Title

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Publication Date
1983-12-01

REPORT NO.
UCB/SESM-83/05

STRUCTURAL ENGINEERING AND
STRUCTURAL MECHANICS

REMARKS ON RATE CONSTITUTIVE EQUATIONS FOR FINITE DEFORMATION PROBLEMS: COMPUTATIONAL IMPLICATIONS

by

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DECEMBER 1983

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UNIVERSITY OF CALIFORNIA
BERKELEY, CALIFORNIA

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1. Introduction

The mechanical behavior of solids undergoing finite deformation is often characterized by a *spatial* rate constitutive equation relating an *objective rate* of the *Kirchoff* (or *Cauchy*) stress tensor, $\overset{\triangledown}{\boldsymbol{\tau}}$, to the *rate* of *deformation* tensor $\mathbf{d}$; e.g., $\overset{\triangledown}{\boldsymbol{\tau}} = \mathbf{a}:\mathbf{d}$. Typically, these rate constitutive equations arise in the formulation of continuum models characterizing *inelastic* response, such as finite deformation plasticity. Within this context, an additive decomposition of the rate of deformation tensor $\mathbf{d}$ is introduced, and the rate constitutive equation with $\mathbf{d}$ replaced by its "elastic" part is then postulated in order to characterize the *elastic response*. (This approach is characteristic of most of the finite element plasticity codes in use). Lack of experimental evidence supporting a particular form of $\mathbf{a}$ often leads to the choice of the *constant isotropic elasticity tensor* of the linearized theory. The question is then often reduced to a search for the "proper" objective rate compatible with this *ad−hoc* choice†. The purpose of this paper is to show that rate constitutive models of this type widely employed in computational mechanics are in fact, not only incompatible with the notion of hyperelasticity, in the sense that a stored energy function does not exist, but even fail to define an elastic material in the nonlinear range. Our results are summarized as follows.

First, in the context of elasticity we show that a nonlinear elastic material cannot have (spatial) elasticities that are a **constant** *isotropic* tensor for all possible configurations, unless $\lambda + \mu \equiv 0$, where λ, μ are the Lame constants of the linearized theory. Such a condition is

†Although many different definitions of objective rate have been proposed (see Truesdell & Toupin [1961], Sects. 148-151 for a fairly complete catalog) formally any two choices lead to equivalent formulations by suitably adjusting the tensor $\mathbf{a}$ (Truesdell & Noll, [1965], p.402). In fact, all the objective rates are particular cases of the Lie derivative (Marsden & Hughes [1983], Sect. 1.6).

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ABSTRACT

It is explicitly shown that if the (spatial) elasticity tensor of an elastic material is taken as isotropic for all possible configurations then its coefficients cannot be constants, they must depend *non−trivially* on the jacobian determinant of the deformation gradient. Moreover, the assumption typically made for computational purposes that its coefficients remain constant for all possible configurations is incompatible with elasticity. It is further shown that an assumption widely used in the computational literature in the context of finite deformation plasticity, namely, relating an objective stress rate to the rate of deformation tensor through a fourth rank constant isotropic tensor, is also incompatible with elasticity, thus furnishing an example of hypoelastic material which is not elastic.

CONTENTS

1. Introduction.
2. Some Basic Notation.
3. Restrictions on the Elasticities of an Elastic Material.
4. Elastic Materials with Anisotropic Elasticities.
5. Integrability Conditions for Generalized Hypoelasticity.
   5.1. Spatial Description: Classical Hypoelasticity.
   5.2. Rotated Description: Generalized Hypoelasticity.
6. Concluding Remarks.
   References.
   APPENDIX

March 8, 1984

clearly unacceptable. Since this assumption is widely used in computation, it is of interest to characterize hyperelastic materials with isotropic (although non-constant) elasticities. We show that if the (spatial) elasticities of the material are *isotropic* in all possible configurations; i.e., $c_{ijkl} = \alpha \delta_{ij} \delta_{kl} + \beta [\delta_{ik} \delta_{jl} + \delta_{il} \delta_{jk}]$, then the coefficients α and β must depend non-trivially on the jacobian J for a stored energy function to exist. In fact the explicit form of the stored energy function corresponds to a neo-Hookean material extended to the compressible range by adding a function of J; i.e., $W \equiv U(J) + \frac{1}{2}\mu [I - 3]$. Since for infinitesimal deformation one must have $\alpha(J)\Big|_{J=1} = \lambda$, and $\beta(J)\Big|_{J=1} = 2\mu$, it follows that for deformations which are approximately isochoric, an assumption typically found in finite deformation metal plasticity, it is a reasonable approximation to regard the elasticities of the material as constant. Such an assumption, however, might not always be realistic since, as pointed out by Lee [1969], large elastic volumetric strains are indeed the most likely to occur in finite deformation plasticity.

Next, we consider hypoelastic behavior, i.e., the tensor **a** in the rate equation does not explicitly depend on the deformation gradient; it is only dependent on the current stress $\boldsymbol{\tau}$. By making use of conditions due essentially to Bernstein [1960], we show that rate equations involving several objective rates with **a** assumed to be constant and isotropic, are incompatible with elasticity.

Finally, we consider the generalized notion of hypoelasticity due to Green & McInnis [1967] which, as opposed to Truesdell's [1955] original proposal, does include anisotropic elasticity as a particular subset. Such an extension is achieved by establishing rate equations in terms of the *rotated* stress tensor and the *rotated* rate of deformation tensor. These *material* tensors are obtained by rotating back to the reference configuration the spatial stress and rate of deformation tensors with the rotation part of the deformation gradient. In Section 5. we derive appropriate conditions under which one recovers elasticity from this generalized notion of hypoelasticity. Our motivation for this is the recent use in finite deformation codes (e.g., Hallquist [1983]) of an objective rate which appears to have been first proposed by Green & Naghdi [1965], and which has recently received considerable attention particularly in connection with finite deformation plasticity (Dienes [1979], Johnson & Bammann [1983], Dafalias [1983]). This rate is obtained by rotating back to the *current* configuration the material time derivative of the rotated stress tensor. Our results show that *if the so-called Green-Naghdi rate is connected to the rate of deformation tensor through an isotropic tensor, the resulting model is incompatible with elasticity.*

Acknowledgments. We thank Tom Hughes, Jerry Marsden and Robert Taylor for helpful comments and many discussions.

2. Some Basic Notation.

Most of our discussion is concerned with both hyperelastic and hypoelastic rate constitutive equations formulated in the spatial description. For elasticity, the analog in the spatial description of the material formula relating the second Piola-Kirchhoff stress to Lagrangian strain, involves the Cauchy stress tensor and *the metric* $\mathbf{g}$ *of the ambient space.* Thus, even within the usual context of an Euclidean structure, it is essential for our discussion to employ general coordinates in order to keep track of the metric tensor.

Let B be the *reference configuration* of a body and S the *ambient space*. For simplicity we simply assume that $S \equiv \mathbb{R}^3$ and $B \subset \mathbb{R}^3$ is open bounded. We write $x = \phi(X,t) \equiv \phi_t(X)$ for a *motion* of the body, and denote by $\mathbf{F}(X)$ the *deformation gradient* at a material point $X \in B$. The metric tensors in the reference and current configurations B and $\phi(B)$, are denoted by $\mathbf{G}$ and $\mathbf{g}$, respectively. The *jacobian* J of $\mathbf{F}$ relative to $\mathbf{g}$ and $\mathbf{G}$ is then given by $J = \det(\mathbf{F}) \sqrt{\det(\mathbf{g})}/\sqrt{\det(\mathbf{G})}$. The right *Cauchy–Green* tensor $\mathbf{C}$ is defined as $\mathbf{C} = \mathbf{F}^T \mathbf{F}$. $\boldsymbol{\sigma}$ designates the *Cauchy* stress tensor and $\boldsymbol{\tau} \equiv J\, \boldsymbol{\sigma}$ the *Kirchhoff* stress tensor. The *first* and *second Piola-Kirchhoff* stress tensors are given by $\mathbf{P} = \boldsymbol{\tau} \cdot \mathbf{F}^{-T}$ and $\mathbf{S} = \mathbf{F}^{-1} \cdot \boldsymbol{\tau} \cdot \mathbf{F}^{-T}$, respectively. Next, we summarize the alternative descriptions employed in this paper. Further details are given in Simo & Marsden [1984].

Material Description. For isothermal *hyperelasticity* the stored energy function W depends on the motion through the *point values* of $\mathbf{C}(X)$; since $\mathbf{C} = \mathbf{F}^T \mathbf{F}$, with the standard abuse in notation we write $W = \tilde{W}(X,\mathbf{C}(X)) = \overline{\overline{W}}(X,\mathbf{F}(X))$. We then have the classical constitutive equations

$$\mathbf{S} = 2\rho_o \frac{\partial \tilde{W}(X,\mathbf{C})}{\partial \mathbf{C}} , \qquad \mathbf{P} = \rho_o \frac{\partial \overline{\overline{W}}(X,\mathbf{F})}{\partial \mathbf{F}} , \tag{2.1}$$

where ρ_o is the density in the reference configuration B and, by *conservation of mass*, $\rho = \rho_o / J$ is the density in the current configuration $\phi_t(B)$. Associated with (2.1) one defines the elasticity tensors

$$\mathbf{C} = 4\rho_o \frac{\partial^2 \tilde{W}}{\partial \mathbf{C} \partial \mathbf{C}} , \qquad \mathbf{A} = \rho_o \frac{\partial^2 \overline{\overline{W}}}{\partial \mathbf{F} \partial \mathbf{F}} , \tag{2.2}$$

with components C^{IJKL} and $A_i{}^J{}_k{}^L$, relative to material and spatial bases $\{\hat{\mathbf{E}}_I\}$ and $\{\hat{\mathbf{e}}_i\}$, respectively. We then have the basic relation

$$\mathbf{A} = \mathbf{F} \cdot \mathbf{C} \cdot \mathbf{F} + \mathbf{S} \otimes \mathbf{g}^{-1} , \quad or: \quad A^{iJkL} = F^i{}_I\, C^{IJKL}\, F^k{}_K + S^{JL}\, g^{ik} . \tag{2.3}$$

For simplicity we shall often employ the standard *pull–back/push–forward* notation of analysis in manifolds. (See e.g., Abraham, Marsden & Ratiu [1983], Sec. 4.2). As an example, for the right Cauchy-Green tensor we have the expression

$$C_{AB} = F^a{}_A F^b_B \, g_{ab} \circ \phi_t \ , \qquad i.e., \qquad \mathbf{C} = \phi_t{}^*(\mathbf{g}) \ . \tag{2.4}$$

Similarly, since $S^{AB} = (F^{-1})^A{}_a (F^{-1})^B{}_b \tau^{ab} \circ \phi_t$, we simply write: $\mathbf{S} = \phi_t{}^*(\boldsymbol{\tau})$; or, equivalently: $\boldsymbol{\tau} = \phi_{t*}(\mathbf{S})$.

Spatial Description. Due to relation (2.4) we may regard the stored energy as a function of the spatial metric $\mathbf{g}$ and $\mathbf{F}$ and write $\overline{W}(x,\mathbf{F}(X),\mathbf{g}(x))$ to express this dependence. For simplicity, we shall often omit explicit indication of the arguments in $\overline{W}$. We then have the following *spatial* constitutive equation for the Cauchy stress $\boldsymbol{\sigma}$ and associated *spatial* elasticity tensor $\mathbf{c}$

$$\boldsymbol{\sigma} = 2\rho \frac{\partial \overline{W}}{\partial \mathbf{g}} \ , \qquad \mathbf{c} \equiv 4\rho \frac{\partial^2 \overline{W}}{\partial \mathbf{g} \, \partial \mathbf{g}} \ . \tag{2.5}$$

Formula $(2.5)_1$ is due to Doyle & Ericksen [1956] and, as emphasized by Marsden & Hughes [1983] and Simo & Marsden [1984], plays a crucial role in a covariant formulation of elasticity. We note that the spatial elasticity tensor $\mathbf{c}$ is related to the material (second) elasticity tensor $\mathbb{C}$ through the Piola transformation:

$$\mathbf{c} = \frac{2}{J} \phi_{t*}(\mathbb{C}) \ , \qquad i.e., \qquad c^{ijkl} = \frac{2}{J} \mathbb{C}^{IJKL} F^i{}_I F^j{}_J F^k{}_K F^l{}_L \ . \tag{2.6}$$

Rotated (Material) Description. This description is obtained by rotating spatial objects back to the reference configuration with the rotation tensor as follows. By the polar decomposition theorem we have $\mathbf{F}(X) = \mathbf{R}(X) \cdot \mathbf{U}(X)$, where the *(two-point) rotation tensor* $\mathbf{R}(X)$ and the *material stretch* tensor $\mathbf{U}(X)$ satisfy the relations

$$G_{AB} = R^a{}_A R^b{}_B \, g_{ab} \circ \phi_t \ , \qquad C_{IJ} = U^A_I U^B_J G_{AB} \tag{2.7a}$$

Introducing the notions of *pull-back/push-forward* under either the *rotation part* $\mathbf{R}$ of $\mathbf{F}$, or the *stretching part* $\mathbf{U}$ of $\mathbf{F}$, relations (2.7a) may be written in the following compact form

$$\mathbf{G} = \mathbf{R}^*(\mathbf{g}) \ , \qquad \mathbf{C} = \mathbf{U}^*(\mathbf{G}) \ . \tag{2.7b}$$

The *rotated* stress tensor $\boldsymbol{\Sigma}$ is obtained by rotating $\boldsymbol{\sigma}$ back to the reference configuration, so that it is given by

$$\boldsymbol{\Sigma} \equiv \mathbf{R}^*(\boldsymbol{\sigma}) \ , \qquad i.e., \qquad \sigma^{ij} = R^i{}_I R^j{}_J \Sigma^{IJ} \circ \phi_t{}^{-1} \tag{2.8}$$

Remarkably, the material version of formula $(2.5)_1$ involves $\boldsymbol{\Sigma}$ and the metric tensor $\mathbf{G}$ as follows. By $(2.7a)_2$ we may regard the stored energy function, depending on $\mathbf{C}(X)$, as a function of the metric $\mathbf{G}(X)$ and $\mathbf{U}(X)$ and, accordingly, write $\hat{W}(X,\mathbf{G}(X),\mathbf{U}(X))$. The chain rule then leads to the following constitutive equation for $\boldsymbol{\Sigma}$ and the associated elasticity tensor $\boldsymbol{\Xi}$

$$\boldsymbol{\Sigma} = 2\rho \frac{\partial \hat{W}}{\partial \mathbf{G}} , \qquad \boldsymbol{\Xi} = 4\rho \frac{\partial^2 \hat{W}}{\partial \mathbf{G}\, \partial \mathbf{G}} \tag{2.9}$$

Formula $(2.9)_1$ is the material version of the Doyle-Ericksen formula $(2.5)_1$, Simo & Marsden [1984]. The *rotated elasticity tensor* $\boldsymbol{\Xi}$, with components Ξ^{ABCD}, is related to $\mathbf{C}$ and $\mathbf{c}$ according to

$$\boldsymbol{\Xi} = \frac{2}{J} \mathbf{U}_*(\mathbf{C}) , \qquad \boldsymbol{\Xi} = \mathbf{R}^*(\mathbf{c}) . \tag{2.10}$$

3. Restrictions on the Elasticities of an Elastic Material.

It is known (see, e.g., Truesdell & Noll [1965, pp.309]) that if a material is *elastic* then the major symmetries of any of its elasticity tensors furnish the necessary and sufficient conditions for a stored energy function to exist; i.e., for the *elastic* material to be *hyperelastic*. This result is simply the statement of Vainberg's theorem for potential operators applied to elasticity (see e.g., Marsden & Hughes [1983, p.250] or Oden & Reddy [1976, p.42]). It is essential to note that the material must be elastic for the result stated above to hold. Considering, for example, the material (convected) description, the condition that the material is elastic implies that a one-to-one map relating $\mathbf{C}$ to $\mathbf{S}$ must exist; i.e.,

$$\mathbf{S} = \hat{\mathbf{S}}(X, \mathbf{C}) , \qquad X \in B \tag{3.1}$$

To illustrate the role played by condition (3.1) consider the converse problem. Suppose one is given a material tensor

$$\mathbb{C}(X,\mathbf{C}) = \mathbb{C}^{IJKL}(X,\mathbf{C})\, \hat{\mathbf{E}}_I \otimes \hat{\mathbf{E}}_J \otimes \hat{\mathbf{E}}_K \otimes \hat{\mathbf{E}}_L , \tag{3.2}$$

which is *fully symmetric* and depends only on $\mathbf{C}$. For (3.2) to define the (material) second elasticity tensor of a hyperelastic material one must first verify whether a function of the form (3.1) exists such that

$$\frac{\partial \hat{\mathbf{S}}(X,\mathbf{C})}{\partial \mathbf{C}} = \mathbb{C}(X,\mathbf{C}) . \tag{3.3}$$

Equivalently, given $\mathbb{C}(X,\mathbf{C})$ which is assumed *fully symmetric* one must ensure that the system (3.3) is integrable. By Vainberg's theorem, the necessary and sufficient conditions are the following symmetry conditions :

$$\frac{\partial \mathbf{C}^{IJKL}}{\partial C_{MN}} = \frac{\partial \mathbf{C}^{IJMN}}{\partial C_{KL}}. \tag{3.4}$$

The example discussed below shows that one can construct fully symmetric tensors (indeed infinitely many) depending only on **C** which violate condition (3.4) and thus *do not* define an elastic material. We note that this example corresponds to one of the most widely used assumptions in computational mechanics (see, e.g., Key & Krieg, [1982]).

Remarks. (i) The argument sketched above can be carried out in the spatial description: Given a spatial tensor

$$\mathbf{c}(x,\mathbf{g},\mathbf{F}) = c^{ijkl}(x,\mathbf{g},\mathbf{F})\ \hat{\mathbf{e}}_i \otimes \hat{\mathbf{e}}_j \otimes \hat{\mathbf{e}}_k \otimes \hat{\mathbf{e}}_l\,, \tag{3.5}$$

which is *fully symmetric*, the necessary and sufficient conditions for the integrability of the system

$$\frac{\partial \hat{\sigma}(x,\mathbf{g},\mathbf{F})}{\partial \mathbf{g}} = \mathbf{c}(x,\mathbf{g},\mathbf{F}) \tag{3.6}$$

which gives $\sigma = \hat{\sigma}(x,\mathbf{g},\mathbf{F})$, are the symmetry conditions:

$$\frac{\partial c^{ijkl}}{\partial g_{mn}} \equiv \frac{\partial c^{ijmn}}{\partial g_{kl}} \tag{3.7}$$

(ii) Similar conditions can also be expressed in the *rotated* and the Lagrangian descriptions. In the former one is given a fourth order *material* tensor: $\Xi(X,\mathbf{G},\mathbf{U}) \equiv \Xi^{IJKL}\ \hat{\mathbf{E}}_I \otimes \hat{\mathbf{E}}_J \otimes \hat{\mathbf{E}}_K \otimes \hat{\mathbf{E}}_L$, whereas in the latter one is given a fourth order *two−point* tensor $\mathbf{A}(X,\mathbf{F})$, depending on the deformation gradient **F**. In these descriptions necessary and sufficient conditions analogous to (3.4) or (3.7) take the form

$$\frac{\partial \Xi^{IJKL}}{\partial G_{MN}} = \frac{\partial \Xi^{IJMN}}{\partial G_{KL}}\,, \quad \text{and} \quad \frac{\partial \mathbf{A}^{i\ j}_{\ I\ J}}{\partial F^k{}_K} = \frac{\partial \mathbf{A}^{i\ k}_{\ I\ K}}{\partial F^j{}_J} \ \square \tag{3.8}$$

Example: It is often assumed, particularly for computational purposes, that in any possible configuration of the body of interest, the spatial elasticity tensor **c** is the *constant isotropic* tensor of the linearized theory; i.e

$$\mathbf{c}^{ijkl} = \alpha\, g^{ij} g^{kl} + \beta [g^{ik} g^{jl} + g^{il} g^{jk}]\,, \tag{3.9a}$$

where α and β are taken equal to the Lame constants λ and μ of the linearized theory. Equivalently, by (2.6) the material second elasticity tensor takes the form

$$\mathbf{C}^{IJKL} = \frac{J}{2}\Big[\lambda\,(C^{-1})^{IJ}(C^{-1})^{KL} + \mu[(C^{-1})^{IK}(C^{-1})^{JL} + (C^{-1})^{IL}(C^{-1})^{JK}]\Big]\,, \tag{3.9b}$$

and from $(2.10)_2$ the rotated elasticity tensor is thus given by

$$\Xi^{IJKL} = \lambda\, G^{IJ}\, G^{KL} + \mu\, [G^{IK}\, G^{JL} + G^{IL}\, G^{JK}]\,. \tag{3.9c}$$

Notice that $\mathbf{C}$ is a fully symmetric tensor which depends only on $\mathbf{C}$. To check whether such an assumption defines an elastic material we may use any of the conditions (3.4), (3.7) or $(3.8)_1$. A straightforward computation then shows that condition (3.4) reduces to the following expression:

$$\frac{J}{4}\,[\lambda + \mu]\Big\{[(C^{-1})^{IK}\,(C^{-1})^{JL} + (C^{-1})^{IL}\,(C^{-1})^{JK}]\,(C^{-1})^{MN}$$
$$- [(C^{-1})^{IM}\,(C^{-1})^{JN} + (C^{-1})^{IN}\,(C^{-1})^{JM}]\,(C^{-1})^{KL}\Big\} \equiv 0 \tag{3.10}$$

Contraction of (3.10) with $C_{IK}\, C_{JL}\, C_{MN}$ shows that (3.10) holds provided $\lambda + \mu \equiv 0$. The condition $\lambda + \mu = 0$, although compatible with the (*strong ellipticity*) condition $\lambda + 2\mu > 0$, violates the (*pointwise* stability) condition of positive bulk modulus, $(3\lambda + 2\mu)/3 > 0$ (see Marsden & Hughes [1983, p.241]). Furthermore, the only possible response function compatible with the condition $\lambda + \mu = 0$ is a constant hydrostatic pressure; i.e.,

$$\lambda + \mu \equiv 0 \quad <=> \quad \boldsymbol{\sigma} = \lambda\, \mathbf{g} \tag{3.11}$$

We thus conclude that: *the assumption that the spatial elasticity tensor* $\mathbf{c} \equiv J^{-1}\partial(J\,\boldsymbol{\sigma})/\partial\mathbf{g}$ *of a non-linear material is isotropic and remains* **constant** *for every possible configuration, is incompatible with elasticity.*

In the next section we shall see that if the (spatial) elasticities of a material are isotropic of the form (3.9a), its coefficients must be non-trivial functions of J which, of course, must also reduce to the Lame constants for $J \equiv 1$. Explicit expressions for the stored energy and elasticities will also be given.

4. Hyperelasticity with Isotropic Elasticities.

In this Section we focus attention directly on hyperelasticity. In view of the example discussed above we first consider the form of the stored energy function characterizing an *hyperelastic* material with *isotropic* although *non−constant* spatial elasticity tensor.

Assume that the material is *hyperelastic* and *isotropic* so that the stored energy function is given by $W = \overline{W}(I, II, J)$, where I, II and $III = J^2$ are the principal invariants of $\mathbf{C}$ (and of $\mathbf{b} = \mathbf{F}\mathbf{F}^T$, by isotropy). Differentiation with respect to $\mathbf{C}$ together with the chain rule and

$(2.1)_1$ leads to the following classical material and spatial representations† (subindices I,II,and J denote derivatives with respect to the invariants):

$$\mathbf{S} = 2\left(\overline{W}_I + I\,\overline{W}_{II}\right)\mathbf{G}^{-1} - 2\,\overline{W}_{II}\,\mathbf{C} + J\,\overline{W}_J\,\mathbf{C}^{-1} \tag{4.1a}$$

$$\sigma = \left[\overline{W}_J + \frac{2}{J}\,II\,\overline{W}_{II}\right]\mathbf{g}^{-1} + \frac{2}{J}\,\overline{W}_I\,\mathbf{b} - 2J\,\overline{W}_{II}\,\mathbf{b}^{-1} \tag{4.1b}$$

Isotropic hyperelastic materials possessing a *spatial isotropic* elasticity tensor may now be easily characterized as follows. By further differentiating (4.1a) with respect to $\mathbf{C}$ and enforcing that the resulting elasticity tensor, which is given by $(2.2)_1$, is of the form $(2.9)_2$ we obtain the conditions:

$$\mathbf{C}^{IJKL} = \tfrac{1}{2}\frac{\partial}{\partial J}\left(J\,\overline{W}_J\right)(C^{-1})^{IJ}\,(C^{-1})^{KL} - \frac{J}{2}\,\overline{W}_J\,[(C^{-1})^{IK}\,(C^{-1})^{JL} + (C^{-1})^{JK}\,(C^{-1})^{IL}]$$

$$\overline{W}_{II} \equiv 0\,, \quad \text{and} \quad \overline{W}_{IJ} = 0\,, \quad \Rightarrow \quad \overline{W}(I,J) = \overline{U}(J) + \tfrac{1}{2}\mu\,I\,, \tag{4.2}$$

where μ = *constant*. Since the reference configuration B is chosen to be *stress free*, setting $\overline{U}(J) \equiv \lambda\,U(J) - \mu\log J$, where $U(J) \geqslant 0$ and $U(J) \equiv dU(J)/dJ = 0$ iff $J = 1$, we are led to a constitutive model which, in the spatial description, is given by

$$\overline{W} = \lambda\,U(J) + \tfrac{1}{2}\mu\,I - \mu\log J$$

$$\sigma^{ij} = \lambda\,\frac{dU(J)}{dJ}\,g^{ij} + \frac{\mu}{J}\,(b^{ij} - g^{ij}) \tag{4.3}$$

$$c^{ijkl} = \lambda\,\frac{d}{dJ}\left[J\,\frac{dU(J)}{dJ}\right]g^{ij}\,g^{kl} + \frac{1}{J}\left[\mu - \lambda\,J\,\frac{dU(J)}{dJ}\right](g^{ik}\,g^{jl} + g^{il}\,g^{jk})$$

It is evident from $(4.3)_3$ that it is not possible for c^{ijkl} (or for $J\,c^{ijkl}$) to be an isotropic tensor and at the same time have coefficients independent of J unless $\lambda + \mu = 0$, in agreement with our result of Section 3.

Remarks. (i) The form of stored energy function $(4.3)_1$ corresponds to a Neo-Hookean material which is extended to the *compressible* range by adding an extra function depending on J. Extensions of incompressible constitutive models, such as the Mooney-Rivlin or Neo-Hookean models, to the compressible regime are often considered in the context of the so-called *penalty method* (see e.g., Simo & Taylor [1982], Oden [1978]). The function $\overline{U}(J)$ is chosen so that the conditions $\lim_{J\to 0}\overline{U}(J) = \lim_{J\to\infty}\overline{U}(J) = \infty$ hold, and such that the (undeformed)

†Eq. (4.1b) can be derived directly from the spatial Doyle-Ericksen formula $(2.5)_1$. See Simo & Marsden [1984].

reference configuration $\phi = Identity$ is stress free. The choice of $\overline{U}(J)$ is, evidently, not unique. One possibility is

$$\overline{U}(J) = \frac{\lambda}{2}(\log J)^2 - \mu \log J \quad => \quad \alpha(J) = \frac{\lambda}{J}, \quad \beta(J) = \frac{1}{J}(\mu - \lambda \log J) \tag{4.4}$$

where $\alpha(J)$ and $\beta(J)$ are the coefficients appearing in (3.9a).

(ii) Clearly, the linearization of (4.3) and (4.4) at the reference configuration $\phi = Identity$ yields the classical infinitesimal model.

(iii) Consider the following *rate* constitutive equations

$$\dot{\mathbf{S}} = \mathbf{C}(X,\mathbf{C}) : \dot{\mathbf{C}}, \qquad \overset{\circ}{\sigma} = \mathbf{c}(x,\mathbf{g}) : \mathbf{d}, \tag{4.5}$$

where $\overset{\circ}{\sigma}$ is the Truesdell rate of Cauchy stress, and $\mathbf{c}$ is related to $\mathbf{C}$ through (2.6), so that $(4.5)_1$ and $(4.5)_2$ are *equivalent*, the latter being the spatial version of the former. The results of the previous section then show that *if* $\mathbf{c}$ *is the constant isotropic tensor given by* (3.9a), *so that* $\mathbf{C}$ *is given by* (3.9b), *equation* (4.5) *defines a material which is not elastic.* For $\mathbf{c}$ constant and isotropic, equation $(4.5)_2$ is a particular instance of a hypoelastic material (of grade 0) often employed in finite deformation computational plasticity (e.g., Pinsky [1981]). The result stated above then implies that (4.5) are not integrable, whence: $(4.5)_2$ *with* $\mathbf{c}$ *constant and isotropic furnishes a non-trivial example of a hypoelastic material which is not elastic.* Further examples of hypoelastic models which are not elastic will be discussed in the next section.

(iv) It is noted that, as a result of (4.3)-(4.4), if the class of deformations under consideration is approximately isochoric, then the coefficients in the isotropic elasticity tensor $(4.3)_3$ are approximately constant. Thus, the assumption often made, particularly in the context of finite deformation metal plasticity, that $\mathbf{c}$ remains constant in the rate constitutive equation $(4.5)_2$ is valid provided large volumetric strains do not occur. As pointed out by Lee [1969] large volumetric *elastic* strains are most likely to occur in finite deformation plasticity, since the "deviatoric" strains are limited by the yield condition which, at least for metals, is often regarded as pressure insensitive. □

5. Integrability Conditions for Generalized Hypoelasticity.

In this Section we address conditions under which rate constitutive equations for both classical and generalized hypoelasticity do indeed define an elastic material. Again our objective is to show that widely used rate constitutive equations in the computational mechanics literature, particularly within the context of finite deformation plasticity, fail to meet these conditions and thus define materials which in the finite deformation range are not elastic. A complete treatment of classical hypoelasticity, which employs the *spatial* description, and its interrelation with elasticity is due to Bernstein [1960]. We summarize the relevant conditions below. Subsequently, we develop analogous conditions for generalized hypoelasticity, which is formulated using the *rotated* description, in terms of the rotated stress tensor, and the rotated rate of deformation tensor.

5.1. Spatial Description: Classical Hypoelasticity

Let $\overset{\nabla}{\boldsymbol{\tau}}$ denote *any* (spatial) *objective rate* of the Kirchhoff stress tensor (Truesdell & Toupin [1960] Sect. 147-152). Constitutive equations for classical hypoelasticity (Truesdell & Noll Sect. 99) may be formulated as

$$\overset{\nabla}{\boldsymbol{\tau}} = \mathbf{a}(\mathbf{g},\boldsymbol{\tau}) : \mathbf{d} \;, \qquad i.e., \quad \overset{\nabla}{\tau}{}^{ij} = a^{ijkl}\, d_{kl} \;, \tag{5.1}$$

where $\mathbf{d} = \frac{1}{2}\phi_t{}^*(\dot{\mathbf{C}}) \equiv \frac{1}{2}\mathbf{F}^{-T}\,\dot{\mathbf{C}}\,\mathbf{F}^{-1}$ is the rate of deformation tensor. Equation (5.1) may be rewritten in terms of the material time derivative $\dot{\boldsymbol{\tau}} \equiv D\boldsymbol{\tau}/Dt$ of the Kirchhoff stress tensor as

$$\dot{\boldsymbol{\tau}} = \mathbf{b}(\mathbf{g},\boldsymbol{\tau}) : \nabla\mathbf{v}_t + \mathbf{a}(\mathbf{g},\boldsymbol{\tau}) : \mathbf{d} \equiv \mathbf{h}(\mathbf{g},\boldsymbol{\tau}) : \nabla\mathbf{v}_t \;, \tag{5.2}$$

where $\nabla\mathbf{v}_t$ designates the spatial velocity gradient and $\mathbf{b}(\mathbf{g},\boldsymbol{\tau}) = b^{ijkl}(\mathbf{g},\boldsymbol{\tau})\,\hat{\mathbf{e}}_i \otimes \hat{\mathbf{e}}_j \otimes \hat{\mathbf{e}}_k \otimes \hat{\mathbf{e}}_l$ is a spatial tensor depending on the assumed stress rate $\overset{\nabla}{\boldsymbol{\tau}}$. Necessary and sufficient conditions for (5.1) to define an elastic material, i.e., for a function $\boldsymbol{\tau} = \hat{\boldsymbol{\tau}}(\mathbf{g},\boldsymbol{\tau})$ to exist, are due to Bernstein (see Truesdell & Noll [1965] pp.409, for a summary account) and may be written as

$$\frac{\partial h^{ijkl}}{\partial \tau^{rs}}\, h^{rsmn} - \frac{\partial h^{ijmn}}{\partial \tau^{rs}}\, h^{rskl} + h^{ijml}\, g^{kn} - h^{ijkn}\, g^{ml} = 0 \tag{5.3}$$

If equation (5.1) is expressed in terms of the Cauchy stress tensor, the appropriate conditions are again (5.3) with $\boldsymbol{\tau}$ replaced by $\boldsymbol{\sigma}$.

The following two examples, the first one already treated in Section 3., give instances in which conditions (5.3) are violated.

Examples. (i) Let the spatial tensor $\mathbf{a}(\mathbf{g},\boldsymbol{\tau})$ be the *constant isotropic* elasticity tensor of the linear theory, and let the left hand side of (5.1) be the *Truesdell* rate of Cauchy stresses. Equation (5.2) then takes the form:

$$\dot{\sigma}^{ij} = h^{ijkl}\, v_{k|l} \equiv [a^{ijkl} + g^{ik}\,\sigma^{jl} + g^{il}\,\sigma^{jk}]\, v_{k|l} \;, \tag{5.4}$$

with $a^{ijkl} \equiv \lambda g^{ij}\, g^{kl} + \mu\,[g^{ik}\, g^{jl} + g^{il}\, g^{jk}]$. Substitution of (5.4) into (5.3) yields after lengthy but otherwise straightforward manipulation, the condition

$$[\lambda + \mu]\left\{ g^{ln}\,(g^{ik}\, g^{jm} + g^{im}\, g^{jk}) - g^{km}\,(g^{in}\, g^{jl} + g^{il}\, g^{jn}) \right\} = 0 \,, \tag{5.5}$$

which, upon contraction with $g_{ln} g_{ik} g_{jm}$, again reduces to the condition $\lambda + \mu \equiv 0$, already derived in Section 3. Conditions (5.3) are also violated if the left hand side of (5.1) is replaced by the Lie derivative of the Kirchhoff stresses (often referred to as convected derivative).

(ii) Consider next the *co−rotational* stress rate, often associated with the names Zaremba, Jaumann and Noll. Rate constitutive equations (5.1) then take the form

$$\dot{\boldsymbol{\tau}} = \mathbf{w} \cdot \boldsymbol{\tau} + \boldsymbol{\tau} \cdot \mathbf{w}^T + \mathbf{a}(\mathbf{g},\boldsymbol{\tau}) : \mathbf{d} , \tag{5.6}$$

where $\mathbf{w} = \frac{1}{2} [\mathbf{d} - \mathbf{d}^T]$ is the *spin* tensor. The tensor $\mathbf{b}$ associated with this stress rate then has the explicit expression

$$b^{ijkl} \equiv \tfrac{1}{2}[g^{ik} \tau^{lj} + g^{kj} \tau^{il} - g^{lj} \tau^{ik} - g^{il} \tau^{jk}] . \tag{5.7}$$

A lengthy calculation again reveals that conditions (5.3) are violated if the tensor $\mathbf{a}(\mathbf{g},\boldsymbol{\tau})$ is assumed to be the constant isotropic tensor of the linearized theory. We omit the details. Thus, *assuming* $\mathbf{a}(\mathbf{g},\boldsymbol{\tau})$ *constant isotropic in*(5.6) *for all possible configurations is incompatible with elasticity.*

Remarks. (i) If the material is elastic, thus conditions (5.3) are satisfied, one can immediately write down the *spatial* elasticities $\mathbf{c} \equiv J^{-1} \partial \boldsymbol{\tau} / \partial \mathbf{g}$. Noting that the spatial rate form of the hyperelastic constitutive equation $(2.5)_1$ may be written as

$$\mathrm{L}_{\mathbf{v}} \boldsymbol{\tau} \equiv \dot{\boldsymbol{\tau}} - \nabla \mathbf{v} \cdot \boldsymbol{\tau} - \boldsymbol{\tau} \cdot \nabla^T \mathbf{v}_t = J \, \mathbf{c}(\mathbf{g},\mathbf{F}) : \mathbf{d} , \tag{5.8}$$

where $\mathrm{L}_{\mathbf{v}} \boldsymbol{\tau}$ is the Lie derivative of Kirchhoff stresses (see, e.g., Simo & Marsden [1984]), and $\mathbf{c}(\mathbf{g},\mathbf{F})$ is the spatial elasticity tensor given by $(2.5)_2$; by comparing (5.2) and (5.8) we obtain

$$c^{ijkl} \equiv J^{-1} [a^{ijkl} + b^{ijkl}] - g^{ik} \tau^{jl} - g^{jk} \tau^{il} , \tag{5.9}$$

where $\mathbf{b}(\mathbf{g},\boldsymbol{\tau})$ depends on the assumed objective rate.

(ii) If conditions (5.3) are satisfied, the symmetry conditions $c^{ijkl} = c^{klij}$ are necessary and sufficient conditions for the elastic material to be hyperelastic. It is essential to observe, however, that these symmetry conditions must hold *in addition to conditions* (5.3). Indeed, the two examples discussed above have tensors $\mathbf{c}$ defined by (5.9) which are symmetric and yet they do not even define an elastic material. The symmetry conditions $c^{ijkl} = c^{klij}$ alone guarantee the existence of the so-called incremental potentials (Hill [1958]). □

5.2. Rotated Description: Generalized Hypoelasticity.

We consider the following rate constitutive equations which generalize those of hypoelasticity (Green & McInnis [1967])

$$\dot{\mathcal{T}} = \Gamma(G,\mathcal{T}) : \Lambda\,, \tag{5.10}$$

where $\Lambda \equiv \mathbf{R}^*(\mathbf{d})$ is the *rotated rate of deformation* tensor. Our objective is to establish integrability conditions analogous to (5.3) under which rate equations (5.10) reduce to elasticity. The duality existing between the spatial and rotated descriptions enables one to construct the following argument analogous to that of Bernstein.

Integrability Conditions. If the material is elastic, one must have the following representation for the rotated stress tensor:

$$\mathcal{T} = \tilde{\mathcal{T}}(G,U) \tag{5.11}$$

In the rotated description, the kinematic tensor analogous to the spatial velocity gradient is defined as

$$\mathbf{L} \equiv \dot{\mathbf{U}}\mathbf{U}^{-1}, \qquad i.e., \qquad L^I{}_J = \dot{U}^I{}_A\,(U^{-1})^A{}_J \tag{5.12}$$

We note that the rotated rate of deformation tensor Λ is the *symmetric* part of the tensor $\mathbf{L}$,

$$\Lambda = [\dot{\mathbf{U}}\cdot\mathbf{U}^{-1}]^S\,, \quad i.e., \quad \Lambda_{IJ} = \tfrac{1}{2}[G_{IA}\,L^A{}_J + G_{JA}\,L^A{}_I]\,. \tag{5.13}$$

Taking the material time derivative of (5.11) and making use of (5.12) we have

$$\dot{\mathcal{T}} = \frac{\partial\tilde{\mathcal{T}}(G,U)}{\partial U}\,\mathbf{U}^T : \mathbf{L} \tag{5.14}$$

Comparing (5.10) and (5.14) we arrive at a system of partial differential equations which in component form reads

$$\frac{\partial\tilde{\mathcal{T}}^{IJ}}{\partial U^K{}_A} = \Gamma^{IJ}{}_K{}^L\,(U^{-1})^A{}_L \tag{5.15}$$

Since the integrability conditions for (5.15) are the symmetry conditions: $\partial\mathcal{T}^{IJ}/\partial U^K{}_A\,\partial U^L{}_B = \partial\mathcal{T}^{IJ}/\partial U^L{}_B\,\partial U^K{}_A$, we are led to the following conditions, analogous to (5.3):

$$\frac{\partial\Gamma^{IJKL}}{\partial\mathcal{T}^{RS}}\Gamma^{RSMN} - \frac{\partial\Gamma^{IJMN}}{\partial\mathcal{T}^{RS}}\Gamma^{RSKL} + \Gamma^{IJML}\,G^{KN} - \Gamma^{IJKN}\,G^{ML} = 0 \tag{5.16}$$

Next, we exhibit an example of practical interest, which has been considered in recent literature, and which fails to satisfy conditions (5.16).

Example. Consider the rate of Kirchhoff (or Cauchy) stress tensor obtained by *rotating back to the current configuration the material time derivative of the rotated Kirchhoff* (or rotated Cauchy) stress tensor. Denoting this rate by $\overset{\square}{\tau}$, we have

$$\overset{\square}{\tau} \equiv \mathbf{R}_{*}\left[\frac{\partial}{\partial t}\mathbf{R}^{*}(\tau)\right] = \dot{\tau} - \boldsymbol{\Omega}_{v}\cdot\tau - \tau\cdot\boldsymbol{\Omega}_{v}^{T}, \tag{5.17}$$

where $\boldsymbol{\Omega}_{v} \equiv \dot{\mathbf{R}}\cdot\mathbf{R}^{T}$ is skew-symmetric, and $\mathbf{R}$ is the rotation tensor obtained from the deformation gradient through the polar decomposition $\mathbf{F} = \mathbf{R}\cdot\mathbf{U}$. This is the objective rate first proposed by Green & Naghdi [1965], in a different context and for another purpose, and recently considered by Dienes [1979], Johnson & Bammann [1983], Dafalias [1983], among others. By $\mathbf{R}$-rotating the (material) rate constitutive equations (5.10) to the current configuration we obtain

$$\overset{\square}{\tau} = \mathbf{R}_{*}\left[\boldsymbol{\Gamma} : \boldsymbol{\Lambda}\right] = \mathbf{R}_{*}(\boldsymbol{\Gamma}) : \mathbf{d}, \tag{5.18}$$

that is, rate constitutive equations of the form (5.1) with $\mathbf{a} \equiv \mathbf{R}_{*}(\boldsymbol{\Gamma})$ and the rate of stress taken to be the *rotated rate* of *rotated stress* (5.17). If it is assumed (see e.g. Dienes [1979]) that for this type of rate constitutive equation $\mathbf{a}$ is a (constant) *isotropic* tensor; i.e., $a^{ijkl} = \lambda\, g^{ij}\, g^{kl} + \mu\, (g^{ik}\, g^{jl} + g^{il}\, g^{jk})$, then, since $\boldsymbol{\Gamma} = \mathbf{R}^{*}(\mathbf{a})$, by (5.18) we have

$$\Gamma^{IJKL} = \lambda\, G^{IJ}\, G^{KL} + \mu\, (G^{IK}\, G^{JL} + G^{IL} G^{JK}) \tag{5.19}$$

To check whether the choice for $\boldsymbol{\Gamma}$ expressed by (5.19) defines an elastic material, we substitute (5.19) into (5.16), obtaining the conditions:

$$\mu\left\{G^{KN}\, [G^{IM}\, G^{JL} + G^{IL}\, G^{JM}] - G^{LM}\, [G^{IK}\, G^{JN} + G^{IN}\, G^{JK}]\right\} \equiv 0 \tag{5.20}$$

Contracting (5.20) with $G_{KN}\, G_{IM}\, G_{JL}$ we obtain the condition: $\mu \equiv 0$. Thus, *The rate constitutive equation* (5.1) *formulated in terms of the Green-Naghdi rate* (5.17), *with* $\mathbf{a}(\mathbf{g},\tau)$ *being the constant isotropic tensor of the linear theory, does not define an elastic material, unless* $\mu \equiv 0$. Clearly, such a condition is inadmissible and one must conclude that this model does not represent an elastic material.

Remarks. (i) The fact that rate constitutive equations (5.10) do not define an hyperelastic material if Γ is given by (5.19) can be checked by a direct computation starting from the stored energy function. In the Appendix, the general expression for the tensor Γ associated with an isotropic elastic material is derived. By direct inspection it is clear that Γ can never be an isotropic tensor (except, of course, at the configuration $\phi = Identity$).

(ii) If the material is elastic, the tensor $\mathbf{\Gamma}$ should not be confused with the *rotated* elasticity tensor $\mathbf{\Xi}$ which is defined by $(2.9)_2$ and connected to the spatial and material elasticities through formulae (2.10). $\mathbf{\Xi}$ is associated with the rate equation $\mathbf{R}^T \cdot \overset{\circ}{\boldsymbol{\sigma}} \cdot \mathbf{R} \equiv \mathbf{\Xi} : \mathbf{\Lambda}$, where $\mathbf{R}^T \cdot \overset{\circ}{\boldsymbol{\sigma}} \cdot \mathbf{R}$ is the rotated Truesdell rate. This is simply a particular Lie derivative (see Simo & Marsden [1984]).

6. Concluding Remarks.

It has been shown that many of the rate constitutive equations currently in use in the field of computational mechanics, especially with reference to inelasticity, define hypoelastic materials which in the finite deformation range are not elastic. Therefore, not only does a stored energy function fail to exist but, more dramatically, an explicit stress response function cannot be obtained. An unacceptable physical implication of this result is that, according to a theorem of Bernstein [1960], the net work produced in a closed cycle must be positive. It should be noted, however, that as our results of Section 4. demonstrate, assumptions such as that of constant spatial elasticities might be reasonable in certain situations, provided that an additional hypothesis such as infinitesimal elastic volume change holds.

From a computational standpoint it will be shown in a forthcoming paper that, for finite deformation rate-independent plasticity, the fact that an explicit expression for the potential associated with the elastic part is available plays a crucial role in the formulation of efficient numerical algorithms. We note that this is at variance with most of the algorithms currently employed which operate directly with the tangent elasticities.

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APPENDIX

The following results will be needed. Let I, II, and III be the principal invariants of $\mathbf{C}$, and Λ the rotated rate of deformation tensor. Then, one has

$$\dot{I} = 2\,tr(\mathbf{C}\cdot\Lambda)\,, \quad \dot{II} = 2\,tr[(II\,\mathbf{I} - III\,\mathbf{C}^{-1})\cdot\Lambda]\,, \quad \dot{III} = 2\,III\,tr(\Lambda) \tag{A.1}$$

For simplicity, we introduce the following notation: Let $\mathbf{A}$ be any symmetric second rank tensor. We denote by $\mathbf{I}_{\mathbf{A}}$ the fourth rank symmetric tensor with components:

$$\mathbf{I}_{\mathbf{A}}^{IJKL} = \tfrac{1}{2}[A^{IK}A^{JL} + A^{IL}A^{JK}] \tag{A.2}$$

The following results can be shown to hold:

$$\dot{\mathbf{C}} = 2\,\mathbf{I}_{\mathbf{U}} : \Lambda\,, \quad \text{and} \quad [\mathbf{C}^{-1}]^{\cdot} = -2\,\mathbf{I}_{\mathbf{U}^{-1}} : \Lambda\,, \tag{A.3}$$

where $\mathbf{U}$ is the stretching tensor. Since $\boldsymbol{\mathcal{T}} = \mathbf{R}^T\cdot\boldsymbol{\tau}\cdot\mathbf{R}$, from (4.1b) one has the representation:

$$\boldsymbol{\mathcal{T}} = 2\left\{\alpha\,\mathbf{G} + \overline{W}_I\,\mathbf{C} - III\,\overline{W}_{II}\,\mathbf{C}^{-1}\right\} \tag{A.4}$$

$$\text{where :} \qquad \alpha \equiv [II\,\overline{W}_{II} + III\,\overline{W}_{III}]$$

Taking the material time derivative of (A.4) and using (A.1)-(A.3) together with the chain rule, leads to the following expression for the tensor $\boldsymbol{\Gamma}$ in constitutive equation $\dot{\boldsymbol{\mathcal{T}}} = \boldsymbol{\Gamma} : \Lambda$,

$$\begin{aligned}\boldsymbol{\Gamma} \equiv\ & 8\,\alpha_I\,[\mathbf{G}\otimes\mathbf{C}]^S - 8\,III\,\alpha_{II}\,[\mathbf{G}\otimes\mathbf{C}^{-1}]^S - 8\,III\,\overline{W}_{I\,II}\,[\mathbf{C}\otimes\mathbf{C}^{-1}]^S \\ & + 4\,(II\,\alpha_{II} + III\,\alpha_{III})\,\mathbf{G}\otimes\mathbf{G} + 4\,\overline{W}_{I\,I}\,\mathbf{C}\otimes\mathbf{C} - 4\,III^2\,\overline{W}_{II\,II}\,\mathbf{C}^{-1}\otimes\mathbf{C}^{-1} \\ & + 4\,\overline{W}_I\,\mathbf{I}_{\mathbf{U}} + 4\,III\,\overline{W}_{II}\,\mathbf{I}_{\mathbf{U}^{-1}}\end{aligned} \tag{A.5}$$

where $[\ \cdot\ ]^S$ indicates symmetric part.