( \langle \gamma^{a}_{bc} H^b_A u^c + \frac{\partial u^a}{\partial X^A} \right)
\]

(99)

In the above equation, \( u \) is an incremental displacement field superimposed on an deformation \( \varphi_0 \) with deformation gradient \( H \) and \( \gamma^{a}_{jk} \) are the connection coefficients of the deformed configuration. The second term in Eq. [99] accounts for non-trivial connection associated with the configuration \( \varphi_0 \), the proof of the above equation can be found in [15]. The components of the connections in spherical coordinate system is given as,

\[
\gamma^r = \begin{bmatrix} -\frac{1}{r} \partial_r f & \frac{1}{r} \partial_\theta f & \frac{1}{r} \partial_\xi f \\ -\frac{1}{r} \partial_\theta f & -r \sin \xi & 0 \\ -\frac{1}{r} \partial_\xi f & 0 & -r \end{bmatrix}; \gamma^\theta = \begin{bmatrix} 0 & \frac{1}{r} - \frac{1}{2} \partial_r f & \frac{1}{r} \partial_\theta f \\ 0 & -\frac{1}{2} \partial_\theta f & \cot \xi - \frac{1}{2} \partial_\xi f \\ 0 & 0 & 0 \end{bmatrix};
\]

\[
\gamma^\xi = \begin{bmatrix} -\frac{1}{r} \partial_r f & -r \cos \xi & \frac{1}{r} - \frac{1}{2} \partial_r f \\ -\frac{1}{r} \partial_\theta f & 0 & -\frac{1}{2} \partial_\theta f \\ \frac{1}{r} \partial_\xi f & 0 & 0 \end{bmatrix}
\]

(100)

The residual force can then be computed using the relation,

\[
R = \frac{d}{dc_{\epsilon=0}} W(\epsilon)
\]

(101)

Where, \( W(\epsilon) \) denotes the perturbed stored energy about the configuration \( \varphi_0 \), which is obtained using the relation \( \varphi_0 + \epsilon u \), here \( \epsilon \) is a small parameter. The perturbed deformation gradient is
obtained using the relation Eq. (99). The finite element approximation for the incremental radial displacement \( u_r \) is denoted by \( u^h_r \) and it is given by,

\[
\sum_{i=1}^{i=N} N_i u^i_r
\]

In the above equation \( u^i_r \) and \( N_i \) denotes the incremental radial displacement and shape function at the \( i^{th} \) node. The incremental radial displacement and the nodal shape function at all nodes are denoted by \( u^h \) and \( \Upsilon \) respectively. In terms of the nodal displacement and stored energy function, the condition for discrete mechanical equilibrium can be written as,

\[
\frac{\partial W}{\partial u^h} = 0
\]

The above equation is nothing but the necessary condition of an extrema for a finite dimensional extremization problem. For the assumed stored energy function, the discrete equilibrium equation is given by,

\[
\frac{\mu}{2} \frac{\partial I_1}{\partial u^h} + \frac{1}{J}(\lambda \log(J) - \mu) \frac{\partial J}{\partial u^h} = 0
\]

The variables \( \frac{\partial I_1}{\partial u^h} \) and \( \frac{\partial J}{\partial u^h} \) denotes the directional derivatives computed using the perturbation given in Eq. (99) whose expressions are given as,

\[
\frac{\partial I_1}{\partial u} = 2 \left( \frac{dr}{dR} - \frac{u_r dr}{dR} + \frac{du}{dR} \right) \left( -\frac{1}{2} \frac{df}{dR} \frac{dr}{dR} + \frac{df}{dR} \right) \left( 1 + u_r \left( \frac{1}{r} - \frac{1}{2} \frac{df}{dR} \right) \right) \left( \frac{1}{r} - \frac{1}{2} \frac{df}{dR} \right) \Upsilon \]

\[
\frac{\partial J}{\partial u} = \left( 1 + u_r \left( \frac{1}{r} - \frac{1}{2} \frac{df}{dR} \right) \right)^2 \left( -\frac{1}{2} \frac{df}{dR} \frac{dr}{dR} + \frac{df}{dR} \right) \left( \frac{1}{r} \right)^2 \left( 1 + u_r \left( \frac{1}{r} - \frac{1}{2} \frac{df}{dR} \right) \right)
\]

\[
\left( \frac{dr}{dR} - \frac{u_r dr}{dR} + \frac{du}{dR} \right) \left( \frac{1}{r} - \frac{1}{2} \frac{df}{dR} \right) \left( \frac{1}{r} \right)^2 \Upsilon
\]

In the above equation, \( u_r \) denotes the displacement computed from the last iteration and \( r \) denotes the last converged radius and \( \frac{df}{dR} \) denotes the derivative of the nodal basis with respect to the radial co-ordinates. The Hessian (tangent stiffness matrix) required for Newtons’ method for the assumed stored energy function is given by,

\[
\frac{\partial^2 W}{\partial u \partial u} = \frac{\mu}{2} \frac{\partial^2 I_1}{\partial u \partial u} + \frac{1}{J^2}(\lambda + \mu - \lambda \log J) \frac{\partial J}{\partial u} \otimes \frac{\partial J}{\partial u}
\]

The second derivatives of \( I_1 \) and \( J \) are computed as,

\[
\frac{\partial I_1}{\partial u \partial u} = 2 \left( \frac{dr}{dR} - \frac{u_r dr}{dR} + \frac{du}{dR} \right) \left( -\frac{1}{2} \frac{df}{dR} \frac{dr}{dR} + \frac{df}{dR} \right) \left( \frac{1}{r} - \frac{1}{2} \frac{df}{dR} \right) \left( \frac{1}{r} \right)^2 \Upsilon \otimes \Upsilon
\]

\[
\frac{\partial J}{\partial u \partial u} = 2 \left( 1 + u_r \left( \frac{1}{r} - \frac{1}{2} \frac{df}{dR} \right) \right) \left( \frac{1}{r} - \frac{1}{2} \frac{df}{dR} \right) \left( \Upsilon \otimes \left( \frac{1}{r} - \frac{1}{2} \frac{df}{dR} \right) \frac{dr}{dR} + \frac{df}{dR} \right) + \left( \frac{1}{r} - \frac{1}{2} \frac{df}{dR} \right) \left( \frac{dr}{dR} \right)^2 \Upsilon \otimes \Upsilon
\]
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