Duality, inverse problems and nonlinear problems in solid mechanics

Configurational forces as dissipative mechanisms: a revisit

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Abstract

A variational argument is used to obtain a necessary and sufficient condition for interpreting the work done by configurational forces as the net dissipation. This condition is the Euler–Lagrange equation associated with the variational integral. We use this simple proposition to re-interpret classical results and also gain insight into recently obtained configurational forces in the stress space. *To cite this article: A. Gupta, X. Markenscoff, C. R. Mecanique 336 (2008).*
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Résumé

Les forces configurationnelles vues comme des mécanismes dissipatifs : un ré-examen. Un argument variationnel est utilisé pour obtenir une condition nécessaire et suffisante permettant d'interpréter le travail effectué par les forces configurationnelles comme une dissipation nette. Cette condition est l'équation d'Euler–Lagrange associée à l'intégrale variationnelle. Nous utilisons cette proposition simple pour ré-interpréter des résultats classiques et aussi approfondir l'interprétation de forces configurationnelles récemment définies dans l'espace des contraintes. *Pour citer cet article : A. Gupta, X. Markenscoff, C. R. Mecanique 336 (2008).*
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Configurational forces are the driving forces associated with the dissipative mechanisms which result as a consequence of material rearrangements. In the mechanics of solids they are related to the concept of the force acting on a defect [1]. These forces are manifested as energy release rates in the study of crack growth [2,3], delamination [4] and epitaxial growth of thin films [5]. In classical dislocation theory they appear in the form of Peach–Koehler force [6], and as a driving traction for a moving phase boundary [7]. For an elastic body, one can obtain expressions for configurational forces using a variational method which follows the procedure of Noether's theorem [8]. Dissipation is quantified by a variation in energy under an infinitesimal rearrangement in the material body and is equal to the work done by the configurational force. We show below (in Section 1) as a simple proposition that this is true if and only if the Euler–Lagrange equations associated with the energy are satisfied.

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In classical elasticity, the energy is given by the quadratic (in strain) strain energy, and the corresponding Euler–Lagrange equations are the equilibrium equations. The compatibility of strain is assumed. Therefore, in this case, the dissipation as a result of material rearrangement is given by the work done due to configurational forces if and only if equilibrium is maintained in the body. We thus have a physical interpretation of our proposition: the consequence that configurational forces act as dissipative mechanisms, is necessary and sufficient for the equilibrium equations to remain valid during the infinitesimal rearrangement in the material body. We discuss this in more detail in Section 2.

We are then led to the question of obtaining a dissipative mechanism when the Euler–Lagrange equations are the Beltrami–Michell (B–M) compatibility conditions. We therefore consider a *generalized energy* in the stress space whose Euler–Lagrange equations are the B–M compatibility conditions [9–11]. Here equilibrium is satisfied trivially. Classical complementary energy principles like Hellinger–Reissner [12] assume the existence of a displacement field a-priori and therefore are not suitable for this purpose. Our proposition is then used (in Section 3) to impart a physical meaning to a recently obtained invariant integral in stress space [11].

1. A variational argument

Consider the following functional (for $\Omega \subset \mathbf{R}^3$):

$$\Pi(u_i, u_{i,j}) = \int_{\Omega} W(x_i, u_i, u_{i,j}) \, \mathrm{d}V \tag{1}$$

where x_i and $u_i(x_i)$ are the independent and the dependent variables, respectively and the function W is assumed to be defined almost everywhere on Ω. All variables are expressed in terms of their Cartesian coordinates, where the subscript indices vary from one to three. In the above relation $u_{i,j}$ denotes the gradient (total derivative) of u_i with respect to x_j. We will also represent the total derivative (with respect to x_i for example) by $\frac{\mathrm{d}}{\mathrm{d}x_i}$ and denote the partial derivative by $\frac{\partial}{\partial x_i}$. We consider smooth transformations in x_i and u_i such that the new independent variables are $y_i = \hat{y}_i(x_i, \epsilon_i)$ and the new dependent variables are $v_i(y_i) = \hat{v}_i(x_i, \epsilon_i)$ where ϵ_i represent the transformation parameters satisfying the condition, $x_i = \hat{y}_i(x_i, 0)$ and $u_i = \hat{u}_i(x_i, 0)$. One can expand y_i and u_i for small ϵ_i as $y_i = x_i + \phi_i + \mathrm{O}(\epsilon^2)$ and $v_i = u_i + \psi_i + \mathrm{O}(\epsilon^2)$, respectively, where ϕ_i and ψ_i are the terms in the expansion which are linear in ϵ_i. For small ϵ_i (i.e. if $|\epsilon_i| \ll 1$), the change in the functional under such a transformation can then be obtained as ([13], page 173)

$$\delta\Pi = \int_{\Omega} \frac{\mathrm{d}}{\mathrm{d}x_i}\left(\frac{\partial W}{\partial u_{k,i}}\bar{\psi}_k + W\phi_i\right)\mathrm{d}V + \int_{\Omega} \Psi_i \bar{\psi}_i \, \mathrm{d}V \tag{2}$$

where $\bar{\psi}_k = \psi_k - u_{k,j}\phi_j$ and

$$\Psi_i = \frac{\partial W}{\partial u_i} - \frac{\mathrm{d}}{\mathrm{d}x_j}\frac{\partial W}{\partial u_{i,j}} \tag{3}$$

In rest of the article we will not consider any independent variations in u_i, i.e. take $\psi_i = 0$. Therefore $\bar{\psi}_k = -u_{k,j}\phi_j$ and Eq. (2) reduces to

$$\delta_x\Pi = \int_{\Omega} B_{i,i} \, \mathrm{d}V - \int_{\Omega} \Psi_i u_{i,j}\phi_j \, \mathrm{d}V \tag{4}$$

where

$$B_i = \left(W\delta_{ij} - u_{k,j}\frac{\partial W}{\partial u_{k,i}}\right)\phi_j \tag{5}$$

and the notation δ_x denotes the variation with respect to x_i.

Observe that $\Psi_i \equiv 0$ represent the Euler–Lagrange equations corresponding to the functional given in (1). The relation (4) also provides us with a special case of Noether's theorem which can be stated as: "if the integral Π is invariant with respect to the group of transformations induced by ϵ_i, then linearly independent combinations of

the Lagrange expressions become divergences. The converse is also true". By Lagrange expressions we refer to Ψ_i. Therefore if the integral Π is invariant under considered transformations then $\delta_x \Pi = 0$, which implies

$$B_{i,i} = \Psi_i u_{i,j} \phi_j \tag{6}$$

as stated in the Noether's theorem above. If the Euler–Lagrange equations hold true then $\Psi_i = 0$ and we obtain conservation laws. For a complete proof, the interested reader is referred to the original paper [14] and the book by Gelfand and Fomin [13].

For the ease of discussion we denote the flux term in (4) by F, i.e.

$$F = \int_{\Omega} B_{i,i} \, \mathrm{d}V \tag{7}$$

We state a simple proposition:

(P) "$\delta_x \Pi = F$ if and only if $\Psi_i = 0$"

whose validity can be easily verified: assume $\Psi_i = 0$, then (4) implies $\delta_x \Pi = F$. Assume $\delta_x \Pi = F$, then owing to the arbitrariness of ϕ_i, we have $u_{i,j} \Psi_i = 0$ and assuming $u_{i,j}$ to be invertible it follows that $\Psi_i = 0$ (we also use the arbitrariness of Ω and the fact that the fields are smooth almost everywhere on Ω). We demonstrate the physical significance of this proposition by considering examples from elasticity.

2. An interpretation of energy release rates in the classical formulation of elasticity

Let W denote the elastic strain energy density, such that $W = W(x_i, u_{i,j})$ and $p_{ij} = \frac{\partial W}{\partial u_{i,j}}$, where p_{ij} is the first Piola stress tensor (equivalent to the Cauchy stress tensor for small strains). The vectors x_i and $u_i(x_i)$ have the usual meaning of the (reference) position and the displacement, respectively. We restrict our attention to the transformation corresponding to a translation, i.e. $\phi_i = \epsilon_i$. Assume that there are no body forces and only displacement boundary conditions are prescribed. Under these conditions, Eq. (4) is reduced to

$$\delta_x \Pi = \int_{\partial \Omega} (W \delta_{ij} - u_{k,j} p_{ki}) \epsilon_j n_i \, \mathrm{d}A + \int_{\Omega} p_{ik,k} u_{i,j} \epsilon_j \, \mathrm{d}V \tag{8}$$

where we have used the divergence theorem to replace the volume integral by a surface integral (assuming that the fields are smooth), with n_i being the surface normal. The flux term here is given in terms of the Eshelby Energy Momentum tensor E_{ij} as

$$F = \int_{\partial \Omega} E_{ij} \epsilon_j n_i \, \mathrm{d}A \tag{9}$$

where $E_{ij} = (W \delta_{ij} - u_{k,j} p_{ki})$. The term conjugate to ϵ_j is defined to be as the *configurational force*, which in this case is given by $\int_{\partial \Omega} E_{ij} n_i \, \mathrm{d}A$. The Euler–Lagrange equations are the equilibrium conditions: $p_{ik,k} = 0$. Eq. (8) can be rewritten using the notation introduced in Eq. (9) as

$$\delta_x \Pi = F + \int_{\Omega} p_{ik,k} u_{i,j} \epsilon_j \, \mathrm{d}V \tag{10}$$

The proposition (P) as stated in Section 1 then implies the following: the energy release (or the change in energy) $\delta_x \Pi$ is given by the flux F (as defined in (9)) if and only if the equilibrium condition is satisfied. The notion of energy release as obtained from the flux F is a popular concept in defect mechanics and was initial introduced in the context of elasticity by Eshelby [15]. Our proposition says that for such a relation (that of the calculation of energy release through flux F) to hold, it is necessary and sufficient to satisfy the equilibrium condition. We elaborate our point further in the following.

Imagine that the body Ω is homogeneous and smooth. This implies that the explicit derivative of W with respect to x_i, $\frac{\partial W}{\partial x_i} = 0$ everywhere in Ω and we can use the divergence theorem to reduce F to a volume integral. We thus obtain from (10),

$$\delta_x \Pi = \int_\Omega (W\delta_{ij} - u_{k,j}p_{ki})_{,i}\epsilon_j \, dV + \int_\Omega p_{ik,k}u_{i,j}\epsilon_j \, dV$$

$$= \int_\Omega (p_{ki}u_{k,ij} - u_{k,ji}p_{ki} - u_{k,j}p_{ki,i})\epsilon_j \, dV + \int_\Omega p_{ik,k}u_{i,j}\epsilon_j \, dV$$

$$= 0$$

and therefore the energy release $\delta_x \Pi$ is rendered zero.

In a case of an inhomogeneity inside Ω, $\frac{\partial W}{\partial x_i} \neq 0$ and the flux F does not cancel exactly with the last term in (10). The choice of $\phi_i = \epsilon_i$ with small ϵ_i provides with an infinitesimal translation to all the material points (denoted by x_i) in the body. We reinterpret the proposition in this case as follows: the energy release (or the change in energy) is given by the flux F so as to maintain equilibrium (given by $p_{ij,j} = 0$) in the state obtained by an infinitesimal translation of material points. Since the material points in the region without inhomogeneities do not contribute to energy release, we associate this (non-trivial) change in energy to the motion of the inhomogeneity. *Therefore the flux ensures that the body remains infinitesimally close to equilibrium even after a small perturbation of the inhomogeneity position.* We can use similar arguments in the presence of dislocations and cracks.

Note that the issue of compatibility never arises in this case, since we assume existence of a smooth (almost everywhere) displacement field a priori, and therefore a compatible strain/stress field is assumed to persist before and after the infinitesimal translation of the defect. A natural question arises of finding a suitable energy release or flux which associates itself in imposing compatibility as a necessary and sufficient condition.

3. An energy release rate associated with the compatibility of stress field

We now consider a formulation of linear and isotropic elasticity in stress space. A positive definite functional has been introduced by Pobedrya [9–11,16,17], whose Euler–Lagrange equations are the B–M compatibility conditions. The functional is given as

$$\Pi(\sigma_{ij}, \sigma_{ij,k}) = \int_\Omega \left\{ \frac{1}{2}\sigma_{ij,k}\sigma_{ij,k} + \frac{1}{1+\nu}\sigma_{kk,i}\sigma_{ij,j} + \frac{1-\nu}{2\nu(1+\nu)}\left(\sigma_{ik,k}\sigma_{ij,j} + \sigma_{jk,k}\sigma_{ji,i}\right) \right\} dV$$

$$- \int_{\partial\Omega} \chi_{ij}\sigma_{ij} \, dS + \int_{\partial\Omega} \left[\frac{1}{2}\left(\sigma_{ij,j}\sigma_{ik,k} + \sigma_{ij}n_j\sigma_{ik}n_k\right) \right] dS \tag{11}$$

where $\chi_{ij} = \frac{\partial L_\Omega}{\partial \sigma_{ij,k}}n_k$ (L_Ω is the integrand in the volume integral above) and ν is the Poisson's ratio. Here $\sigma_{ij}(x_i)$ denotes the Cauchy stress tensor. The traction forces are assumed to vanish all over the boundary. We also assume body force and incompatibility field distribution to vanish throughout the body Ω. The Euler–Lagrange equations corresponding to the functional above are:

$$\sigma_{ij,kk} + \frac{1}{1+\nu}\sigma_{kk,ij} = 0, \quad \forall x_k \in \Omega \tag{12}$$

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

$$\sigma_{ij,j} = 0, \quad \forall x_k \in \partial\Omega \tag{14}$$

The equilibrium relation $\sigma_{ij,j} = 0$ needs to be satisfied only on the boundary, as a result of which it is satisfied automatically in the domain [9]. Therefore, equilibrium inside the domain is always maintained as long as the equilibrium conditions hold on the boundary. We would now like to express the integral equation (4) for the functional (11) for the case of translation transformation ($\phi_i = \epsilon_i$). We assume that the boundary $\partial\Omega$ is smooth and the boundary terms in (11) remain invariant under the translation transformation [11]. We obtain,

$$\delta_x \Pi = \int_{\partial\Omega} X_{ij}\epsilon_j n_i \, dA - \int_\Omega \Psi_{ij}\sigma_{ij,k}\epsilon_k \, dV \tag{15}$$

where

$$X_{ij} = \frac{1}{2}\sigma_{lm,n}\sigma_{lm,n}\delta_{ij} - \sigma_{mn,j}\sigma_{mn,i} - \frac{1}{1+\nu}\sigma_{mi,j}\sigma_{qq,m} \tag{16}$$

and

$$-\Psi_{ij} = \sigma_{ij,kk} + \frac{1}{1+\nu}\sigma_{kk,ij} \tag{17}$$

The proposition (P) in Section 1 then implies the following: under a coordinate translation, the change in functional Π (as given in (11)) is equal to the flux (second term in (15)) if and only if the compatibility equations in the form of (12) are satisfied almost everywhere in the domain. Note that the functional Π in (11) does not have dimensions of energy. In fact if $\sigma_{ij,k}(x_i) \in L^2(\Omega)$ then under the assumption of equilibrium, the volume part of this functional provides the norm associated with the space $L^2(\Omega)$ [18].

A change of dimensions in Eq. (15) might be useful for its physical interpretation. We define a *generalized energy* $\hat{\Pi}$ such that

$$\hat{\Pi} = \frac{l^2}{\mu}\Pi \tag{18}$$

where μ denotes the shear modulus (material constant) and l represents an internal length scale in the problem. The internal length scale is assumed to be a fixed constant and can be associated to the characteristic length scales involved in gradient elasticity theories. Here, however, we do not formulate a gradient theory, in the sense that there are no higher order stresses in our problem. An interpretation of this internal length scale can also be made as a length parameter at which gradients of stress remain finite. Below such a scale, the gradients might not remain smooth and our formulation would lose its validity. Consequently the scale defined by l defines a lower limit for the length dimension at which the notion of compatibility as expressed by (12) makes sense. Relation (15) can then be rewritten as

$$\delta_x\hat{\Pi} = \int\limits_{\partial\Omega} \hat{X}_{ij}\epsilon_j n_i \,\mathrm{d}A - \frac{l^2}{\mu}\int\limits_{\Omega} \Psi_{ij}\sigma_{ij,k}\epsilon_k \,\mathrm{d}V \tag{19}$$

where $\hat{X}_{ij} = \frac{l^2}{\mu}X_{ij}$. The proposition (P) mentioned in the Section 1 can now be re-interpreted: the flux term $\hat{F}$ is given by

$$\hat{F} = \int\limits_{\partial\Omega} \hat{X}_{ij}\epsilon_j n_i \,\mathrm{d}A \tag{20}$$

and the corresponding *configurational force* is given by $\int_{\partial\Omega} \hat{X}_{ij} n_i \,\mathrm{d}A$. According to the proposition, the change in the energy equals the flux if and only if $\Psi_{ij} = 0$. In the absence of inhomogeneities and defects, we can use the divergence theorem to convert the flux term to a volume integral, which cancels identically with the last term in Eq. (19). Therefore in such a case $\delta_x\hat{\Pi} = 0$.

In the case where there is an inhomogeneity or a defect inside Ω, the flux $\hat{F}$ no longer cancels identically with the last term in (19). *The flux $\hat{F}$ then represents a necessary and sufficient change in energy such that compatibility (in terms of stress) is maintained even after an infinitesimal translation of the inhomogeneity/defect inside Ω.* The equilibrium of stress is satisfied trivially (as a consequence of satisfying the equilibrium on the boundary) during such an infinitesimal translation. It is evident that for large characteristic length scales, such a dissipation is large in comparison to the problems where the internal length scales are small. If $\Psi_{ij} \neq 0$ (see for example [19]), then the dissipation should be evaluated using the complete right-hand side of Eq. (19) (a similar remark can be made for the case in Section 2).

Finally, we relate our interpretation to Kröner's ([20], page 287) 'internal observer' who 'cannot distinguish between compatible deformations', but would be sensitive to an incompatibility. In our settings, it is this observer who is operating the dissipative mechanism which ensures that compatibility is not violated anywhere in the domain.

Acknowledgements

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