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Authors

Govindjee, Sanjay
Zoller, Miklos J
Hackl, Klaus

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A fully-relaxed variationally-consistent framework for inelastic micro-sphere models: Finite viscoelasticity

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Sanjay Govindjee^{a,*}, Miklos J. Zoller^a, Klaus Hackl^b

^a*Structural Engineering, Mechanics, and Materials; Department of Civil and Environmental Engineering; University of California, Berkeley; Berkeley CA 94720-1710, USA*

^b*Lehrstuhl für Allgemeine Mechanik; Ruhr-Universität Bochum; D-44801 Bochum, Germany*

Abstract

The micro-sphere modeling framework provides a popular means by which one-dimensional mechanical models can easily and quickly be generalized into three-dimensional stress-strain models. The essential notion of the framework, similar to homogenization theory, is that one allows the microstructural kinematic fields to relax subject to a constraint connected to a macroscopic deformation measure. In its standard presentation, the micro-sphere modeling framework is strictly applicable to elastic materials. Presentations considering inelastic phenomena invariably, and inconsistently, assume an affine relation between inelastic macroscopic and microscopic phenomena. In this work we present a methodology by which one can lift this modeling restriction using two formally different approaches. In particular, we show how one can construct and apply a homogenization with Biot theory to generate fully-relaxed variationally-consistent macroscopic models for inelastic materials within the context of the micro-sphere model. The primary application example will be finite deformation viscoelasticity.

Keywords: micro-sphere, finite deformation viscoelasticity

1. Introduction

The development of material models of polymeric materials, elastomers in particular, generally follows either a phenomenological track or a micromechanical one. Common successful phenomenological models include, for example, the two-parameter model of Mooney (1940), Rivlin (1948), and Rivlin and Saunders (1951), the principal stretch model of Ogden (1972, 1984), or the multi-parameter model of Yeoh (1993). While successful, these models lack a direct

*Corresponding author.

Email addresses: s_g@berkeley.edu (Sanjay Govindjee), zollermi@berkeley.edu (Miklos J. Zoller), klaus.hackl@rub.de (Klaus Hackl)

connection to the microstructural origins of the mechanical response. Models that attempt to address this issue include the famous 3-, 4-, and 8-chain models proposed, respectively, by James and Guth (1943), Flory and Rehner (1943), and Arruda and Boyce (1993). This category of models also includes the full network models of Treloar and Riding (1979) and Wu and van der Giessen (1993); see also Puso (1994) for a review of these models.

Underlying these latter micromechanical models is a statistical mechanics model for the force-extension relation for a single polymer chain and an imaginative idealization of the topology of the cross-linked polymer network. These models also employ an affine kinematic assumption, the exception being the 4-chain model of Flory and Rehner (1943) which allows the central tetrahedral junction to take up an energetically relaxed position. The remainder of the models, the affine ones, are essentially homogenization models of a particular network arrangement employing a Taylor (1938)-like kinematic condition (see also Zienkiewicz et al., 2014, Chap. 7) – all the network junctions move affinely with respect to the macroscopic deformation (gradient).

Similar to the full network models is the *micro-plane* model of Bažant and Gambarova (1984) that was developed for the modeling of the fracture of brittle materials; see also Bažant and Oh (1985) and Carol et al. (2004) among other papers from the same group. The micro-plane model starts with a one-dimensional model (inelastic) and then proposes a virtual work equivalence between macroscopic and microscopic virtual work on a spherical representation of the material microstructure. To close the model, an affine kinematic assumption is made between the macroscopic deformation measure and the microstructural deformation measures. The framework of the micro-plane models is one that is clearly connected to the notions of homogenization in the spirit of Hill (1972) and others, but omitting gradient fields due to the point nature of the representative volume element in the micro-plane model.

The *micro-sphere* model by Miehe et al. (2004) improved on these earlier works by recognizing that the full network models were in fact like homogenization models, and it was not necessary to impose an affine assumption on the microstructural kinematics. Rather it was possible to allow the stretch in each direction on the micro-sphere to energetically relax, subject to a macroscopic constraint that keeps the p-root average of the local micro-sphere stretches equal to the p-root average of the affine stretches over the micro-sphere. Strikingly, Miehe et al. (2004) were able to show that this minimization problem had a closed-form solution for single chain models with arbitrary complexity. The micro-sphere modeling framework has been widely used in many contexts. In particular, researchers have extended its use to the case where the underlying chain model is no longer elastic; see e.g. Miehe and Göktepe (2005); Dal and Kaliske (2009); Mistry and Govindjee (2014); Guilié et al. (2015) among others. In these extensions, researchers have chosen not to follow the fully variational setting developed by Miehe et al. (2004) when treating the inelastic phenomena, instead they have chosen to connect the macroscopic and microscopic inelastic evolution affinely, with the partial exception of Rastak and Linder (2018). It is the goal of this paper to show how to lift this restriction and arrive at a model

which includes micromechanical evolution that generates variationally relaxed macroscopic evolution of the inelastic phenomena. To keep the presentation compact, we will restrict ourselves to the case of viscoelasticity.

Similar to the viscoelastic extension by Miehe and Göktepe (2005) we will utilize the dissipation potential concept of Biot (1955). In this context we present two model frameworks. Model Framework 1 performs a relaxation as done in the original micro-sphere model and then uses a non-affine evolution equation at the microscopic scale to determine the inelastic evolution of the system based on Biot’s principle. This framework does not require the introduction of macroscopic internal variable fields but does result in a model that naturally appears to require that the internal state of the material be represented by a field on the micro-sphere. In Model Framework 2, we present a re-writing of the relations from Framework 1 that highlights an interesting macroscopic dissipation structure that is fully compatible with the microscopic dissipation potentials at the “chain-level”. The outlined relations are in direct analogy to how macroscopic free energies are constructed from microscopic ones. Thus this second model framework aims to highlight an embedded structure in the non-affine homogenization scheme for the determination of the macroscopic free energy in the presence of internal evolutionary phenomena. Viscoelastic behavior will be incorporated through a proposed extension of the variational framework of Biot (1955) and an additional relaxation process involving macroscopic internal variables. Model Framework 2 introduces a number of observed relations but produces a model which is provably identical to the one generated by Model Framework 1 — as it is fully derivable from Model Framework 1 under certain macro-micro kinematic assumptions. Ultimately, both these frameworks permits the modeling of a wide variety of inelastic polymer behaviors. Following the micro-sphere developments of Tkachuk and Linder (2012) and the micro-plane developments, by for example, Carol et al. (2004), we will additionally utilize tensorial constraints for the micro-sphere relaxation. In the examples, we will do this using the Hencky strain measure as well as the deformation gradient.

2. Preliminaries

We consider deformable continuum bodies with a deformation χ that maps reference points $\mathbf{X}$ to current locations $\mathbf{x} = \chi(\mathbf{X})$. The deformation gradient will be denoted $\mathbf{F} = \partial \mathbf{x} / \partial \mathbf{X}$, the right Cauchy-Green deformation tensor $\mathbf{C} = \mathbf{F}^T \mathbf{F} = \mathbf{U}^2$, where $\mathbf{U}$ is the right stretch tensor computed from the polar decomposition of $\mathbf{F}$; see e.g. Ogden (1984) or Gurtin (1981). Additionally, since $\mathbf{C}$ is symmetric and positive definite, by the spectral decomposition theorem:

$$\mathbf{C} = \mathbf{U}^2 = \sum_{i=1}^3 \lambda_i^2 \mathbf{N}_i \otimes \mathbf{N}_i,$$

and

$$\mathbf{U} = \sum_{i=1}^3 \lambda_i \mathbf{N}_i \otimes \mathbf{N}_i,$$

where λ_i and $\mathbf{N}_i$ are the principal stretches and directions, respectively. The Hencky strain (see Hencky, 1928) can then be expressed as

$$\ln(\mathbf{U}) = \sum_{i=1}^3 \ln(\lambda_i) \mathbf{N}_i \otimes \mathbf{N}_i.$$

We further define the volume preserving parts of $\mathbf{F}$ and $\mathbf{C}$, where $J = \det(\mathbf{F})$, by

$$\begin{aligned} \bar{\mathbf{F}} &= J^{-1/3} \mathbf{F}, \\ \bar{\mathbf{C}} &= \bar{\mathbf{F}}^T \bar{\mathbf{F}} = J^{-2/3} \mathbf{C}. \end{aligned}$$

For one of the viscoelastic models developed below we will additionally adopt the Sidoroff (1974) multiplicative decomposition of the deformation gradient into elastic and inelastic parts:

$$\mathbf{F} = \mathbf{F}^E \mathbf{F}^V;$$

see also Le Tallec and Rahier (1994); Reese and Govindjee (1998).

3. Fully variational microsphere for viscoelastic materials

This section will focus on generalizing the minimization technique of the micro-sphere model with tensorial constraints. The core of the model is a minimization on micro-scale kinematic variables subject to a constraint enforcing that the continuum deformation is equal to the directional integral average of the microscopic deformation, in other words, that the microscopic kinematics are compatible with macroscopic kinematics. Additionally, Biot's principle will be utilized to determine the evolution law of the system via two types of dissipation potentials. This approach allows for extension to other evolutionary microstructural phenomena but this will not be the topic of this work.

The micro-sphere model proposed by Miehe et al. (2004) and Miehe and Göktepe (2005) postulates that the topology of the polymer network can be characterized by a micro-sphere. The micro-sphere is composed of a distribution of polymer chains that all connect to the center of the micro-sphere and whose other ends are distributed on the surface of the sphere, S . More generally one can think of tubes of material connecting the center to the surface of the sphere. To each point on the sphere we will define the outward unit normal to be $\mathbf{n}$, this gives the orientation of the individual chains/tubes of material. The 3-, 4-, 8-chain, and full network models are included in this framework by assuming either a distribution function composed of 3-, 4-, or 8-Dirac masses or as a uniform ($1/|S| \equiv 1/4\pi$) distribution.

To each point on the sphere we postulate a micro-scale tensorial deformation measure that depends on micro-scale kinematic fields on the surface of the sphere. Example micro-scale kinematic fields that can be used to build such tensor fields would include, for example, the local stretch (Miehe et al., 2004) and the local transverse tube strain for each orientation (Edwards and Vilgis, 1988). The micro-scale kinematic fields need not be scalar (Tkachuk and Linder, 2012). To be more concrete, we assume that for each orientation $\mathbf{n}$ there is an associated tensorial micro-scale deformation measure $\mathbf{E}_m$ that depends on these micro-scale kinematic fields. The subscript m will be used to denote micro-scale variables; corresponding macroscopic quantities, $\mathbf{E}$, will not have the subscript. It is emphasized that $\mathbf{E}$ is an arbitrary model dependent deformation/strain measure. Furthermore, we will denote by α_i the elastic micro-scale fields on the sphere. To account for inelastic processes, we will introduce a different set of micro-scale fields β_j over the sphere. In Model Framework 2 there will be the need for an additional viscous measure $\mathbf{E}_m^V$ (dependent on the β_j) to model time dependent relaxation phenomena – along with its macroscopic counter part.

3.1. The elastic case

As a specialization, and to fix ideas in the simplest possible case, we will briefly review the elastic micro-sphere case in the setting just described. For concreteness let us define the micro-scale “right-stretch tensor” as

$$\mathbf{U}_m(\lambda, \nu) = \lambda \mathbf{n} \otimes \mathbf{n} + \nu (\mathbf{1} - \mathbf{n} \otimes \mathbf{n}),$$

where λ and ν are the local stretch and tube contraction of the material oriented at $\mathbf{n}$. This is the primary kinematic assumption on the local deformation. We further introduce the micro-scale Hencky strain as

$$\ln \mathbf{U}_m = \frac{1}{3} \ln j \mathbf{1} + 3 \ln \xi \left(\mathbf{n} \otimes \mathbf{n} - \frac{1}{3} \mathbf{1} \right),$$

where the micro-jacobian $j = \lambda \nu^2$ and the micro-deviatoric stretch $\xi = \sqrt[3]{\lambda/\nu}$. In the general notation $\ln \mathbf{U}_m$ corresponds to $\mathbf{E}_m$, and $\ln j$ and $\ln \xi$ correspond to α_1 and α_2 .

The second ingredient of the micro-sphere model is a micro-scale description of the free energy of the material oriented in the direction $\mathbf{n}$ in terms of the micro-scale kinematic fields. In the present case, this could be an additively split function

$$\psi_m(\ln j, \ln \xi) = \psi_m^{\text{vol}}(\ln j) + \psi_m^{\text{dev}}(\ln \xi),$$

though other choices are certainly possible. Note, however, that the choices are not fully arbitrary. In particular, Carol et al. (2004) have shown for the micro-plane model that certain choices lead to restrictions on material response that do not comport with usual expectations – such as materials with only negative Poisson’s ratios or fixed Poisson’s ratios (in the small strain limit). These issues also hold true for the micro-sphere model, but the choice given above does not suffer from these defects.

For the present choices, the macroscopic free energy density is then postulated to be given by the energetic relaxation

$$\Psi(\ln \mathbf{U}) = \inf_{\ln j, \ln \xi} \left\{ \frac{1}{|S|} \int_S \psi_m(\ln j, \ln \xi) dS \right\}, \quad (1)$$

subject to the kinematic constraint (micro-macro compatibility relation)

$$\ln \mathbf{U} = \frac{1}{|S|} \int_S \ln \mathbf{U}_m dS. \quad (2)$$

The minimization in (1) subject to (2) can be carried out to generate an elastic stress-strain model, where the Lagrange multiplier used to enforce the constraint is the conjugate stress to $\ln \mathbf{U}$; we leave out the details to avoid duplication later. In general the resulting model requires quadrature over the sphere – a point that we will also discuss later. Depending on the choices for the micro-energy densities explicit or implicit models may be obtained. Written in this way, the micro-sphere model is clearly seen to be a type of homogenization model, albeit one that can be computed without having to consider gradient constraints as appear in typical representative volume element homogenization problems.

3.2. The viscoelastic case: General structure Model Framework 1

We now return to the general viscoelastic case where in addition to $\mathbf{E}_m$ and α_i ($i = 1, \dots, n_\alpha$), we also have micro-scale viscous fields β_j ($j = 1, \dots, n_\beta$) on the sphere. As with the elastic case, we will require

$$\mathbf{E} = \frac{1}{|S|} \int_S \mathbf{E}_m(\alpha_i) dS. \quad (3)$$

Here and throughout we always assume that the macro-scale deformation measures are computed as (linear) projections of the micro-scale deformation measures; further we will restrict attention to the case where the micro-scale deformation measure is linear in the micro-scale fields. The macroscopic free energy is constructed through the relaxation of the micro-scale fields α_i in terms of an energy function ψ_m defined for each spatial direction over the micro-sphere (and dependent on α_i as well as β_j):

$$\Psi = \inf_{\alpha_i} \left\{ \frac{1}{|S|} \int_S \psi_m(\alpha_i, \beta_j) dS \right\} \quad (4)$$

subject to (3). Note that Ψ will be a function of $\mathbf{E}$ and a functional of the fields β_j .

We solve this optimization problem using a Lagrange multiplier $\boldsymbol{\tau}$ via the Lagrangian

$$\mathcal{L}(\alpha_i, \beta_j, \boldsymbol{\tau}) = \frac{1}{|S|} \int_S \psi_m(\alpha_i, \beta_j) dS + \boldsymbol{\tau} : \left[\mathbf{E} - \frac{1}{|S|} \int_S \mathbf{E}_m(\alpha_i) dS \right].$$

The stationary conditions for this Lagrangian yield:

$$\delta_{\alpha_i} \mathcal{L} = \frac{1}{|S|} \int_S \left(\frac{\partial \psi_m}{\partial \alpha_i} - \boldsymbol{\tau} : \frac{\partial \mathbf{E}_m}{\partial \alpha_i} \right) \delta \alpha_i dS = 0, \quad (5)$$

$$\delta_{\boldsymbol{\tau}} \mathcal{L} = \delta \boldsymbol{\tau} : \left[\mathbf{E} - \frac{1}{|S|} \int_S \mathbf{E}_m(\alpha_i) dS \right] = 0. \quad (6)$$

Thus, the Euler-Lagrange equations are:

$$\left(\frac{\partial \psi_m}{\partial \alpha_i} - \boldsymbol{\tau} : \frac{\partial \mathbf{E}_m}{\partial \alpha_i} \right) = 0, \quad (7)$$

along with the macroscopic residual equation enforcing the micro-macro kinematic relation:

$$\left[\mathbf{E} - \frac{1}{|S|} \int_S \mathbf{E}_m(\alpha_i) dS \right] = 0. \quad (8)$$

In general, the free energy ψ_m couples the variables α_i and β_j in a nonlinear way, requiring equations (7) be solved via an iterative method. When done so, the fields α_i are given in terms of the β_j and the macro-scale Lagrange multiplier $\boldsymbol{\tau}$, which is straightforwardly shown to be the macroscopic stress conjugate to $\mathbf{E}$; viz. $\boldsymbol{\tau} = \partial \Psi / \partial \mathbf{E}$ (see Appendix A). When the solution field for α_i is inserted into (8), one obtains the micro-sphere's macroscopic stress-strain model (strain in terms of stress). Not specified yet is a means for determining the evolution of the viscous fields β_j .

To proceed further, following Miehe and Göktepe (2005), we postulate the existence of a micro-scale dissipation potential $\Delta_m(\beta_j, \dot{\beta}_j)$ in the sense of Biot (1955) such that the inelastic micro-field evolution is governed by the minimization problem:

$$\inf_{\dot{\beta}_j} \left[\dot{\psi}_m + \Delta_m \right]. \quad (9)$$

In this framework, satisfaction of second law requirements is relatively easy. For example, all functions Δ_m that are non-negative homogenous of degree n in the second argument will work. Note that for economy of presentation, we will assume henceforth that Δ_m is only a function of $\dot{\beta}_j$.

The resulting optimality relations from (9) are given by

$$\frac{\partial \psi_m}{\partial \beta_j} + \frac{\partial \Delta_m}{\partial \dot{\beta}_j} = 0, \quad (10)$$

which furnish a closure for Model Framework 1 without the introduction of any affine assumptions. In particular (7), (8), and (10) allow for the computation of the stress (or strain) history, given the strain (or stress history). The process is mediated by the relaxed micro-fields α_i and non-affine viscous micro-fields β_j .

3.3. Time incremental form

Due to the complexity of the system of constitutive equations, they, like most inelastic models, are often evaluated in a time incremental fashion. The time incremental equations can be derived from the above where time derivatives are replaced by difference approximations. This methodology follows closely the ideas pioneered by Honein and Simo (1990); Simo and Govindjee (1991); Ortiz and Stainier (1999); Ortiz et al. (2000); Carstensen et al. (2002) (and references therein) and analyzed by Mielke (2004). In what follows, we will use subscripts n and $n + 1$ to denote quantities evaluated at times t_n and $t_{n+1} = t_n + h$, where $h > 0$ denotes the time step. In this setting, all quantities at time t_n are assumed known, as is $\mathbf{E}_{n+1}$.

Following this approach, (9) is replaced by

$$\inf_{\beta_{j,n+1}} \left[\psi_m(\alpha_{i,n+1}, \beta_{j,n+1}) - \psi_m(\alpha_{i,n}, \beta_{j,n}) + h \cdot \Delta_m \left(\frac{\beta_{j,n+1} - \beta_{j,n}}{h} \right) \right].$$

This allows one to determine $\beta_{j,n+1}$ in terms of $\alpha_{i,n+1}$ and the history $\beta_{j,n}$. Insertion into (7) determines $\alpha_{i,n+1}$ in terms of the history and $\boldsymbol{\tau}$. Consequently substitution into (8) gives the *inelastic* relation between $\boldsymbol{\tau}$ and $\mathbf{E}$. This comes about without any need for recourse to additive or multiplicative splits of the macroscopic measures into elastic and viscous parts. Despite the simplicity of Model Framework 1, it should be noted that it appears to rely upon a set of internal variable *fields* β_j that must be carried by the model at each material point.

3.4. The viscoelastic case: General structure Model Framework 2

Model Framework 1 provides a complete variationally consistent model for inelastic micro-sphere behavior. In this section we present a second model framework that results in the same final model equations, but provides a scheme by which macroscopic inelastic kinematic measures may be introduced and in which a macroscopic inelastic stress tensor appears. As the final equations are identical, Model Framework 2 does not involve new mechanics, rather it presents an alternate vantage point from which to reason about the proposed model and highlights an alternate algorithmic possibility.

In addition to the macro-micro kinematic relation (3) between $\mathbf{E}$ and $\mathbf{E}_m(\alpha_i)$, in Model Framework 2 we also allow for the introduction of a macroscopic kinematic measure of the viscous response $\mathbf{E}^V$ that is the directional/surface average of a new microscopic kinematic viscous measure $\mathbf{E}_m^V$ (assumed linearly) dependent on β_j ($j = 1, \dots, n_\beta$):

$$\mathbf{E}^V = \frac{1}{|S|} \int_S \mathbf{E}_m^V(\beta_j) dS. \quad (11)$$

With these relations between the micro and macro kinematic measures, the macroscopic free energy is constructed through the relaxation of the micro-scale fields α_i and β_j in terms of the energy function ψ_m ,

$$\Psi = \inf_{\alpha_i, \beta_j} \left\{ \frac{1}{|S|} \int_S \psi_m(\alpha_i, \beta_j) dS \right\} \quad (12)$$

subject to (3) and (11).

We solve this optimization problem using two Lagrange multipliers $\boldsymbol{\tau}$ and $\boldsymbol{\tau}^V$ via the Lagrangian

$$\begin{aligned}\mathcal{L}(\alpha_i, \beta_j, \boldsymbol{\tau}, \boldsymbol{\tau}^V) &= \frac{1}{|S|} \int_S \psi_m(\alpha_i, \beta_j) dS \\ &+ \boldsymbol{\tau} : \left[\mathbf{E} - \frac{1}{|S|} \int_S \mathbf{E}_m(\alpha_i) dS \right] \\ &+ \boldsymbol{\tau}^V : \left[\mathbf{E}^V - \frac{1}{|S|} \int_S \mathbf{E}_m^V(\beta_j) dS \right].\end{aligned}$$

In addition to the residual (8) and the Euler-Lagrange equation (7), in this setting we also find:

$$\left(\frac{\partial \psi_m}{\partial \beta_j} - \boldsymbol{\tau}^V : \frac{\partial \mathbf{E}_m^V}{\partial \beta_j} \right) = 0, \quad (13)$$

along with the macroscopic residual equation:

$$\left[\mathbf{E}^V - \frac{1}{|S|} \int_S \mathbf{E}_m^V(\beta_j) dS \right] = 0. \quad (14)$$

In general, the free energy ψ_m couples the variables α_i and β_j in a nonlinear way, requiring equations (7) and (13) be solved via an iterative method. When done so, the fields α_i and β_j are given in terms of the macro-scale Lagrange multipliers $\boldsymbol{\tau}$ and $\boldsymbol{\tau}^V$, which are straightforwardly shown to be the macroscopic stresses conjugate to $\mathbf{E}$ and $\mathbf{E}^V$; viz. $\boldsymbol{\tau} = \partial \Psi / \partial \mathbf{E}$ and $\boldsymbol{\tau}^V = \partial \Psi / \partial \mathbf{E}^V$ (see Appendix A). When the solution fields for α_i and β_j are inserted into (8) and (14), one obtains the micro-sphere's macroscopic stress-strain model (strain in terms of stress).

Model Framework 2 proceeds by noting that one can construct a macroscopic dissipation potential Δ from an additional relaxation process on the microscopic dissipation potential Δ_m in terms of the rate of the viscous internal variables $\dot{\beta}_j$:

$$\Delta = \inf_{\dot{\beta}_j} \left\{ \frac{1}{|S|} \int_S \Delta_m(\dot{\beta}_j) dS \right\}, \quad (15)$$

subject to the time derivative of constraint (11):

$$\dot{\mathbf{E}}^V = \frac{1}{|S|} \int_S \overline{\dot{\mathbf{E}}_m^V(\beta_j)} dS. \quad (16)$$

Note that our assumption that $\mathbf{E}_m^V$ depends linearly on β_j is crucial for the optimization of (15) subject to (16) to be sensible, as $\dot{\beta}_j$ is merely a formal parameter in (15) and (16).

To determine the macroscopic dissipation potential, one can employ a third Lagrange multiplier $\boldsymbol{\tau}^d$ to enforce equation (16):

$$\begin{aligned}\mathcal{L}(\dot{\beta}_j, \boldsymbol{\tau}^d) &= \frac{1}{|S|} \int_S \Delta_m(\dot{\beta}_j) dS \\ &+ \boldsymbol{\tau}^d : \left[\dot{\mathbf{E}}^V - \frac{1}{|S|} \int_S \overline{\mathbf{E}_m^V(\beta_j)} dS \right].\end{aligned}$$

The resulting variational equations yield:

$$\delta_{\dot{\beta}_j} \mathcal{L} = \frac{1}{|S|} \int_S \left(\frac{\partial \Delta_m}{\partial \dot{\beta}_j} - \boldsymbol{\tau}^d : \frac{\partial \overline{\mathbf{E}_m^V(\beta_j)}}{\partial \dot{\beta}_j} \right) \delta \dot{\beta}_j dS = 0, \quad (17)$$

$$\delta_{\boldsymbol{\tau}^d} \mathcal{L} = \delta \boldsymbol{\tau}^d : \left[\dot{\mathbf{E}}^V - \frac{1}{|S|} \int_S \overline{\mathbf{E}_m^V(\beta_j)} dS \right] = 0. \quad (18)$$

Satisfaction of equation (17) requires

$$\left(\frac{\partial \Delta_m}{\partial \dot{\beta}_j} - \boldsymbol{\tau}^d : \frac{\partial \overline{\mathbf{E}_m^V(\beta_j)}}{\partial \dot{\beta}_j} \right) = 0. \quad (19)$$

If one now considers a macroscopic version of (9):

$$\inf_{\dot{\mathbf{E}}^V} [\dot{\Psi} + \Delta], \quad (20)$$

then

$$\frac{\partial \Psi}{\partial \mathbf{E}^V} + \frac{\partial \Delta}{\partial \dot{\mathbf{E}}^V} = 0 \quad \Rightarrow \quad \boldsymbol{\tau}^V + \boldsymbol{\tau}^d = 0. \quad (21)$$

Using this result, one can add (19) to (13), which in turn shows that the formal parameters $\dot{\beta}_j$ in (19) are in fact the time derivatives of β_j ; note that Δ_m is assumed convex and we always assume the microscopic Biot principle to hold.

Examining the governing equations up to this point we see that we have three macroscopic residual equations (3), (11), and (16) plus the equality relation for the Lagrange multipliers (21); further, there are three microscopic residual equations (7), (13), and (19) that allow one to evaluate the macroscopic residuals in terms of the Lagrange multipliers. Macroscopically there are four tensors to be determined by the constitutive framework $(\mathbf{E}^V, \boldsymbol{\tau}, \boldsymbol{\tau}^V, \boldsymbol{\tau}^d)$, assuming that $\mathbf{E}$ is given, and thus the system of equations is closed.

Remarks:

1. Note that in this setting equations (13) and (16) together with (19) provide the evolution equations for the viscous (internal) variables, and “Biot’s principle” in this setting provides the inter-relation between the Lagrange multipliers.

2. Not only does one in general have that $\partial \mathbf{E}_m^V / \partial \beta_j = \overline{\partial \mathbf{E}_m^V(\beta_j) / \partial \dot{\beta}_j}$, but in our case these derivatives are independent of β_j . This is what allows us to identify the formal parameters in the optimization problem for the dissipation potential as the rates of the viscous micro-scale fields. It is under these conditions that the inelastic evolution of Model Framework 2 is identical to that of Model Framework 1. Thus the two models are in fact identical under the assumption that viscous micro-scale deformation measures are linear with respect to the viscous micro-scale fields. The two frameworks only provide alternate perspectives. No new principles are asserted in Model Framework 2; it is strictly a re-writing of Model Framework 1 with an interesting mathematical structure.
3. Model Framework 2 also highlights the fact that at a material point, the inelastic history need not be represented by the entire set of fields β_j when $\mathbf{E}_m^V$ is linear in β_j (the natural case), rather it is sufficient to carry this information in the aggregate variable $\mathbf{E}^V$. There is an added CPU cost for this change do to the costs associated with the additional structure, but it does result in a great memory savings – especially if high order quadrature rules are used in the evaluation of the micro-sphere relations.
4. It should also be further noted that if quadratic potentials are chosen, and $\mathbf{E}$ and $\mathbf{E}^V$ are taken as the total and viscous infinitesimal strain tensors, respectively, then closed form solutions are easily found and the theory of linear viscoelasticity is exactly recovered; see Appendix B where we additionally provide a comparison to the affine case.

3.5. Time incremental form

Within the Model Framework 2, the time incremental form of the equations starts by discretizing the expression for the macroscopic dissipation potential (15) as:

$$\Delta \left(\frac{\mathbf{E}_{n+1}^V - \mathbf{E}_n^V}{h} \right) = \inf_{\beta_{j,n+1}} \left\{ \frac{1}{|S|} \int_S \Delta_m \left(\frac{\beta_{j,n+1} - \beta_{j,n}}{h} \right) dS, \right\}$$

subject to the time incremental constraint

$$\frac{\mathbf{E}_{n+1}^V - \mathbf{E}_n^V}{h} = \frac{1}{|S|} \int_S \frac{\mathbf{E}_m^V(\beta_{j,n+1}) - \mathbf{E}_m^V(\beta_{j,n})}{h} dS. \quad (22)$$

Constructing the Lagrangian for this problem, one arrives at the time incremental Euler-Lagrange equations

$$D \Delta_m \left(\frac{\beta_{j,n+1} - \beta_{j,n}}{h} \right) - \boldsymbol{\tau}^d : \frac{\partial \mathbf{E}_{m,n+1}^V}{\partial \beta_{j,n+1}} = 0,$$

which furnishes the time incremental evolution equation for the micro-scale inelastic fields. Note the operator D indicates differentiation with respect to the function's entire argument.

As with the time continuous case, we employ the macroscopic version of Biot's principle to close the system of equations – this time in its time incremental form. Thus we require

$$\inf_{\mathbf{E}_{n+1}^V} \left[\Psi_{n+1} \left(\mathbf{E}_{n+1}, \mathbf{E}_{n+1}^V \right) - \Psi_n \left(\mathbf{E}_n, \mathbf{E}_n^V \right) + h \cdot \Delta \left(\mathbf{E}_{n+1}^V, \mathbf{E}_n^V \right) \right]. \quad (23)$$

As before this relation informs us that $\boldsymbol{\tau}^V = -\boldsymbol{\tau}^d$.

3.6. Second law satisfaction

To show that the second law of thermodynamics is directly satisfied in Model Framework 2, let $\Delta_m(\dot{\boldsymbol{\beta}})$ be a differentiable, convex and symmetric function (i.e., it holds $\Delta_m(\dot{\boldsymbol{\beta}}) = \Delta_m(-\dot{\boldsymbol{\beta}})$), where $\boldsymbol{\beta} = \dot{\boldsymbol{\beta}}(\mathbf{n})$ is a vector collection of the n_β micro-scale fields. Then it holds

$$\frac{\partial \Delta_m}{\partial \dot{\boldsymbol{\beta}}} \cdot \dot{\boldsymbol{\beta}} \geq 0, \quad (24)$$

i.e., the second law is satisfied at the micro-scale. Let now a macro-dissipation potential be defined as

$$\Delta = \inf_{\dot{\boldsymbol{\beta}}} \left\{ \frac{1}{|S|} \int_S \Delta_m(\dot{\boldsymbol{\beta}}) dS \right\}, \quad (25)$$

subject to the constraint

$$\dot{\mathbf{E}}^V = \frac{1}{|S|} \int_S \mathbb{A}(\mathbf{n}) \cdot \dot{\boldsymbol{\beta}} dS, \quad (26)$$

where $\mathbb{A}(\mathbf{n}) = \mathbb{A}_{ijk}(\mathbf{n})$, $i, j = 1, \dots, 3$, $k = 1, \dots, n_\beta$. Then it holds

$$\frac{\partial \Delta}{\partial \dot{\mathbf{E}}^V} : \dot{\mathbf{E}}^V \geq 0, \quad (27)$$

i.e., Δ satisfies the second law as well.

Proof:

Enforcing constraint (26) via a Lagrange multiplier $\boldsymbol{\tau}^d$ gives

$$\frac{\partial \Delta_m}{\partial \dot{\boldsymbol{\beta}}} = \boldsymbol{\tau}^d : \mathbb{A}(\mathbf{n}). \quad (28)$$

The Legendre transformation Δ_m^* of Δ_m is given as

$$\Delta_m^*(z) = \sup_{\dot{\boldsymbol{\beta}}} \left\{ z \cdot \dot{\boldsymbol{\beta}} - \Delta_m(\dot{\boldsymbol{\beta}}) \right\}, \quad (29)$$

and is a differentiable, convex and symmetric function once again, satisfying

$$\frac{\partial \Delta_m^*}{\partial z} \cdot z \geq 0. \quad (30)$$

Equation (28) can now be inverted to give

$$\dot{\beta} = \frac{\partial \Delta_m^*}{\partial \mathbf{z}}(\boldsymbol{\tau}^d : \mathbb{A}(\mathbf{n})). \quad (31)$$

Substitution of (31) into (25) and differentiation with respect to $\dot{\mathbf{E}}^V$ gives

$$\begin{aligned} & \frac{\partial \Delta}{\partial \dot{\mathbf{E}}^V} \\ &= \frac{1}{|S|} \int_S \frac{\partial \Delta_m}{\partial \dot{\beta}} \left(\frac{\partial \Delta_m^*}{\partial \mathbf{z}}(\boldsymbol{\tau}^d : \mathbb{A}(\mathbf{n})) \right) \cdot \frac{\partial^2 \Delta_m^*}{\partial \mathbf{z}^2}(\boldsymbol{\tau}^d : \mathbb{A}(\mathbf{n})) \cdot \mathbb{A}(\mathbf{n})^T dS : \frac{\partial \boldsymbol{\tau}^d}{\partial \dot{\mathbf{E}}^V} \end{aligned} \quad (32)$$

Making use of

$$\frac{\partial \Delta_m}{\partial \dot{\beta}} = \left(\frac{\partial \Delta_m^*}{\partial \mathbf{z}} \right)^{-1}, \quad (33)$$

(32) simplifies to

$$\frac{\partial \Delta}{\partial \dot{\mathbf{E}}^V} = \boldsymbol{\tau}^d : \frac{1}{|S|} \int_S \mathbb{A}(\mathbf{n}) \cdot \frac{\partial^2 \Delta_m^*}{\partial \mathbf{z}^2}(\boldsymbol{\tau}^d : \mathbb{A}(\mathbf{n})) \cdot \mathbb{A}(\mathbf{n})^T dS : \frac{\partial \boldsymbol{\tau}^d}{\partial \dot{\mathbf{E}}^V}. \quad (34)$$

Furthermore, differentiation of (26) with respect to $\dot{\mathbf{E}}^V$ and substitution of (31) gives

$$\mathbf{I} = \frac{1}{|S|} \int_S \mathbb{A}(\mathbf{n}) \cdot \frac{\partial^2 \Delta_m^*}{\partial \mathbf{z}^2}(\boldsymbol{\tau}^d : \mathbb{A}(\mathbf{n})) \cdot \mathbb{A}(\mathbf{n})^T dS : \frac{\partial \boldsymbol{\tau}^d}{\partial \dot{\mathbf{E}}^V}. \quad (35)$$

From (34) and (35) we deduce

$$\frac{\partial \Delta}{\partial \dot{\mathbf{E}}^V} = \boldsymbol{\tau}^d. \quad (36)$$

Finally, (26) together with (28) and (36) yields

$$\frac{\partial \Delta}{\partial \dot{\mathbf{E}}^V} : \dot{\mathbf{E}}^V = \frac{1}{|S|} \int_S \boldsymbol{\tau}^d : \mathbb{A}(\mathbf{n}) \cdot \frac{\partial \Delta_m^*}{\partial \mathbf{z}}(\boldsymbol{\tau}^d : \mathbb{A}(\mathbf{n})) dS. \quad (37)$$

Inequality (30) states that the integrand in (37) is always positive. Hence, the integral is positive, which gives the desired result.

4. Nonlinear viscoelasticity with Hencky measures

To illustrate the application of the general theory, we now consider its application to the case of a material that can be modeled using Hencky strain measures. We will first do so using the Model Framework 2 and then comment on the model equations that result from the use of Model Framework 1. To begin, we postulate at the microstructural level that the chain deformation is

described via a tensor, $\mathbf{U}_m = \lambda \mathbf{n} \otimes \mathbf{n} + \nu (\mathbf{1} - \mathbf{n} \otimes \mathbf{n})$, where λ is the chain stretch, ν is the stretch tranverse to the chain, and $\mathbf{n}$ is the unit chain orientation vector. As is common in elastomer models, we wish to decouple these variables into volumetric and isochoric components. This is achieved by first defining a micro-jacobian $j = \lambda \nu^2$ and a purely deviatoric kinematic variable $\xi = \sqrt[3]{\lambda/\nu}$. From here we can define the isochoric part of the micro-strain tensor:

$$\bar{\mathbf{U}}_m = j^{-1/3} \mathbf{U}_m = \xi^2 \mathbf{n} \otimes \mathbf{n} + \xi^{-1} (\mathbf{1} - \mathbf{n} \otimes \mathbf{n}),$$

or equivalently

$$\mathbf{U}_m = j^{1/3} \bar{\mathbf{U}}_m = j^{1/3} \xi^2 \mathbf{n} \otimes \mathbf{n} + j^{1/3} \xi^{-1} (\mathbf{1} - \mathbf{n} \otimes \mathbf{n}).$$

The strain measure we will use will be the Hencky (logarithmic) strain:

$$\ln \mathbf{U}_m = \frac{1}{3} \ln j \mathbf{1} + 3 \ln \xi \mathbb{D}(\mathbf{n}),$$

where $\mathbb{D}(\mathbf{n}) = \mathbf{n} \otimes \mathbf{n} - \frac{1}{3} \mathbf{1}$. The viscous micro-strain will be assumed to be purely deviatoric and thus to have the following form:

$$\ln \mathbf{U}_m^V = \sum_{i=1}^{n_v} 3 \ln \xi_i^V \mathbb{D}(\mathbf{n}). \quad (38)$$

The factor of 3 in front of the $\ln \xi_i^V$ terms is used for convenience. The parameter n_v in the summation above denotes how many viscous relaxation terms are needed to accurately represent a particular material's mechanical response. For simplicity of presentation we will assume $n_v = 1$ and drop the summation.

For the micro-scale free energy we will assume an additive structure with equilibrium and non-equilibrium terms and one that also splits deviatoric from volumetric contributions:

$$\psi_m(\ln j, \ln \xi, \ln \xi^V) = \psi_m^{\text{vol,eq}}(\ln j) + \psi_m^{\text{dev,eq}}(\ln \xi) + \psi_m^{\text{dev,neq}}(\ln \xi, \ln \xi^V).$$

Setting up the free energy Lagrangian with Lagrange multipliers $\boldsymbol{\tau}$ and $\boldsymbol{\tau}^V$, we have:

$$\begin{aligned} \mathcal{L}(\ln j, \ln \xi, \ln \xi^V, \boldsymbol{\tau}, \boldsymbol{\tau}^V) &= \frac{1}{|S|} \int_S \psi_m(\ln j, \ln \xi, \ln \xi^V) dS \\ &+ \boldsymbol{\tau} : \left[\ln \mathbf{U} - \frac{1}{|S|} \int_S \ln \mathbf{U}_m dS \right] + \boldsymbol{\tau}^V : \left[\ln \mathbf{U}^V - \frac{1}{|S|} \int_S \ln \mathbf{U}_m^V dS \right]. \end{aligned}$$

Here $\ln \mathbf{U}$ represents the total macroscopic Hencky strain and $\ln \mathbf{U}^V$ represents the macroscopic viscous Hencky strain. The resulting Euler-Lagrange equations are:

$$\frac{\partial \psi_m^{\text{vol,eq}}}{\partial \ln j} - \boldsymbol{\tau} : \frac{1}{3} \mathbf{1} = 0, \quad (39)$$

$$\frac{\partial \psi_m^{\text{dev,eq}}}{\partial \ln \xi} + \frac{\partial \psi_m^{\text{dev,neq}}}{\partial \ln \xi} - \boldsymbol{\tau} : 3 \mathbb{D}(\mathbf{n}) = 0, \quad (40)$$

$$\frac{\partial \psi_m^{\text{dev,neq}}}{\partial \ln \xi^V} - \boldsymbol{\tau}^V : 3 \mathbb{D}(\mathbf{n}) = 0, \quad (41)$$

along with the two constraint equations:

$$\ln \mathbf{U} - \frac{1}{|S|} \int_S \ln j \frac{1}{3} \mathbf{1} + 3 \ln \xi \mathbb{D}(\mathbf{n}) dS = 0, \quad (42)$$

$$\ln \mathbf{U}^V - \frac{1}{|S|} \int_S 3 \ln \xi^V \mathbb{D}(\mathbf{n}) dS = 0. \quad (43)$$

The conjugate stresses, the Lagrange multipliers, are the rotated Kirchhoff stresses; see Hoger (1987).

It is interesting to observe that (39) implies that $\ln j$ is a constant over the micro-sphere. Thus $\ln j$ behaves affinely, $j = J$. This result provides justification for the arbitrary assumption in Miehe et al. (2004) that the energetic relaxation for the micro-sphere construction is only performed on the deviatoric part of the motion. The two other micro-fields $\ln \xi$ and $\ln \xi^V$ are coupled via (40) and (41). If we denote the solution of the equations for the micro-fields with a superscript $*$, then we see that they are a function of $\boldsymbol{\tau}$ and $\boldsymbol{\tau}^V$ and orientation $\mathbf{n}$:

$$\ln \xi^*(\boldsymbol{\tau}, \boldsymbol{\tau}^V, \mathbf{n}) \quad \text{and} \quad \ln \xi^{V*}(\boldsymbol{\tau}, \boldsymbol{\tau}^V, \mathbf{n}) \quad \text{and} \quad \ln j^*(\boldsymbol{\tau}),$$

which implies that (42) and (43) become at time t_{n+1}

$$\ln \mathbf{U}_{n+1} - \frac{1}{|S|} \int_S \ln j^*(\boldsymbol{\tau}) \frac{1}{3} \mathbf{1} + 3 \ln \xi^*(\boldsymbol{\tau}, \boldsymbol{\tau}^V, \mathbf{n}) \mathbb{D}(\mathbf{n}) dS = 0, \quad (44)$$

$$\ln \mathbf{U}_{n+1}^V - \frac{1}{|S|} \int_S 3 \ln \xi^{V*}(\boldsymbol{\tau}, \boldsymbol{\tau}^V, \mathbf{n}) \mathbb{D}(\mathbf{n}) dS = 0. \quad (45)$$

To complete the system of equations, we can apply the developments of Sec. 3.5 to the present case. Doing so results in the time incremental relation for the inelastic micro-scale field as

$$D\Delta_m \left(\frac{\ln \xi_{n+1}^V - \ln \xi_n^V}{h} \right) + 3\boldsymbol{\tau}^V : \mathbb{D}(\mathbf{n}) = 0, \quad (46)$$

where we have used the macroscopic version of Biot's principle (20) to eliminate the third Lagrange multiplier. If we solve (46) for the inelastic micro-fields and then plug back into the time incremental constraint (22), we find

$$\ln \mathbf{U}_{n+1}^V = \ln \mathbf{U}_n^V + \frac{h}{|S|} \int_S [D\Delta_m]^{-1} (-3\boldsymbol{\tau}^V : \mathbb{D}(\mathbf{n})) 3\mathbb{D}(\mathbf{n}) dS, \quad (47)$$

as the incremental update formula for the macroscopic inelastic Hencky strains. Equations (44), (45), and (47) constitute the macroscopic constitutive equations for the model. They represent 3 tensor equations in the three unknowns $\ln \mathbf{U}_{n+1}^V$, the inelastic strains, $\boldsymbol{\tau}$, the total stress, and $\boldsymbol{\tau}^V$ the viscous stress; they are fully macroscopic. (For convenience we have omitted the time step subscript for the stress tensors).

If Model Framework 1 is used to derive the governing equations, the result is equations (39), (40), (42) together with

$$D\Delta_m \left(\frac{\ln \xi_{n+1}^V - \ln \xi_n^V}{h} \right) + \frac{\partial \psi_m^{\text{dev,neq}}}{\partial \ln \xi^V} (\ln \xi_{n+1}, \ln \xi_{n+1}^V). \quad (48)$$

Even though these equations result in the same solution as those from Model Framework 2, they are not amenable to the manipulation that resulted in the strictly macroscopic update (47). Thus, in this form the carried history must include the entire field $\ln \xi^V$. Further, while it is possible to reconstruct $\ln \mathbf{U}^V$ as a post processing – simply by definition – the reconstruction of a viscous stress is not accessible within Model Framework 2. It is however to be observed that simplicity of the Model Framework 1 equations does make them amenable to faster algorithms for solution, and the resulting stress-strain responses are identical.

4.1. Numerical Algorithm

The solution of the governing equations in either framework requires two issues to be addressed when used in the conventional strain driven setting. The first is that the equations are implicit in terms of the stress and thus have to be inverted. This is easily done using a Newton-Raphson iteration. The other numerical issue that arises is that one needs to evaluate integrals on the sphere to compute the terms in the governing equations. This can be achieved by a quadrature, whereby

$$\frac{1}{|S|} \int_S f(x) dS \approx \sum_{i=1}^{n_q} f(x_i) w_i,$$

where the x_i are the quadrature points, w_i are the weights, and n_q are the number of quadrature points. Recent studies have shown problems with the accuracy and reliability of common numerical integration methods over the sphere. Verron (2015), for example, compares various numerical integration methods for evaluating constitutive equations over the micro-sphere and has concluded that the number of quadrature points for a given scheme is very important in yielding accurate results. However, further work done by Itskov (2016) shows that numerical integration is still a reliable and accurate tool for full network models. A majority of the disagreement seems to be in the smoothness of the functions used. We took this into account and have studied the accuracy of integrating micro-free energies on the micro-sphere for a variety of points and different integration schemes. We omit the details here and simply note that the symmetric 21 point integration rule formulated by Bažant and Oh (1986) provided reasonable accuracy for the moderate levels of finite deformation show below. Good results can also be found with the more expensive rules of Fliege and Maier (1999), Sloan and Womersley (2004), Burkhardt (2010), and Freund et al. (2011).

4.2. Comparison to data: Tire derived materials

As an application of the model, we consider the experiments on tire-derived materials (TDMs) from Montella et al. (2016), who showed that Hencky based continuum models were appropriate for such materials. TDMs are made by cold forging a mix of styrene-butadiene rubber fibers from recycled vehicle tires and grains with a polyurethane binder. This results in a material composed of about 90 percent styrene-butadiene fibers and about 10 percent grains with varying densities. In addition, TDMs are compressible, so the original micro-sphere model for nearly incompressible materials will not suffice here. This utilizes the $\ln j$ component of our micro-sphere model unlike common rubber elasticity models which inherently assume incompressibility.

We choose to compare our model to a TDM with a density of 500 kg/m^3 , excited in uniaxial compression and simple shear at a loading frequency of 0.1 Hz . For the uniaxial compression test, there was a static pre-strain of 10% followed by a superimposed sinusoidal compression varying in amplitude in the range of 1% to 20%. The second test was a dynamic lap-shear test in which the sample specimen was loaded up to 100% shear strain. The reader is referred to Montella et al. (2016) for more details.

Since the authors used a modified version of the exponentiated Hencky strain energy, Neff et al. (2015), we choose to use microscopic potentials with a similar structure, given by (49)–(52). The exponentiated energies are important to achieve proper energy growth at large deformations. Note that the choice of these functions is somewhat arbitrary and any one-dimensional micromechanical model can be employed within the proposed framework. The functions chosen are only intended for illustration purposes. A set of non-optimized material parameters are given in Table 4.2.

$$\psi_{\text{m}}^{\text{vol,eq}} = \frac{E_v}{2} (\ln j)^2 \quad (49)$$

$$\psi_{\text{m}}^{\text{dev,eq}} = \frac{E_{d1}}{2} (\ln \xi)^2 + \frac{E_{d2}}{4} (\ln \xi)^4 + \frac{E_{d3}}{2\kappa_1} \exp(\kappa_1 (\ln \xi)^2) \quad (50)$$

$$\begin{aligned} \psi_{\text{m}}^{\text{dev,neq}} &= \frac{\mu_1}{2} (\ln \xi - \ln \xi^V)^2 + \frac{\mu_2}{4} (\ln \xi - \ln \xi^V)^4 \\ &+ \frac{\mu_3}{2\kappa_2} \exp(\kappa_2 (\ln \xi - \ln \xi^V)^2) \end{aligned} \quad (51)$$

$$\Delta_{\text{m}} = \frac{\eta_1}{2} (\ln \xi^{\dot{V}})^2 + \frac{\eta_2}{4} (\ln \xi^{\dot{V}})^4 \quad (52)$$

Figures 1 and 2 show the results for our model compared to the data for the tire-derived material. The plots of the total stretch $\lambda = j^{1/3} \xi^2$ and the ratio of the total stretch to $\lambda^V = (\xi^V)^2$ illustrate that once the macroscopic material response has been computed, the micro-fields are available via function evaluation/post-processing to allow investigation of local effects. For these two loading cases, our model performs reasonably well in simulating the experimental data. We are able to accurately obtain the stress for the largest deformations while still predicting the overall response of the stress-strain curve. However,

E_v (MPa)	E_{d1} (MPa)	E_{d2} (MPa)	E_{d3} (MPa)	κ_1 (-)	μ_1 (MPa)	μ_2 (MPa)	μ_3 (MPa)	κ_2 (-)
0.5	0.215	0.2	0.16	1.18	0.2	0.4	0.55	1.0

η_1 (MPa·s)	η_2 (MPa·s)
0.115	3.25

Table 1: Material parameters for Figures 1 and 2.

we do note that the compression stress/strain simulation is not as accurate as in the shear case due to the slightly anisotropic microstructure of the tire derived material. The overall response of the model is, of course, also tightly connected to the quality of the one-dimensional micro-scale potentials used, and we have not attempted to optimize these in this work, as our main focus is on the overall modeling framework.

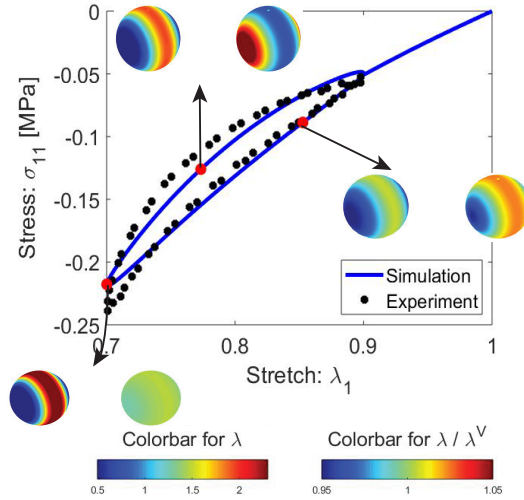


Figure 1: Data from Montella et al. (2016). The left sphere represents the total stretch along various orientations for the micro-sphere, while the right sphere represents the non-equilibrium stretch.

5. Nonlinear viscoelasticity with a multiplicative split

In this section we illustrate the use of our Model Framework 2 to extend the maximal advance path constraint scheme presented in Tkachuk and Linder (2012) to include viscous relaxation phenomena. The “strain measure” used here will be the deformation gradient $\mathbf{F}$. In the spirit of the multiplicative

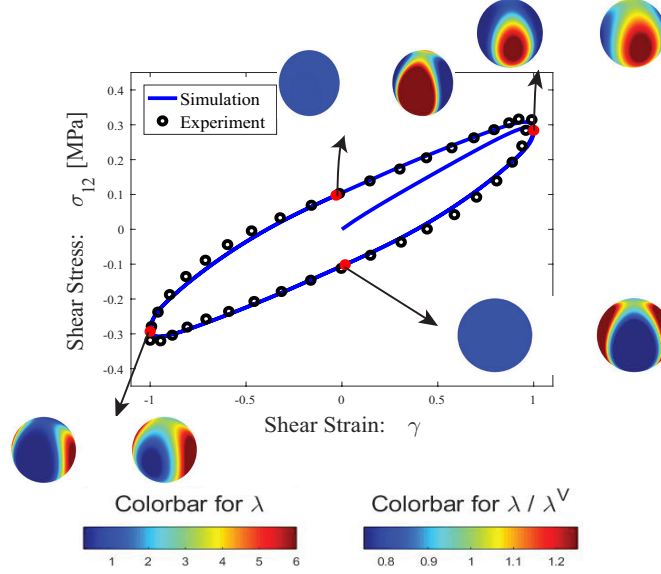


Figure 2: Data from Montella et al. (2016). The left sphere represents the total stretch along various orientations for the micro-sphere, while the right sphere represents the non-equilibrium stretch.

decomposition $\mathbf{F} = \mathbf{F}^E \mathbf{F}^V$ (Sidoroff, 1974), we assume micro-scale elastic and viscous deformation gradients of the form:

$$\mathbf{F}_m^E = \alpha \cdot \mathbf{n} \otimes \mathbf{n}^V, \quad (53)$$

$$\mathbf{F}_m^V = \mathbf{n}^V \otimes \mathbf{n}_0, \quad (54)$$

$$\mathbf{F}_m = \mathbf{F}_m^E \mathbf{F}_m^V = \mathbf{n} \otimes \mathbf{n}_0. \quad (55)$$

Here, the total micro-strain is the outer product of the deformed orientation vector $\mathbf{n}$ and the original directional vector $\mathbf{n}_0$ over the surface of the sphere; i.e. $\mathbf{n}_0$ maps to $\mathbf{n}$. We extend Tkachuk and Linder (2012) using a similar kinematic assumption for the viscous micro-scale deformation gradient and introduce a new variable $\mathbf{n}^V$ accounting for the mapping of $\mathbf{n}_0$ from the reference to intermediate configuration; $\alpha = 1/\|\mathbf{n}^V\|$ to ensure that we recover $\mathbf{F}_m = \mathbf{n} \otimes \mathbf{n}_0$ when multiplying $\mathbf{F}_m^E$ and $\mathbf{F}_m^V$ together.

The requisite constraint equations for the relaxations are now given in terms of the *vectorial* micro-fields $\mathbf{n}$ and $\mathbf{n}^V$:

$$\frac{1}{3} \mathbf{F} = \frac{1}{|S|} \int_S \mathbf{F}_m(\mathbf{n}) dS, \quad (56)$$

$$\frac{1}{3} \mathbf{F}^V = \frac{1}{|S|} \int_S \mathbf{F}_m^V(\mathbf{n}^V) dS. \quad (57)$$

(The factor of 1/3 as noted in Tkachuk and Linder (2012) is due to the fact that for no deformation $\frac{1}{|S|} \int_S \mathbf{n}_0 \otimes \mathbf{n}_0 dS = \frac{1}{3} \mathbf{1}$.) Continuing with the framework,

we again assume a decoupled micro free energy into equilibrium ψ_m^{eq} and non-equilibrium ψ_m^{neq} components, where ψ_m^{eq} will depend on the norm of $\mathbf{n}$ and ψ_m^{neq} will depend on $\|\mathbf{n} - \mathbf{n}^{\text{V}}\|$. Additionally, the microscopic dissipation potential is defined in terms of $\|\dot{\mathbf{n}}^{\text{V}}\|$:

$$\begin{aligned}\psi_m(\mathbf{n}, \mathbf{n}^{\text{V}}) &= \psi_m^{\text{eq}}(\|\mathbf{n}\|) + \psi_m^{\text{neq}}(\|\mathbf{n} - \mathbf{n}^{\text{V}}\|), \\ \Delta_m(\dot{\mathbf{n}}^{\text{V}}) &= \Delta_m(\|\dot{\mathbf{n}}^{\text{V}}\|).\end{aligned}$$

The remainder of the model details follow in exactly the same fashion as above. Perhaps the only point of note is that the conjugate stresses that appear in this formulation are 1st Piola-Kirchhoff stress (and they appear as one-third times the Lagrange multipliers).

5.1. Comparison to data: Tire derived materials

As with the Hencky example we will apply this model to the TDM data of Montella et al. (2016). The potential functions chosen, as before, are for illustrative purposes:

$$\begin{aligned}\psi_m^{\text{eq}} &= \frac{E_1}{2} \exp(\|\mathbf{n}\|^2) + \frac{E_2}{2} \|\mathbf{n}\|^2 + K (\log \|\mathbf{n}\|)^2, \\ \psi_m^{\text{neq}} &= \frac{\mu}{2} \|\mathbf{n} - \mathbf{n}^{\text{V}}\|^2, \\ \Delta_m &= \frac{\eta_1}{2} \|\dot{\mathbf{n}}^{\text{V}}\|^2 + \frac{\eta_2}{4} \|\dot{\mathbf{n}}^{\text{V}}\|^4.\end{aligned}$$

The (non-optimized) material parameter used are shown in Table 2.

The model is seen to be able to model large deformations and with large amounts of dissipation. We can see that for roughly the same accuracy as the Hencky model, one needs half as many material parameters with our viscoelastic extension of the maximal advance path constraint structure from Tkachuk and Linder (2012). This highlights the importance of good micro-scale models when using the micro-sphere framework to model materials.

E_1 (MPa)	E_2 (MPa)	K (MPa)	μ (MPa)	η_1 (MPa·s)	η_2 (MPa·s)
0.10	0.10	1.254	10.0	0.10	0.15

Table 2: Material parameters for Figures 3 and 4.

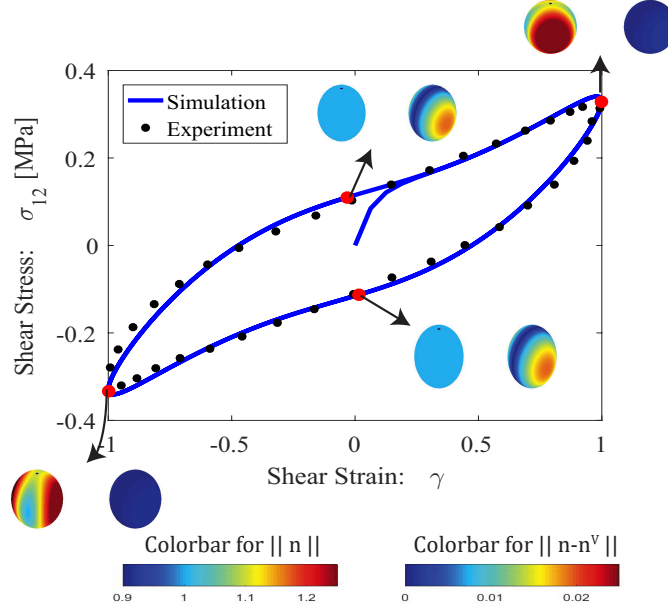


Figure 3: Data from Montella et al. (2016). The left sphere colorbar shows the norm of the elastic vector $\mathbf{n}$, while the right sphere colorbar shows the norm of the difference $\mathbf{n} - \mathbf{n}^V$.

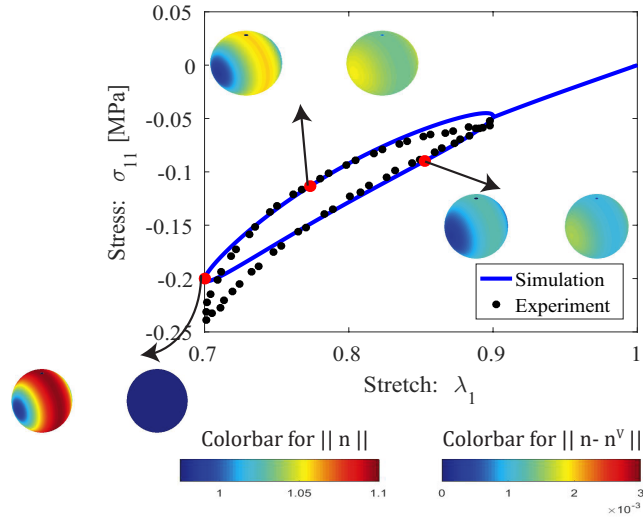


Figure 4: Data from Montella et al. (2016). The left sphere colorbar shows the norm of the elastic vector $\mathbf{n}$, while the right sphere colorbar shows the norm of the difference $\mathbf{n} - \mathbf{n}^V$.

6. Conclusion

The micro-sphere framework is a popular framework for extending one-dimensional elastic models into three dimensions via energetic relaxation of micro-scale energies subject to macro-micro relational constraints. Outside of the elastic case, efforts to date have always relied upon an affine connection between macroscopic and microscopic inelasticity. In this work we have presented a structure for dispensing with this affine assumption.

The construction requires that the micro-scale material response be governed by one-dimensional models that admit a Biot variational representation. In particular we have shown via examples that this applies to linear and non-linear viscoelasticity (at both finite and small deformations). We also note that it applies to many models of plasticity, strain crystallization, and other transformation phenomena.

The modeling framework can be developed in two formally equivalent manners – one using known relaxation principles with a micro-scale Biot principle and a second involving the construction of a relaxed macro-scale dissipation potential coupled to a macro-scale Biot-like relation. In both presentations, the resulting model provides a macroscopic three-dimensional evolutionary model for inelastic behavior that is variationally fully consistent with the microscopic material model that one assumes. The frameworks only differ in the character of the representation of the internal state of the material. In the first framework, the internal state is represented by a field which implies high storage costs in a computational setting. In the second framework, the internal state can be represented (in most cases) by a single tensor leading to lower storage costs but resulting in equations that involve a higher computational cost to solve.

While we have applied our relaxation schemes to the micro-sphere, we also note that the idea of constructing macroscopic inelastic models from microscopic models based on dissipation potentials applies more generally. In particular, it naturally extends to inelastic composite materials, where one, however, must also deal with the issue of gradient constraints should one desire to do better than Voigt averaging.

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Appendix A. Lagrange multipliers and conjugate stresses

The conjugate stresses to the macroscopic variables are straightforwardly show to be equal to the Lagrange multipliers in our relaxation problems. Consider a micro-scale free energy in terms of a two sets of micro-fields α_i (elastic) and β_j (viscous), subject to averaging constraints, such that the governing Lagrangian is given by

$$\begin{aligned}\mathcal{L}(\alpha_i, \beta_j, \boldsymbol{\tau}, \boldsymbol{\tau}^V) &= \frac{1}{|S|} \int_S \Psi_m(\alpha_i, \beta_j) dS \\ &+ \boldsymbol{\tau} : \left[\mathbf{E} - \frac{1}{|S|} \int_S \mathbf{E}_m(\alpha_i) dS \right] \\ &+ \boldsymbol{\tau}^V : \left[\mathbf{E} - \frac{1}{|S|} \int_S \mathbf{E}_m^V(\beta_j) dS \right]\end{aligned}$$

The corresponding stationary conditions yield:

$$\delta_{\alpha_i} \mathcal{L} = \frac{1}{|S|} \int_S \left(\frac{\partial \Psi_m}{\partial \alpha_i} - \boldsymbol{\tau} : \frac{\partial \mathbf{E}_m}{\partial \alpha_i} \right) \delta \alpha_i dS = 0 \quad (\text{A.1})$$

$$\delta_{\beta_j} \mathcal{L} = \frac{1}{|S|} \int_S \left(\frac{\partial \Psi_m}{\partial \beta_j} - \boldsymbol{\tau}^V : \frac{\partial \mathbf{E}_m^V}{\partial \beta_j} \right) \delta \beta_j dS = 0 \quad (\text{A.2})$$

$$\delta_{\boldsymbol{\tau}} \mathcal{L} = \mathbf{E} - \frac{1}{|S|} \int_S \mathbf{E}_m(\alpha_i) dS = 0 \quad (\text{A.3})$$

$$\delta_{\boldsymbol{\tau}^V} \mathcal{L} = \mathbf{E}^V - \frac{1}{|S|} \int_S \mathbf{E}_m^V(\beta_j) dS = 0 \quad (\text{A.4})$$

Taking the derivative of equation (A.3) with respect to $\mathbf{E}$ yields:

$$\mathbb{I}^{\text{sym}} - \frac{1}{|S|} \int_S \frac{\partial \mathbf{E}_m}{\partial \alpha_i} \frac{\partial \alpha_i}{\partial \mathbf{E}} dS = 0.$$

Taking the derivative of equation (A.4) with respect to $\mathbf{E}^V$ yields:

$$\mathbb{I}^{\text{sym}} - \frac{1}{|S|} \int_S \frac{\partial \mathbf{E}_m^V}{\partial \beta_j} \frac{\partial \beta_j}{\partial \mathbf{E}^V} dS = 0.$$

It is also useful to note, that by the assumed independence of $\mathbf{E}$ and $\mathbf{E}^V$:

$$\begin{aligned} \mathbf{0} &= \frac{1}{|S|} \int_S \frac{\partial \mathbf{E}_m}{\partial \alpha_i} \frac{\partial \alpha_i}{\partial \mathbf{E}^V} dS \\ \mathbf{0} &= \frac{1}{|S|} \int_S \frac{\partial \mathbf{E}_m^V}{\partial \beta_j} \frac{\partial \beta_j}{\partial \mathbf{E}} dS \end{aligned}$$

From (A.1) and (A.2), we have the following Euler-Lagrange equations:

$$\begin{aligned} \frac{\partial \Psi_m}{\partial \alpha_i} &= \boldsymbol{\tau} : \frac{\partial \mathbf{E}_m}{\partial \alpha_i}, \\ \frac{\partial \Psi_m}{\partial \beta_j} &= \boldsymbol{\tau}^V : \frac{\partial \mathbf{E}_m^V}{\partial \beta_j}. \end{aligned}$$

If their solution is denoted by α_i^* and β_j^* then our macroscopic energy becomes:

$$\Psi(\mathbf{E}, \mathbf{E}^V) = \frac{1}{|S|} \int_S \Psi_m(\alpha_i^*, \beta_j^*) dS.$$

The conjugate stress will be given by $\partial \Psi / \partial \mathbf{E}$ and $\partial \Psi / \partial \mathbf{E}^V$.

$$\begin{aligned} \frac{\partial \Psi}{\partial \mathbf{E}} &= \frac{1}{|S|} \int_S \frac{\partial \Psi_m}{\partial \alpha_i^*} \frac{\partial \alpha_i^*}{\partial \mathbf{E}} + \frac{\partial \Psi_m}{\partial \beta_j^*} \frac{\partial \beta_j^*}{\partial \mathbf{E}} dS \\ &= \frac{1}{|S|} \int_S \boldsymbol{\tau} : \frac{\partial \mathbf{E}_m}{\partial \alpha_i^*} \frac{\partial \alpha_i^*}{\partial \mathbf{E}} + \boldsymbol{\tau}^V : \frac{\partial \mathbf{E}_m^V}{\partial \beta_j^*} \frac{\partial \beta_j^*}{\partial \mathbf{E}} dS \\ &= \boldsymbol{\tau} : \mathbb{I}^{\text{sym}} + \boldsymbol{\tau}^V : \mathbf{0} \\ &= \boldsymbol{\tau}. \end{aligned}$$

Similarly, for the viscous conjugate stress:

$$\begin{aligned} \frac{\partial \Psi}{\partial \mathbf{E}^V} &= \frac{1}{|S|} \int_S \frac{\partial \Psi_m}{\partial \alpha_i^*} \frac{\partial \alpha_i^*}{\partial \mathbf{E}^V} + \frac{\partial \Psi_m}{\partial \beta_j^*} \frac{\partial \beta_j^*}{\partial \mathbf{E}^V} dS \\ &= \frac{1}{|S|} \int_S \boldsymbol{\tau} : \frac{\partial \mathbf{E}_m}{\partial \alpha_i^*} \frac{\partial \alpha_i^*}{\partial \mathbf{E}^V} + \boldsymbol{\tau}^V : \frac{\partial \mathbf{E}_m^V}{\partial \beta_j^*} \frac{\partial \beta_j^*}{\partial \mathbf{E}^V} dS \\ &= \boldsymbol{\tau} : \mathbf{0} + \boldsymbol{\tau}^V : \mathbb{I}^{\text{sym}} \\ &= \boldsymbol{\tau}^V. \end{aligned}$$

Appendix B. Linear Viscoelasticity

Following Model Framework 2, in the linear case the strain measure chosen is the infinitesimal strain tensor $\boldsymbol{\varepsilon}$. We assume a microscopic strain tensor, $\boldsymbol{\varepsilon}_m = \boldsymbol{\varepsilon}_m^e + \boldsymbol{\varepsilon}_m^v$, which is decomposed into a total elastic strain and a viscous strain. The micro-scale tensors are constructed from three scalar fields ε_{vol} , ε_{dev} , and $\varepsilon_{\text{dev}}^v$ accounting for the total volumetric, total deviatoric, and viscous deviatoric deformations, respectively. These correspond to α_1 , α_2 , and β_1 from the general theory. The micro-scale strains are given by:

$$\boldsymbol{\varepsilon}_m = \varepsilon_{\text{vol}} \frac{\mathbf{1}}{3} + \varepsilon_{\text{dev}} \left(\mathbf{n} \otimes \mathbf{n} - \frac{\mathbf{1}}{3} \right), \quad (\text{B.1})$$

$$\boldsymbol{\varepsilon}_m^v = \varepsilon_{\text{dev}}^v \left(\mathbf{n} \otimes \mathbf{n} - \frac{\mathbf{1}}{3} \right). \quad (\text{B.2})$$

Here we assume that the viscous strain is purely deviatoric and the vector $\mathbf{n}$ denotes orientation on the sphere. An alternate micro-strain decomposition is to have $\alpha_1 = \varepsilon_a$ correspond to an axial stretch and $\alpha_2 = \varepsilon_c$ correspond to a transverse contraction. This is similar to the approach in Miehe et al. (2004) and Bažant and Gambarova (1984) leading to:

$$\boldsymbol{\varepsilon}_m = \varepsilon_a \mathbf{n} \otimes \mathbf{n} + \varepsilon_c (\mathbf{1} - \mathbf{n} \otimes \mathbf{n}), \quad (\text{B.3})$$

$$\boldsymbol{\varepsilon}_m^v = \varepsilon_a^v \mathbf{n} \otimes \mathbf{n} + \varepsilon_c^v (\mathbf{1} - \mathbf{n} \otimes \mathbf{n}). \quad (\text{B.4})$$

In the setting with axial and transverse micro-fields it is attractive, considering only the elastic case (i.e. no $\boldsymbol{\varepsilon}_m^v$), to have a micro-scale energy of the form $\psi_m = \psi_{m,a}(\varepsilon_a) + \psi_{m,c}(\varepsilon_c)$, where the $\psi_{m,a}$ and $\psi_{m,c}$ are quadratic. However this Ansatz leads to Poisson ratios that are strictly negative for all positive microscopic moduli. The negative values respect the thermodynamic limits of the Poisson ratio being greater than -1 , but one is not able to reach positive values. This is not a result of the form of micro-scale strain measure, but due to the postulated structure of the free energy. Since physically these terms are coupled via a Poisson ratio effect, we cannot neglect a coupled free energy term. Therefore, our model utilizes the volumetric and deviatoric kinematic variables so that we are able to obtain the full range of thermodynamically admissible Poisson ratios in the linear elastic case (no viscous phenomena). A similar problem with the Poisson ratio was also seen in the original affine micro-plane model formulated by Bažant and Gambarova (1984), where it was only able to take on values of 0.25 for two-dimensional problems and $1/3$ for three-dimensional problems. In the original formulation, only normal and tangential strain components were considered for each micro-plane, which corresponds to equation (B.3). This problem was fixed in Bažant (1988) by considering an additional shear strain on each micro-plane along with decoupling the normal strain into volumetric and deviatoric components; see also Carol et al. (2004).

Continuing, we can employ quadratic potentials for the microscopic free

energy and dissipation potential:

$$\psi_m = \frac{1}{2}K(\varepsilon_{\text{vol}})^2 + \frac{1}{2}G_\infty(\varepsilon_{\text{dev}})^2 + \frac{1}{2}G_1(\varepsilon_{\text{dev}} - \varepsilon_{\text{dev}}^v)^2 \quad (\text{B.5})$$

$$\Delta_m = \frac{1}{2}\eta_G(\dot{\varepsilon}_{\text{dev}}^v)^2 \quad (\text{B.6})$$

Here K , G_∞ , and G_1 are the microscopic bulk modulus, equilibrium shear modulus, and viscous shear modulus, respectively; η_G is a microscopic measure of internal viscosity.

Following the procedure outlined in the previous section, the macroscopic free energy is defined as in equation (12) with the corresponding Lagrangian in terms of the micro-kinematic variables and two Lagrange multipliers $\boldsymbol{\tau}$ and $\boldsymbol{\tau}^v$:

$$\begin{aligned} \mathcal{L}(\varepsilon_{\text{vol}}, \varepsilon_{\text{dev}}, \varepsilon_{\text{dev}}^v, \boldsymbol{\tau}, \boldsymbol{\tau}^v) = & \\ & \frac{1}{|S|} \int_S \left[\frac{1}{2}K(\varepsilon_{\text{vol}})^2 + \frac{1}{2}G_\infty(\varepsilon_{\text{dev}})^2 + \frac{1}{2}G_1(\varepsilon_{\text{dev}} - \varepsilon_{\text{dev}}^v)^2 \right] dS \\ & + \boldsymbol{\tau} : \left(\boldsymbol{\varepsilon} - \frac{1}{|S|} \int_S \boldsymbol{\varepsilon}_m dS \right) + \boldsymbol{\tau}^v : \left(\boldsymbol{\varepsilon}^v - \frac{1}{|S|} \int_S \boldsymbol{\varepsilon}_m^v dS \right). \end{aligned}$$

As before, we define $\mathbb{D}(\mathbf{n}) = \mathbf{n} \otimes \mathbf{n} - \frac{1}{3}\mathbf{1}$. The stationary conditions yield:

$$\delta_{\varepsilon_{\text{vol}}} \mathcal{L} = \frac{1}{|S|} \int_S \left[K\varepsilon_{\text{vol}} - \boldsymbol{\tau} : \frac{\mathbf{1}}{3} \right] \delta\varepsilon_{\text{vol}} dS = 0, \quad (\text{B.7})$$

$$\begin{aligned} \delta_{\varepsilon_{\text{dev}}} \mathcal{L} &= \frac{1}{|S|} \int_S [G_\infty(\varepsilon_{\text{dev}}) + G_1(\varepsilon_{\text{dev}} - \varepsilon_{\text{dev}}^v) - \boldsymbol{\tau} : \mathbb{D}(\mathbf{n})] \delta\varepsilon_{\text{dev}} dS \\ &= 0, \end{aligned} \quad (\text{B.8})$$

$$\delta_{\varepsilon_{\text{dev}}^v} \mathcal{L} = \frac{1}{|S|} \int_S [-G_1(\varepsilon_{\text{dev}} - \varepsilon_{\text{dev}}^v) - \boldsymbol{\tau}^v : \mathbb{D}(\mathbf{n})] \delta\varepsilon_{\text{dev}}^v dS = 0, \quad (\text{B.9})$$

$$\delta_{\boldsymbol{\tau}} \mathcal{L} = \delta\boldsymbol{\tau} : \left(\boldsymbol{\varepsilon} - \frac{1}{|S|} \int_S \varepsilon_{\text{vol}} \frac{\mathbf{1}}{3} + \varepsilon_{\text{dev}} \mathbb{D}(\mathbf{n}) dS \right) = 0, \quad (\text{B.10})$$

$$\delta_{\boldsymbol{\tau}^v} \mathcal{L} = \delta\boldsymbol{\tau}^v : \left(\boldsymbol{\varepsilon}^v - \frac{1}{|S|} \int_S \varepsilon_{\text{dev}}^v \mathbb{D}(\mathbf{n}) dS \right) = 0. \quad (\text{B.11})$$

This set of linear equations is easily solved for the micro-kinematic variables in terms of the Lagrange multipliers. If we then plug these results back into the constraint equations, we can solve for the Lagrange multipliers in terms of the macroscopic strains by splitting them into deviatoric and volumetric parts. With this procedure one finds that the macroscopic free energy:

$$\begin{aligned} \Psi = & \frac{1}{2}3K\boldsymbol{\varepsilon} : \mathbb{I}^{\text{vol}} : \boldsymbol{\varepsilon} + \frac{1}{2}G_\infty \frac{15}{2} [\boldsymbol{\varepsilon} : \mathbb{I}^{\text{dev}} : \boldsymbol{\varepsilon}] \\ & + \frac{1}{2}G_1 \frac{15}{2} [(\boldsymbol{\varepsilon} - \boldsymbol{\varepsilon}^v) : \mathbb{I}^{\text{dev}} : (\boldsymbol{\varepsilon} - \boldsymbol{\varepsilon}^v)], \end{aligned} \quad (\text{B.12})$$

where $\mathbb{I} = \mathbb{I}^{\text{dev}} + \mathbb{I}^{\text{vol}}$, $\mathbb{I}^{\text{vol}} = \frac{1}{3}\mathbf{1} \otimes \mathbf{1}$.

The conjugate stresses are the derivatives of the free energy with respect to the strains, yielding:

$$\begin{aligned}\boldsymbol{\tau} &= \frac{\partial \Psi}{\partial \boldsymbol{\varepsilon}} = 3K\boldsymbol{\varepsilon} : \mathbb{I}^{\text{vol}} + G_{\infty} \frac{15}{2} \boldsymbol{\varepsilon} : \mathbb{I}^{\text{dev}} \\ &+ G_1 \frac{15}{2} (\boldsymbol{\varepsilon} - \boldsymbol{\varepsilon}^{\text{v}}) : \mathbb{I}^{\text{dev}},\end{aligned}\quad (\text{B.13})$$

$$\boldsymbol{\tau}^{\text{v}} = \frac{\partial \Psi}{\partial \boldsymbol{\varepsilon}^{\text{v}}} = -G_1 \frac{15}{2} (\boldsymbol{\varepsilon} - \boldsymbol{\varepsilon}^{\text{v}}) : \mathbb{I}^{\text{dev}}. \quad (\text{B.14})$$

The evolution of the viscous strain is determined through the use of a dissipation potential. The Lagrangian associated with relaxation problem (15) subject to (16) is given by

$$\mathcal{L}(\dot{\boldsymbol{\varepsilon}}_{\text{dev}}^{\text{v}}, \boldsymbol{\tau}^{\text{d}}) = \frac{1}{|S|} \int_S \frac{1}{2} \eta_G (\dot{\boldsymbol{\varepsilon}}_{\text{dev}}^{\text{v}})^2 dS + \boldsymbol{\tau}^{\text{d}} : \left[\dot{\boldsymbol{\varepsilon}}^{\text{v}} - \frac{1}{|S|} \int_S \dot{\boldsymbol{\varepsilon}}_{\text{dev}}^{\text{v}} \mathbb{D}(\mathbf{n}) dS \right]$$

Following the same procedure above, the resulting variational equations are:

$$\delta_{\dot{\boldsymbol{\varepsilon}}_{\text{dev}}^{\text{v}}} \mathcal{L} = \frac{1}{|S|} \int_S [\eta_G \cdot \dot{\boldsymbol{\varepsilon}}_{\text{dev}}^{\text{v}} - \boldsymbol{\tau}^{\text{d}} : \mathbb{D}(\mathbf{n})] \delta \dot{\boldsymbol{\varepsilon}}_{\text{dev}}^{\text{v}} dS = 0, \quad (\text{B.15})$$

$$\delta_{\boldsymbol{\tau}^{\text{d}}} \mathcal{L} = \delta \boldsymbol{\tau}^{\text{d}} : \left[\dot{\boldsymbol{\varepsilon}}^{\text{v}} - \frac{1}{|S|} \int_S \dot{\boldsymbol{\varepsilon}}_{\text{dev}}^{\text{v}} \mathbb{D}(\mathbf{n}) dS \right] = 0. \quad (\text{B.16})$$

Solving these linear equations, and plugging back into the expression for the macroscopic dissipation potential, gives the macroscopic dissipation potential as:

$$\Delta = \frac{1}{2} \eta_G \frac{15}{2} [\dot{\boldsymbol{\varepsilon}}^{\text{v}} : \mathbb{I}^{\text{dev}} : \dot{\boldsymbol{\varepsilon}}^{\text{v}}]. \quad (\text{B.17})$$

Again it is easily shown that the conjugate stress to the dissipation potential is the new Lagrange multiplier,

$$\boldsymbol{\tau}^{\text{d}} = \frac{\partial \Delta}{\partial \dot{\boldsymbol{\varepsilon}}^{\text{v}}} = \eta_G \frac{15}{2} \dot{\boldsymbol{\varepsilon}}^{\text{v}} : \mathbb{I}^{\text{dev}}. \quad (\text{B.18})$$

Combining equations (B.12) and (B.17) with the Biot framework will determine the evolution equation of the system:

$$\inf_{\dot{\boldsymbol{\varepsilon}}^{\text{v}}} \left[\dot{\Psi}(\boldsymbol{\varepsilon}, \boldsymbol{\varepsilon}^{\text{v}}) + \Delta(\dot{\boldsymbol{\varepsilon}}^{\text{v}}) \right],$$

or equivalently,

$$\frac{\partial \Psi}{\partial \boldsymbol{\varepsilon}^{\text{v}}} + \frac{\partial \Delta}{\partial \dot{\boldsymbol{\varepsilon}}^{\text{v}}} = 0, \quad (\text{B.19})$$

$$\boldsymbol{\tau}^{\text{v}} + \boldsymbol{\tau}^{\text{d}} = 0. \quad (\text{B.20})$$

Substituting these relations back into the equation above:

$$\dot{\boldsymbol{\varepsilon}}^{\text{v}} - \frac{G_1}{\eta_G} (\boldsymbol{\varepsilon} - \boldsymbol{\varepsilon}^{\text{v}}) : \mathbb{I}^{\text{dev}} = 0. \quad (\text{B.21})$$

Considering (B.13) and (B.21), we see we have exactly the macroscopic model for the standard linear solid when one identifies K as the macroscopic bulk modulus, $\frac{15}{2}G_\infty$ as the macroscopic equilibrium modulus, $\frac{15}{2}G_1$ as the macroscopic non-equilibrium modulus, and $\frac{15}{2}\eta_G$ as the macroscopic viscosity.

Remarks:

1. If Model Framework 1 had been used in this linear context, the exact same model would have resulted including the ability to fully convert the model equations to a strictly macroscopic model.
2. As an illustration of the difference in the response of our fully variationally consistent frameworks and that of the affine model, in Figure B.5 we compare the hysteresis loops for a cyclic uniaxial simulation in the linear setting. The material parameters were $G_\infty = 2.5$, $G_1 = 1.2$, $K = 100$, $\tau = \eta_G/G_1 = 1.1$, with a uniaxial stress loading of $\sigma_{11}(t) = \sin(t)$. The results are generally indicative of an observed phenomena of lower than expected hysteresis (Mistry and Govindjee, 2014) when using affine evolution equations with the micro-sphere model.

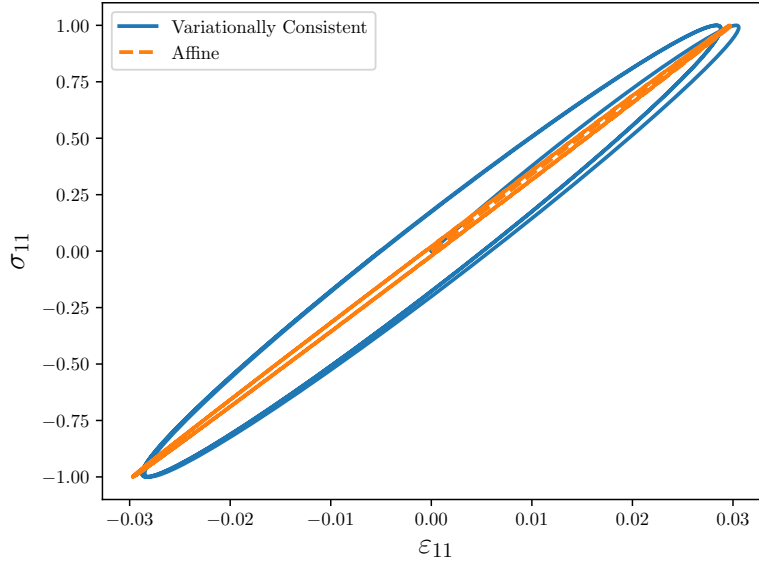


Figure B.5: Comparison of the variationally relaxed model in the linear setting to the affine model of Miehe and Göktepe (2005) using the same micro-scale properties.

Appendix C. Surface Integrals

For the derivations in Appendix B, the following results are helpful to know:

$$\frac{1}{|S|} \int_{S^2} \mathbf{n} \otimes \mathbf{n} dS = \frac{1}{3} \mathbf{1},$$

$$\frac{1}{|S|} \int_{S^2} \mathbf{n} \otimes \mathbf{n} \otimes \mathbf{n} \otimes \mathbf{n} dS = \frac{1}{15} (\mathbf{1} \otimes \mathbf{1} + 2\mathbb{I}^{\text{sym}}),$$

and

$$\frac{1}{|S|} \int_S \mathbb{D}(\mathbf{n}) \otimes \mathbb{D}(\mathbf{n}) dS = \frac{2}{15} \mathbb{I}^{\text{dev}}.$$