An anisotropic elastic formulation for configurational forces in stress space

Anurag Gupta · Xanthippi Markenscoff

Abstract A new variational principle for an anisotropic elastic formulation in stress space is constructed, the Euler–Lagrange equations of which are the equations of compatibility (in terms of stress), the equilibrium equations and the traction boundary condition. Such a principle can be used to extend recently obtained configurational balance laws in stress space to the case of anisotropy.

Keywords Configurational forces · Stress formulation · Anisotropy

1 Introduction

Configurational forces (in solid mechanics) provide us with the forces necessary for driving the dissipative mechanisms which are responsible for the kinetics of defect flow. In case of a thermodynamic equilibrium, vanishing of configurational forces are additional relations required for a complete determination of the system. Popular examples are dislocation motion, crack propagation, delamination etc. (Eshelby 1956; Maugin 1993; Gupta and Markenscoff 2007 and references therein). A systematic way of obtaining expressions for these forces follows from Noether's theorem (Noether 1918; Gelfand and Fomin 2000), where given a variational principle, conserved integrals (path independent in 2D) are obtained as necessary and sufficient conditions for satisfying respective symmetries of the variational principle. Configurational forces are then interpreted as these conserved integrals which vanish in case of a non-dissipative flow, but fail to vanish if dissipative mechanisms are active (i.e. when symmetries are broken) (Eshelby 1975).

In (Li et al. 2005), the authors use a variational principle of Pobedrya (Pobedrja 1980; Pobedria and Holmatov 1982) to obtain a class of conservation laws. The Euler–Lagrange equations of this principle were the Beltrami–Michell compatibility equations in the domain and stress equilibrium with traction boundary condition on the boundary. It was shown by Pobedrya (1980) and Kucher et al. (2004) that such a boundary value problem in terms of stress is well defined and it is sufficient to satisfy equilibrium on the boundary to satisfy it in the domain. The conservation laws were obtained assuming the case of linear, homogeneous and isotropic elasticity with vanishing body forces and incompatibility. In a sequel paper (Markenscoff and Gupta 2007) these were extended for non-vanishing incompatibility and body force distribution and applicability of such quantities was demonstrated using examples from dislocation theory and heat flow in a domain with a spherical cavity. More recently these

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conserved quantities (or configurational forces) were interpreted as the necessary and sufficient dissipative mechanisms so as to maintain compatibility during the propagation of a inhomogeneity (or a defect) (Gupta and Markenscoff 2007).

The present paper aims at formulating a variational principle which would extend the earlier principle of Pobedrya (1980) to the case of anisotropy. Such a variational principle can then be used to obtain the configurations balance laws in stress space (Li et al. 2005; Markenscoff and Gupta 2007) for the case of anisotropic elasticity. Before constructing a variational principle in Sect. 3, we first discuss Pobedrya's formulation of the boundary value problem of anisotropic linear elasticity in stress space.

2 Formulation

The classical problem of linear and homogeneous elasticity in terms of stress involves equilibrium and compatibility equations in the bulk (bulk is denoted by $\Omega \in \mathbf{R}^3$) and a traction boundary condition (boundary is denoted by $\partial\Omega \equiv \Omega \cap \mathbf{R}^3/\Omega$). Assuming absence of body forces and inertial terms, the equilibrium equation is given as follows,

$$\sigma_{ij,j} = 0, \quad \forall x_k \in \Omega \tag{1}$$

with $\sigma_{ij}(x_k)$ denoting the stress. The compatibility relations are written in terms of strain $e_{ij}(x_k)$ as,

$$\eta_{ij} \equiv -\epsilon_{ikl}\epsilon_{jmn}e_{ln,km} = 0, \quad \forall x_k \in \Omega \tag{2}$$

where ϵ_{ikl} is the alternating tensor and η_{ij} is the Kröner's incompatibility tensor (Kröner 1981) (vanishing of which ensures compatibility). The compatibility relations in terms of stresses can be obtained by using an appropriate constitutive law in the framework of linear elasticity,

$$e_{ij} = D_{ijkl}\sigma_{kl}, \tag{3}$$

where D_{ijkl} is the (constant) elastic compliance tensor. Denote $\bar{\eta}_{ij}$ as the incompatibility tensor thus obtained as a function of the stress tensor. Therefore the compatibility relations in terms of stresses are,

$$\bar{\eta}_{ij} \equiv -D_{lnpq}\epsilon_{ikl}\epsilon_{jmn}\sigma_{pq,km} = 0, \quad \forall x_k \in \Omega. \tag{4}$$

Equations 1 and 4 are to be supplemented by prescribing traction on the boundary,

$$\sigma_{ij}n_j = p_i, \quad \forall x_k \in \partial\Omega \tag{5}$$

with $p_i(x_k)$ being the prescribed traction and $n_j(x_k)$, the unit normal to $\partial\Omega$. The system of Eqs. 1 and 4 is over-determined as there are nine equations for six unknowns. On the boundary, there is an under-determinacy by three conditions (Georgievskii and Pobedrya 2004). Pobedrya (1994) has introduced a set of equations to deal with this problem. His formulation transfers the equilibrium Eq. 1 to the boundary and therefore leaving only Eq. 4 to be solved in the bulk. The resulting system of equations is well defined over the whole domain (Pobedrja 1980; Kucher et al. 2004). An outline of his theory for anisotropic elasticity is now discussed.

Let $a_{ij}^{(\alpha)}$ be a set of tensors ($\alpha = 1, \ldots, N$) constructed from the invariant basis tensors of the symmetry group $\mathcal{G}$. These invariant basis tensors were originally obtained for the representation of anisotropic tensors and there are systematic procedures for their evaluation corresponding to the symmetry group $\mathcal{G}$ (see (Weyl 1946; Smith and Rivlin 1957; Smith 1970) for foundations and (Markenscoff 1976) for a possible application). The tensors $a_{ij}^{(\alpha)}$ are constructed such that they are pairwise orthogonal and add up to the unit tensor,

$$\frac{a_{ij}^{(\alpha)}a_{ij}^{(\beta)}}{a_{(\alpha)}a_{(\beta)}} = \delta_{\alpha\beta}, \quad \sum_{\alpha=1}^{N} a_{ij}^{(\alpha)} = \delta_{ij}, \tag{6}$$

where $a_{(\alpha)} = \sqrt{a_{ij}^{(\alpha)}a_{ij}^{(\alpha)}}$ (no summation implied under α). A set of linear invariants of the incompatibility tensor can then be constructed as,

$$\eta_{(\alpha)} = \eta_{ij}a_{ij}^{(\alpha)}. \tag{7}$$

Define a tensor H_{ij} as,

$$H_{ij} = \eta_{ij} + \sum_{\alpha=1}^{N} \xi^{(\alpha)}\eta_{(\alpha)}a_{ij}^{(\alpha)}, \tag{8}$$

where $\xi^{(\alpha)}$ are arbitrary scalars. The condition $H_{ij} = 0$ is equivalent to the compatibility condition (2), $\eta_{ij} = 0$ if $\xi^{(\alpha)} \neq -(a_{(\alpha)})^{-2}$ for all α. Indeed if $\eta_{ij} = 0$ then by definitions (7) and (8), $H_{ij} = 0$. If $H_{ij} = 0$, then by Eq. 8, $H_{ij}a_{ij}^{(\beta)} = \eta_{(\beta)} + \xi^{(\beta)}\eta_{(\beta)}(a_{(\beta)})^2 = 0$, where relations (6) and (7) have been used. If $\xi^{(\alpha)} \neq -(a_{(\alpha)})^{-2}$, then $\eta_{(\alpha)} = 0$ and consequently, using $H_{ij} = 0$ in (8) we obtain $\eta_{ij} = 0$.

Define a vector valued function,

$$A_i = R_{ij}\sigma_{jk,k}, \tag{9}$$

where R_{ij} is a positive definite operator. Therefore, condition $A_i = 0$ is equivalent to equilibrium relation (1). Construct a tensor $\mathrm{A}_{ij} = A_{i,j} + A_{j,i}$ whose linear invariants are denoted by $A_{(\alpha)} = \mathrm{A}_{ij} a_{ij}^{(\alpha)}$. Another tensor can then be defined as,

$$\bar{\mathrm{A}}_{ij} = \mathrm{A}_{ij} + \sum_{\alpha=1}^{N} \xi^{(\alpha)} A_{(\alpha)} a_{ij}^{(\alpha)}. \tag{10}$$

Reasoning along the lines of the paragraph following Eq. 8, we note that $\mathrm{A}_{ij} = 0$, if and only if $\bar{\mathrm{A}}_{ij} = 0$ given that $\xi^{(\alpha)} \neq -(a_{(\alpha)})^{-2}$.

Form a tensor,

$$\bar{H}_{ij} = H_{ij}^{\sigma} + \bar{\mathrm{A}}_{ij}, \tag{11}$$

where superscript σ in H_{ij}^{σ} indicates that H_{ij} is expressed in terms of stress rather than strain (using (6)). Therefore $H_{ij}^{\sigma} = \bar{\eta}_{ij} + \sum_{\alpha=1}^{N} \xi^{(\alpha)} \bar{\eta}_{(\alpha)} a_{ij}^{(\alpha)}$ where $\bar{\eta}_{ij}$ is as given in (4) and $\bar{\eta}_{(\alpha)} = \bar{\eta}_{ij} a_{ij}^{(\alpha)}$. The formulation of Pobedrya (Pobedrya 1994) involves satisfying equation,

$$\bar{H}_{ij} = 0, \quad \forall x_k \in \Omega \tag{12}$$

in the bulk and conditions,

$$\sigma_{ij} n_j = p_i, \quad \sigma_{ij,j} = 0, \quad \forall x_k \in \partial\Omega \tag{13}$$

on the boundary. The solution to Eqs. 12 and 13 satisfies equations of equilibrium and of compatibility as given in (1) and (4). From Eqs. 11 and 12 obtain, $\bar{H}_{ij} a_{ij}^{(\beta)} = (\bar{\eta}_{(\beta)} + A_{(\beta)})(1 + \xi^{(\beta)} (a_{(\beta)})^2) = 0$, and therefore if $\xi^{(\alpha)} \neq -(a_{(\alpha)})^{-2}$ is satisfied, we obtain,

$$\bar{\eta}_{(\beta)} + A_{(\beta)} = 0. \tag{14}$$

Differentiate Eq. 11 to get,

$$\bar{H}_{ij,j} = H_{ij,j}^{\sigma} + \bar{\mathrm{A}}_{ij,j} \tag{15}$$

which will now be evaluated term by term. Let $\bar{\eta}$ denote the trace of $\bar{\eta}_{ij}$. Therefore $\bar{\eta} = \bar{\eta}_{ij}\delta_{ij}$ and from (4), $\bar{\eta} = 2(D_{iijk}\sigma_{jk,pp} - D_{mnjk}\sigma_{jk,mn})$. It is easy to see that $\bar{\eta}_{ij,j} = \frac{1}{2}(\bar{\eta})_{,i}$. Also, note that $\bar{\eta} = \bar{\eta}_{ij}\delta_{ij} = \bar{\eta}_{ij} \sum_{\alpha=1}^{N} a_{ij}^{(\alpha)} = \sum_{\alpha=1}^{N} \bar{\eta}_{(\alpha)}$, where the first relation in (6) has been used. Using these results $H_{ij,j}^{\sigma}$ can then be evaluated as,

$$H_{ij,j}^{\sigma} = \sum_{\alpha=1}^{N} \left(\frac{1}{2}\delta_{ij} + \xi^{(\alpha)} a_{ij}^{(\alpha)} \right) \bar{\eta}_{(\alpha),j}. \tag{16}$$

For calculating $\bar{\mathrm{A}}_{ij,j}$, start from (10) and note that $\mathrm{A}_{ij,j} = \Delta A_i + A_{j,ji}$ and $A_{j,j} = \frac{1}{2}\mathrm{A}_{ij}\delta_{ij} = \frac{1}{2}\mathrm{A}_{ij} \sum_{\alpha=1}^{N} a_{ij}^{(\alpha)} = \frac{1}{2}\sum_{\alpha=1}^{N} A_{(\alpha)}$ to obtain,

$$\bar{\mathrm{A}}_{ij,j} = \Delta A_i + \sum_{\alpha=1}^{N} \left(\frac{1}{2}\delta_{ij} + \xi^{(\alpha)} a_{ij}^{(\alpha)} \right) A_{(\alpha),j} \tag{17}$$

and thereafter combine Eqs. 16 and 17 to write,

$$\bar{H}_{ij,j} = \Delta A_i + \sum_{\alpha=1}^{N} \left(\frac{1}{2}\delta_{ij} + \xi^{(\alpha)} a_{ij}^{(\alpha)} \right) \times (\bar{\eta}_{(\alpha)} + A_{(\alpha)})_{,j}. \tag{18}$$

Substitution of relations (12) and (14) into (18) then results into $\Delta A_i = 0$, i.e. A_i is harmonic. The vector A_i vanishes on the boundary (by $(13)_2$) and therefore it vanishes inside Ω (since A_i is harmonic). Therefore equilibrium relation (1) is satisfied in the bulk. As a consequence of this result and Eqs. 11 and 12, obtain $H_{ij}^{\sigma} = 0$. The compatibility relation (4) then follows from this equality. This is exactly the generalization to anisotropy of Pobedrya's method.

3 A New Variational Principle

Consider the following functional,

$$\Pi(\sigma_{ij}, \sigma_{ij,k}) = \int_{\Omega} E_{ijk}\sigma_{ij,k} dV - \int_{\partial\Omega} \left(E_{ijk}\sigma_{ij}n_k - \frac{1}{2}\sigma_{ij,j}\sigma_{ik,k} - \frac{1}{2}\sigma_{ij}n_j\sigma_{ik}n_k + p_i\sigma_{ij}n_j \right) dA, \tag{19}$$

where

$$E_{ijk} = - D_{lnpq}\epsilon_{ikl}\epsilon_{jmn}\sigma_{pq,m} + A_i\delta_{jk} + A_j\delta_{ik} + \sum_{\alpha=1}^{N} \xi^{(\alpha)} (-D_{lnpq}\epsilon_{rkl}\epsilon_{smn}\sigma_{pq,m} + A_r\delta_{sk} + A_s\delta_{rk}) a_{rs}^{(\alpha)} a_{ij}^{(\alpha)} \tag{20}$$

and A_i is as given in (9). Define $L_\Omega = E_{ijk}\sigma_{ij,k}$, then to obtain the Euler–Lagrange equations corresponding to the above functional, evaluate $\frac{\partial L_\Omega}{\partial \sigma_{uv,w}}$ using following formulae,

(i) $$\frac{\partial (D_{lnpq}\epsilon_{ikl}\epsilon_{jmn}\sigma_{pq,m}\sigma_{ij,k})}{\partial \sigma_{uv,w}} = Sym_{uv}[D_{lnpq}\epsilon_{ikl}\epsilon_{jmn}(\delta_{up}\delta_{vq}\delta_{wm}\sigma_{ij,k} + \delta_{ui}\delta_{vj}\delta_{wk}\sigma_{pq,m})] = D_{lnuv}\epsilon_{ikl}\epsilon_{jwn}\sigma_{ij,k} + Sym_{uv}(D_{lnpq}\epsilon_{uwl}\epsilon_{vmn}\sigma_{pq,m})$$

(ii) $$\frac{\partial(D_{lnpq}\epsilon_{rkl}\epsilon_{smn}\sigma_{pq,m}\sigma_{ij,k})}{\partial\sigma_{uv,w}}$$
$$= Sym_{uv}[D_{lnpq}\epsilon_{rkl}\epsilon_{smn}(\delta_{up}\delta_{vq}\delta_{wm}\sigma_{ij,k} + \delta_{ui}\delta_{vj}\delta_{wk}\sigma_{pq,m})]$$
$$= D_{lnuv}\epsilon_{rkl}\epsilon_{swn}\sigma_{ij,k} + Sym_{uv}(D_{lnpq}\epsilon_{rwl}\epsilon_{smn}\delta_{ui}\delta_{vj}\sigma_{pq,m})$$

(iii) $$\frac{\partial(R_{ip}\delta_{qr}\delta_{jk}\sigma_{pq,r}\sigma_{ij,k})}{\partial\sigma_{uv,w}} = Sym_{uv}(R_{iu}\delta_{vw}\sigma_{ij,j}) + Sym_{uv}(R_{up}\delta_{vw}\sigma_{pq,q})$$

(iv) $$\frac{\partial(R_{rp}\delta_{qt}\delta_{sk}\sigma_{pq,t}\sigma_{ij,k})}{\partial\sigma_{uv,w}} = Sym_{uv}(R_{ru}\delta_{vw}\sigma_{ij,s}) + Sym_{uv}(R_{rp}\delta_{iu}\delta_{jv}\delta_{sw}\sigma_{pq,q}),$$

where the notation $Sym_{uv}(\cdot)_{uv} = \frac{1}{2}[(\cdot)_{uv} + (\cdot)_{vu}]$ has been employed. Also note, that for a symmetric tensor σ_{ij}, $\frac{\partial\sigma_{ij}}{\partial\sigma_{uv}} = Sym_{uv}(\delta_{iu}\delta_{jv})$. Using these relations obtain,

$$\frac{\partial L_\Omega}{\partial\sigma_{uv,w}} = Sym_{uv}(E_{uvw}) - D_{lnuv}\epsilon_{ikl}\epsilon_{jwn}\sigma_{ij,k} + 2Sym_{uv}(R_{iu}\delta_{vw}\sigma_{ij,j}) + \sum_{\alpha=1}^{N}\xi^{(\alpha)}(-D_{lnuv}\epsilon_{rkl}\epsilon_{swn}\sigma_{ij,k} + 2Sym_{uv}Sym_{rs}(R_{ru}\delta_{vw}\sigma_{ij,s}))a_{rs}^{(\alpha)}a_{ij}^{(\alpha)}. \quad (21)$$

Taking a variation of the functional (19) with respect to σ_{uv}, we evaluate,

$$\delta\Pi = \int_\Omega -\left(\frac{d}{dx_w}\frac{\partial L_\Omega}{\partial\sigma_{uv,w}}\right)\delta\sigma_{uv}dV - \int_{\partial\Omega}\left(E_{uvw} - \frac{\partial L_\Omega}{\partial\sigma_{uv,w}}\right)\delta\sigma_{uv}n_w dA + \int_{\partial\Omega}\sigma_{ij,j}\delta\sigma_{ik,k}dA + \int_{\partial\Omega}(\sigma_{ik}n_k - p_i)\delta\sigma_{ij}n_j dA, \quad (22)$$

where the 'frozen condition' (Pobedrja 1980): $\delta E_{ijk}n_k = 0$ on $\partial\Omega$ has been assumed. The frozen condition ensures that variation $\delta\sigma_{uv}$ does not introduce a flux of incompatibility across the boundary into the bulk. Noting expression 21, Eqs. 12 and 13 are then recovered as the Euler–Lagrange equations if,

$$-D_{lnuv}\epsilon_{ikl}\epsilon_{jwn}\sigma_{ij,k} + 2(R_{iu}\delta_{vw}\sigma_{ij,j}) + \sum_{\alpha=1}^{N}\xi^{(\alpha)}\big(-D_{lnuv}\epsilon_{rkl}\epsilon_{swn}\sigma_{ij,k} + 2Sym_{rs}(R_{ru}\delta_{vw}\sigma_{ij,s})\big)a_{rs}^{(\alpha)}a_{ij}^{(\alpha)} = 0. \quad (23)$$

These equations give conditions on the arbitrary variables $\xi^{(\alpha)}$ and R_{ij} which make the variational principle suitable. Under such conditions Eq. 22 simplifies to,

$$\delta\Pi = -\int_\Omega E_{uvw,w}\delta\sigma_{uv}dV + \int_{\partial\Omega}\sigma_{ij,j}\delta\sigma_{ik,k}dA + \int_{\partial\Omega}(\sigma_{ik}n_k - p_i)\delta\sigma_{ij}n_j dA. \quad (24)$$

The equation $E_{uvw,w} = 0$ is equivalent to (12). Finally, note that Eq. 23 should be satisfied for arbitrary $\sigma_{ij,k}$ and therefore we obtain necessary and sufficient conditions,

$$-D_{lnuv}\epsilon_{ikl}\epsilon_{jwn} + 2R_{iu}\delta_{vw}\delta_{jk} + \sum_{\alpha=1}^{N}\xi^{(\alpha)}(-D_{lnuv}\epsilon_{rkl}\epsilon_{swn}a_{rs}^{(\alpha)} + 2Sym_{rk}(R_{ru}\delta_{vw}a_{rk}^{(\alpha)}))a_{ij}^{(\alpha)} = 0 \quad (25)$$

which are used as restrictions on the arbitrary variables $\xi^{(\alpha)}$ and R_{ij}.

Functional (19) can be used to derive conservation laws using the formalism of Noether's theorem (Noether 1918; Gelfand and Fomin 2000). Noether's theorem provides a systematic procedure to obtain divergence-free quantities from given symmetries of a variational problem such as one formulated in (19). The divergence-free quantities in an integral form provide conservation laws which in the presence of singularities and inhomogeneities will result into configurational forces acting on these defects. An extension of Noether's theorem to tensorial fields was already achieved (Li et al. 2005; Markenscoff and Gupta 2007) and conservation laws were obtained for translation, rotation, pre-stress and scaling symmetries, which are new and distinct (Gupta and Markenscoff 2007). Application of these conservation laws allowed for the determination of the incompatibility in the interior of the domain by surface data. The variational principle obtained in this paper extends previous work to the case of anisotropy.

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References

Eshelby JD (1975) The elastic energy-momentum tensor. J Elasticity 5:321–335
Eshelby JD (1956) The continuum theory of lattice defects. In: Seitz F, Turnbull D (eds) Solid state physics. Academic Press, New York pp 79–144

Gelfand IM, Fomin SV (2000) Calculus of variations, Dover
Georgievskii DV, Pobedrya BYe (2004) The number of independent compatibility equations in the mechanics of deformable solids. Prikl Mat Mekh 68(6):1043–1048 (trans: J Appl Math Mech 68:941–946 (2004))
Gupta A, Markenscoff X (2007) Configurational forces as dissipative mechanisms: a revisit, Comptes Rendus Mecanique (In press)
Kröner E (1981) Continuum theory of defects. In: Balian R et al (eds) Les Houches, Session 35, 1980 – Physique des defauts. North-Holland, New York, pp 215–315
Kucher V, Markenscoff X, Paukshto M (2004) Some properties of the boundary value problem of linear elasticity in terms of stresses. J Elasticity 74(2):135–145
Li S, Gupta A, Markenscoff X (2005) Conservation laws of linear elasticity in stress formulations. Proc Roy Soc Lon A 461:99–116
Markenscoff X (1976) Independent 4th-order elastic coefficients for quartz. Appl Phys Lett 29(12):768–770
Markenscoff X, Gupta A (2007) Configurational balance laws for incompatibility in stress space. Proc R Soc Lond A, 463:1379–1392
Maugin GA (1993) Material inhomogeneities in elasticity. Chapman & Hall, London
Noether E (1918) Invariante variationsprobleme, Göttinger Nachrichten, (Mathematisch-physikalische Klasse) 2:235–257 (trans: Transport Theory and Statistical Physics 1:186–207 (1971))
Pobedrja BE (1980) A new formulation of the problem in mechanics of a deformable solid body under stress. Soviet Math Doklady 22(1):88–91
Pobedria BE, Holmatov T (1982) On the existence and uniqueness of solutions in the elasticity theory problem with stresses, Vestnik Moskovskogo Universiteta, Seriya 1 (Matematika Mekhanika), 1, pp 50–51
Pobedrya BYe (1994) The problem in terms of a stress tensor for an anisotropic medium. Prikl Mat Mekh 58(1):77–85. (trans: J Appl Math Mech 58(1):81–89 (1994))
Smith GF, Rivlin RS (1957) The anisotropic tensors. Quart Appl Math 15(3):308–314
Smith GF (1970) The crystallographic property tensors of orders 1 to 8. Ann N Y Acad Sci 172(5):57–106
Weyl H (1946) The classical groups, their invariants and representations. Princeton Univ Press, Princeton, NJ