

A counterpoint to Cermelli and Gurtin's criteria for choosing the 'correct' geometric dislocation tensor in finite plasticity

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Abstract

The criteria of Cermelli and Gurtin (2001, J. Mech. Phys. Solids) for choosing a geometric dislocation tensor in finite plasticity are reconsidered. It is shown that physically reasonable alternate criteria could just as well be put forward to select other measures; overall, the emphasis should be on the connections between various physically meaningful measures as is customary in continuum mechanics and geometry, rather than on criteria to select one or another specific measure. A more important question is how the geometric dislocation tensor should enter a continuum theory and it is shown that the inclusion of the dislocation density tensor in the specific free energy function in addition to the elastic distortion tensor is not consistent with the free energy content of a body as predicated by classical dislocation theory. Even in the case when the specific free energy function is meant to represent some spatial average of the actual microscopic free energy content of the body, a dependence on the average dislocation density tensor cannot be adequate.

1. Is a unique geometric dislocation tensor necessary?

With regard to the question of characterizing measures of dislocation/Burgers vector density (\mathbf{G}) appropriate for a continuum theory, Cermelli and Gurtin (2001) (C&G) indicate that “the problem is not the absence of such a field, but rather the plethora of fields that have appeared in the literature.” They then commit themselves to the task of showing that “there is but a single measure of geometrically necessary dislocations consistent with physically motivated requirements.” Thus, the entire justification of this choice seems to rest on these “physically motivated requirements.”

We proceed now to explore these requirements and provide alternative points of view to each of these requirements:

(C&G) (i) - \mathbf{G} should measure the local Burgers vector in the microstructural configuration, per unit area in that configuration;

- While in itself this is a reasonable physical requirement for the use of some measure, it appears unreasonable to use this to rule out other measures of dislocation density. For instance, one could as well stipulate that the intended tensor should measure local, undeformed Burgers vector, per unit area of the current configuration (this also being the only physically available configuration for measurements). Under this definition, the C&G measure would not qualify but the two-point tensor field (Willis, 1967; Acharya, 2004)

$$-\text{curl } \mathbf{F}^{e-1} \quad ; \quad \left(\text{curl } \mathbf{F}^{e-1} \right)_{ij} := \varepsilon_{jmn} F_{in,m}^{e-1} \quad (1)$$

(with the *curl* operation being with respect to the current configuration and a transpose of the C&G definition and the minus sign relates to the definition of the 'true' Burgers vector in the FS convention – see, Willis, 1967) would, but such stipulation is, of course, vacuous in spirit for the student of continuum mechanics. To draw an analogy, this is not

unlike the situation with the Cauchy and the First Piola-Kirchhoff stress tensors, the latter with respect to some (arbitrary) reference configuration. The former measures forces acting on surface elements of the current configuration, measured per unit area of the same area elements; the latter measures the same forces, measured per unit area of the image area element in the reference configuration. Both have clear physical meanings and preference of one or the other based solely on these definitions is arbitrary.

(C&G) (ii) - \mathbf{G} should, at any point, be expressible in terms of the field \mathbf{F}^p in a neighborhood of the point, since, by fiat, \mathbf{F}^p characterizes the defect structure near the point in question;

- It may be argued that there is no physically distinguished reference configuration in the context of plasticity; in fact, as is well known, classical, finite deformation plasticity theory, whether of the single crystal variety or the ‘microstructure-less’ type (e.g. J -2 plasticity theory) can all be formulated without reference to the tensor \mathbf{F}^p under the additive strain rate decomposition (it can be shown that elementary averaging procedures applied to a finite deformation field theory of dislocation mechanics consistent with classical dislocation theory (Acharya, 2004) naturally lead to the additive decomposition of the velocity gradient). Thus, this second requirement of C&G may be argued to be of dubious physical origin.

(C&G) (iii) - \mathbf{G} should be invariant under superposed compatible elastic deformations and also under compatible local changes in reference configuration, since these – being compatible – should not result in an intrinsic change in the distribution of GNDs near any point.

- Like (i), the invariance under superposed compatible elastic deformations is a physically reasonable requirement, but not one that can be used to rule out other measures of dislocation *density*. Being a measure of physical quantities per unit area, it stands to reason that if this area changes under compatible, elastic deformation, the per unit area, density measure should change. Consider, for example, three dislocation lines threading an area patch (at the minimum scale of resolution) in the current configuration. Roughly speaking, if under further deformation this area patch is stretched but it still contains only those three dislocation lines that do not move with respect to the material (i.e. elastic deformation), then the Burgers vector content *per unit area* of the patch should change; what should remain invariant is the local (unstretched) Burgers vector content of the patch, obtained by integrating the density measure over the area patch, as the patch deforms. The measure $\boldsymbol{\alpha} := -\text{curl } \mathbf{F}^{e-1}$ satisfies this requirement and thus would be a good enough measure of dislocation density under the physical definition that it be the Burgers vector density, measured per unit area of the current configuration, just as the tensor $\mathbf{G} := \det(\mathbf{F}^e)(\text{curl } \mathbf{F}^{e-1})\mathbf{F}^{e-T}$ is, under the definition of C&G.

In fact, the change in the $\boldsymbol{\alpha}$ field in arbitrary material area patches under superposed elastic motions of the current configuration for which no dislocations are nucleated in, or transported into, the patches can be made precise. One only need consider

$$\frac{d}{dt} \int_{A(t)} \boldsymbol{\alpha} \mathbf{n} da = \mathbf{0} \quad (2)$$

for any deforming, but material, surface patch $A(t)$ and the answer is obtained by setting the appropriate convected rate (Fox, 1966; Acharya 2004) to zero;

$$(\text{div } \mathbf{v})\boldsymbol{\alpha} + \dot{\boldsymbol{\alpha}} - \boldsymbol{\alpha}\mathbf{L}^T = \mathbf{0} \Rightarrow \dot{\boldsymbol{\alpha}} = \boldsymbol{\alpha}\mathbf{L}^T - (\text{div } \mathbf{v})\boldsymbol{\alpha}. \quad (3)$$

Here, a superposed dot represents a material time derivative, \mathbf{v} represents the material velocity, \mathbf{L} the velocity gradient, and the result may be referred to as a transport theorem for areas. Clearly, if one wished to elevate the measure $\boldsymbol{\alpha}$ to be a unique measure, one could easily adjust the definition of the required measure to include the result (3) stipulating changes in $\boldsymbol{\alpha}$ in superposed elastic motions (it should be clear that a static condition corresponding to (3) is also easily derived involving the deformation between two elastically related configurations).

As for frame-indifference, the tensor $\boldsymbol{\alpha}$ being a kinematical quantity (as opposed to a constitutive response function), its definition itself suggests how it should transform under a superposed rigid body motion and thus it trivially satisfies the transformations expected of it under superposed rigid motions.

In summary, it is our opinion that while physically reasonable criteria can always be specified to single out one measure of dislocation density or another, in essence, such distinctions are superficial. *In particular, the measure $\boldsymbol{\alpha} := -\text{curl } \mathbf{F}^{e-1}$ is an equally physically-valid measure of Burgers vector content as the \mathbf{G} tensor of C&G, as is the measure $\boldsymbol{\alpha}^* := \mathbf{F}^e\boldsymbol{\alpha}$ - a local, elastically stretched Burgers vector per unit area measure in the current configuration - that arises naturally in thermodynamic considerations leading to the definition of the finite deformation Peach-Koehler force¹ (Acharya, 2004). Moreover, what is of fundamental importance is the non-vanishing *curl* of the inverse elastic tensor (or \mathbf{F}^p on the reference configuration, if one chooses to work with this measure) characterizing the presence of defects in the neighborhood of a point (Acharya and Bassani, 2000). Knowing the elastic and plastic distortions, the relationships between all the measures discussed by C&G are clearly established, and this is all that is important at a kinematical level.*

To draw an historical analogy, denying this fact would be, in essence, similar to attributing fundamental importance to the discussion and controversy that plasticity theory has seen in the past regarding the question of the choice of the ‘physically correct’ objective stress rate for posing rate-type constitutive equations for the stress².

2. Dependence of stored energy on the dislocation tensor; is this necessary?

Field equations and a class of constitutive equations that allow the prediction of stress fields of a prescribed dislocation density field (including individual dislocations) on a given configuration are given by (Willis, 1967; Acharya, 2001, 2004):

¹ This energetic force (per unit volume) depends explicitly on the Cauchy stress in contrast to the object called by the same name in Gurtin (2002) that depends on the defect stress in his theory.

² The important matter in this case is the determination of the physically correct rate response from experiment or micromechanical theory which would naturally satisfy frame-indifference; once accomplished, it is a trivial matter to adjust this statement appropriately to pose it in terms of one objective rate or another so that the rate response implied by the adjusted statement is identical to the micromechanical/experimentally determined physically correct rate response.

$$\begin{aligned} \operatorname{curl} \mathbf{F}^{e-1} &= -\boldsymbol{\alpha} \\ \operatorname{div} \mathbf{T} &= \mathbf{0} \quad ; \quad \mathbf{T} = \hat{\mathbf{T}}(\mathbf{F}^e). \end{aligned} \tag{4}$$

In this theory, *that is consistent with classical dislocation theory*, the tensor $\boldsymbol{\alpha}$ plays a fundamental role whereas under the C&G physical requirements it would be an invalid measure. It is also true that this theory (4), along with its counterpart for small deformations introduces a stored energy function that depends only on the elastic distortion and no additional dependence on the dislocation density tensor is introduced. In contrast, Gurtin's (2002) theory (and many other following works in the literature) depends critically on the dependence of the stored energy function on the dislocation tensor to produce non-classical effects.

Restricting the discussion to small deformations to make the essential point, it is a well-known standard result (see, e.g., Kröner, 1981, Sec. 4) that the strain energy density of a dislocation distribution (including individual discrete dislocations) depends only on the elastic strain that results from the dislocation density distribution and not on *both* the elastic strain and the dislocation density. Furthermore, this strain energy density function corresponds to the linear elastic stress and strain fields of the dislocation distribution involved, as the latter fields are understood in classical dislocation theory (e.g., Nabarro, 1987). In what follows in this section, this result is illustrated in the context of standard procedures for solving boundary value problems in continuum inelasticity theory.

Consider the following question: we are interested in determining the state of internal stress and the strain energy in a linear elastic body of given geometry, for a prescribed dislocation density field $\boldsymbol{\alpha}$. For definiteness, the prescribed dislocation density field can be thought of as representing a screw dislocation along a straight cylinder representing its core. While the main conclusion of this section applies at all instants of time in the deformation of a body, it suffices to demonstrate the idea at any one instant and we choose the initial instant for definiteness. Thus, the problem may be thought of as determining the initial condition on the plastic distortion field in a conventional elastoplasticity calculation, where the plastic distortion field, \mathbf{U}^p , has to satisfy

$$\operatorname{curl} \mathbf{U}^p = -\boldsymbol{\alpha}. \tag{5}$$

Thus, we need to solve the equations

$$\begin{aligned} \operatorname{div}[\mathbf{C}\mathbf{U}^e] &= \mathbf{0} \\ \mathbf{U}^e + \mathbf{U}^p &= \operatorname{grad} \mathbf{u} \\ \operatorname{curl} \mathbf{U}^e &= -\operatorname{curl} \mathbf{U}^p = \boldsymbol{\alpha}, \end{aligned} \tag{6}$$

and since we are talking about initial conditions (for an elastoplasticity calculation), the displacement $\mathbf{u} \equiv \mathbf{0}$ at the initial time so that $\mathbf{U}^e = -\mathbf{U}^p$ at this time. Here, \mathbf{C} is the possibly anisotropic linear elastic moduli with major and minor symmetries and \mathbf{U}^e is the elastic distortion. In classical elastoplasticity, (6) is appended with an evolution equation for \mathbf{U}^p or its symmetric part. For this problem (6) at the initial time when the displacement is known, we consider statically consistent traction boundary conditions (possibly vanishing) to be specified. The paper of Willis (1967) shows that solving these equations amounts to solving the problem of internal stress in classical dislocation theory corresponding to the prescribed dislocation density field. The existence of a non-trivial initial dislocation density distribution in the body is an eminently physical statement; the associated possibility of a non-trivial, *initial* plastic distortion in any theory where the fundamental relation (5) is active reflects the physical fact that the

instantaneous dislocation density distribution encodes information of some portion of the past history of dislocation motion/nucleation in the body.

To solve the problem in the format of continuum inelasticity, we first note that it can be shown that there is at most one solution to the problem of calculating the initial distribution of stress, $\mathbf{T} = \mathbf{C}\boldsymbol{\varepsilon}^e$, where $\boldsymbol{\varepsilon}^e$ is the symmetric part of \mathbf{U}^e . Thus, as long as we can solve (6) and the associated boundary conditions by any procedure, the resulting solution would be the correct one. To find this solution, represent the plastic distortion as a sum of a gradient of a vector field and a tensor field whose *curl* does not vanish as

$$\mathbf{U}^p := -\boldsymbol{\chi} + \text{grad } \mathbf{z} \quad (7)$$

so that

$$-\text{curl } \mathbf{U}^p = \boldsymbol{\alpha} \Rightarrow \text{curl } \boldsymbol{\chi} = \boldsymbol{\alpha}. \quad (8)$$

In order to solve for $\boldsymbol{\chi}$ in a well-posed manner, we append the equations

$$\begin{aligned} \text{div } \boldsymbol{\chi} &= \mathbf{0} \\ \boldsymbol{\chi}\mathbf{n} &= \mathbf{0} \text{ on boundary} \end{aligned} \quad (9)$$

to (8) to obtain a Poisson's equation

$$\text{div grad } \boldsymbol{\chi} = -\text{curl } \boldsymbol{\alpha} \quad (10)$$

for the components of the tensor $\boldsymbol{\chi}$ with Dirichlet boundary conditions; this problem may be solved by standard methods of potential theory.

With a solution for $\boldsymbol{\chi}$ in hand, one solves the equilibrium equation

$$\text{div}[-\mathbf{C} \text{grad } \mathbf{z}] = \text{div}[\mathbf{C}\boldsymbol{\chi}] \quad (11)$$

for the vector field \mathbf{z} with Neumann boundary conditions inferred from the prescribed traction boundary condition and the boundary values of the field $\boldsymbol{\chi}$. This is a standard problem in linear elasticity theory. The solution for $\text{grad } \mathbf{z}$ is unique, and this is all that matters for the present purpose.

The fields $\text{grad } \mathbf{z}$ and $\boldsymbol{\chi}$ in conjunction with (7) and $\mathbf{u} \equiv \mathbf{0}$ now deliver the solution to (6) and thus the unique elastic strain and stress fields corresponding to the prescribed dislocation density field $\boldsymbol{\alpha}$, including arbitrary discrete dislocations in finite, anisotropic, linear elastic bodies.

The corresponding elastic strain energy density distribution in the body, consistent with the classical elastic theory of dislocations, is given by

$$\bar{\psi}(\boldsymbol{\varepsilon}^e) := \frac{1}{2}(\mathbf{C}\boldsymbol{\varepsilon}^e) : \boldsymbol{\varepsilon}^e \quad ; \quad \boldsymbol{\varepsilon}^e := (-\text{grad } \mathbf{z} + \boldsymbol{\chi})_{\text{sym}} = \mathbf{U}_{\text{sym}}^e \quad (12)$$

and, consequently, an assumption of the form

$$\psi = \bar{\psi}(\boldsymbol{\varepsilon}^e) + \hat{\psi}(\boldsymbol{\alpha}) \quad (13)$$

would be superfluous and physically inaccurate in this context where core effects are not taken into account.

Of course, it may be argued that a continuum theory of the type proposed in Gurtin (2002) is meant to be a model of dislocation plasticity at scales of resolution much coarser than where every dislocation is well-resolved, so the appropriate form of a stored energy function for such a situation becomes an issue. But even here, if the coarse free energy function is meant to represent the spatially averaged free energy content in a representative volume element for the coarse-scale model, then an added dependence on the average dislocation density tensor cannot be adequate. For it is well understood that for two different spatial distributions of microscopic dislocation

density α_1 and α_2 within an averaging volume with identical averages $\bar{\alpha}_1 = \bar{\alpha}_2$, the averaged free-energy content is, in general, different, i.e. $\bar{\psi}_1 \neq \bar{\psi}_2$, where ψ represents the microscopic (specific) free energy. But a model that proposes to account for the added strain energy of dislocations at the coarse-scale by a unique functional dependence on $\bar{\alpha}$, say $R(\bar{\alpha})$, alone is bound to fail since the evaluation of such a function for the two cases would have to be identical:

$$R(\bar{\alpha}_1) = R(\bar{\alpha}_2) \text{ but } \bar{\psi}_1 \neq \bar{\psi}_2. \quad (14)$$

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