Analogies between continuum dislocation theory, continuum mechanics and fluid mechanics

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Abstract. Continuum Dislocation Theory (CDT) relates gradients of plastic deformation in crystals with the presence of geometrically necessary dislocations. Interestingly, CDT shows striking analogies to other branches of continuum mechanics. The present contribution demonstrates this on two essential kinematical quantities which reflect tensorial dislocation properties: the (resultant) Burgers vector and the dislocation density tensor. First, the limiting process for the (resultant) Burgers vector from an integral to a local quantity is performed analogously to the limiting process from the force vector to the traction vector. By evaluating the balance of forces on a tetrahedral volume element, Cauchy found his famous formula relating traction vector and stress tensor. It is shown how this procedure may be adopted to a continuously dislocated tetrahedron. Here, the conservation of Burger’s vector implicates the introduction of the dislocation density tensor. Second, analogies between the plastic flow of a continuously dislocated solid and the liquid flow of a fluid are highlighted: the resultant Burgers vector of a dislocation ensemble plays a similar role as the (resultant) circulation of a vortex tube. Moreover, both vortices within flowing fluids and dislocations within deforming solids induce discontinuities in the velocity field and the plastic distortion field, respectively. Beyond the analogies, some peculiar properties of the dislocation density tensor are presented as well.

1. Introduction

It is well-established that matter of any kind consists of discrete particles, such as atoms and molecules. In order to understand the material behavior microscopically, discrete physical models and theories need to be applied. As an example, plastic deformation of solids is intrinsically tied to the motion of discrete lattice defects such as dislocations [1, 2]. Discrete Dislocation Dynamics (DDD) simulations take into account dislocation lines and their (microscopic) interactions [3]. Though matter is clearly heterogeneous on these small scales, the material body often seems homogeneous on a larger scale. Then, a continuum theory is appropriate and effective in order to study the body’s meso- and macroscopical physical behavior. One prominent example is continuum mechanics, which aims to predict a body’s motion/deformation under the action of external loads. Different sub-branches with respect to the state of the body have evolved. In this study, the focus is on continuum mechanics applied to fluids and dislocated solids. In Continuum Dislocation Theory (CDT), the material is considered as continuously dislocated. Instead of the (small scale) interaction of individual dislocation lines as in DDD, the collective behavior of dislocation ensembles is of key interest. Surprisingly, CDT shows some striking analogies, both to general continuum mechanics and to fluid mechanics [8, 9]. For simplicity, this is demonstrated on the geometrically linear CDT in the present contribution.
First, section 2 recalls basic dislocation properties on the example of a discrete edge dislocation. This is necessary for section 3, where the analogy between Cauchy’s stress tensor and Krönér’s dislocation density tensor is discussed. Next, section 4 confronts CDT with fluid mechanics and reveals analogous quantities and relations. Finally, section 5 goes beyond the analogies and emphasizes some peculiar properties of the dislocation density tensor.

For the sake of a compact and clear representation, symbolic tensor notation is preferred in this paper. Tensors of \(n\)-th order are denoted by a small or capital letter with \(n\) underscores, e.g. \(U\) is a second-order tensor. The tensor product is denoted by \(\otimes\), the cross product by \(\times\) and the contraction of tensors is written symbolically with a dot (\(\cdot\)). The coefficients with respect to a certain Cartesian coordinate system \(e_a\) are \(U_{ab} = e_a \cdot U \cdot e_b\). Italic indices \(a, b, \ldots\) stand for Cartesian coordinates \(x, y, z\), whereas upright indices are labels (e.g. \(p\) stands for plastic). The arrangement of second-order tensor coefficients in a quadratic matrix is denoted by \(\begin{bmatrix}U_{ab}\end{bmatrix}\).

Differential operators such as divergence and curl are expressed symbolically with the Nabla operator denoted by \(\nabla\).

2. Preliminary considerations about dislocations

For the following sections some basic dislocation properties are recalled: Dislocations are line-shaped crystal defects. They constitute a discontinuity separating plastically slipped regions from unslipped ones (figure 1). A discrete dislocation within a crystal is characterized by two vectorial quantities: the tangent vector \(t\) on the dislocation line and the Burgers vector \(b\). The latter defines both magnitude and direction of the plastic slip carried by the dislocation. Furthermore, \(b\) is constant along the dislocation line whereas the tangent \(t\) varies in case of a curved dislocation.

The Burgers vector is obtained by tracing a loop in the dislocated body and evaluating the vector needed to close the loop in the non-dislocated state. This is the well-known Burgers circuit (figure 1). With respect to some sign convention, the obtained closure failure represents the dislocation’s elementary Burgers vector \(\overset{\_}{b}\). For evident geometrical reasons, dislocations cannot end within a crystal, but only at phase boundaries or junctions with other dislocation segments. Considering \(N\) (discrete) dislocation lines within some crystal volume, this has the following consequence [3]:

\[
\sum_{i=1}^{N} \overset{\_}{b_i} = 0 \quad \text{analogous to} \quad \sum_{i=1}^{N} \overset{\_}{F_i} = 0 ,
\]

which is Newton’s balance of linear momentum for \(N\) (discrete) forces \(\overset{\_}{F}\) acting on some solid body. In this sense, the Burgers vector is a conserved quantity. If the length scale is chosen this large that dislocations seem to be distributed continuously, then each material point of the continuum embraces an ensemble of dislocations. It may be characterized in an average sense by its resultant Burgers vector \(\overset{\_}{b_r}\).
3. The analogy between Cauchy’s stress tensor and dislocation density tensor
In this section the far reaching analogy between the force vector \( F \) / traction vector \( s \) and the resulting Burgers vector \( b_r \) / dislocation vector \( a \) is presented. The analogy is further extended by deriving the dislocation density tensor in the same way the stress tensor is derived. Therefore, the balance laws (1) are evaluated on an elementary tetrahedron-shaped volume element.

3.1. Definition of local and integral quantities
For everything which follows, assume some finite continuous body in space with \( r = x_a e_a \) denoting the position of the material points. Now there are quantities that are integral by nature, such as forces or closure failures as explained in section 2. Hence, a corresponding local quantity must exist in a continuum theory. Consequently, a limiting process should be possible relating the local quantity to the integral/global one. However, having in mind the validity of continuum theories (cf. section 1) care must be taken not to violate the continuum hypothesis: Infinitesimal line, surface, volume and mass elements must not become zero. Instead, the elements always have to remain this large that enough of the material’s relevant microscopic constituents are included [6]. In table 1 this is demonstrated for a simple solid and a dislocated one.

Table 1. Continuum limit for a simple solid and a dislocated solid.

| Integral quantity | Force – Traction | Closure failure – Dislocations |
|-------------------|------------------|--------------------------------|
| Force vector \( F \) | Resultant Burgers vector \( b_r \) |

| Relevant length scale | Atomic lattice: | Edge dislocation array: |
|----------------------|-----------------|------------------------|
| \( a \) | \( \Delta A \) | l |

| Limiting process | \( s = \lim_{\Delta A \to 0} \left( \frac{\Delta F}{\Delta A} \right)_{\Delta A \gg a^2} \) | \( a = \lim_{\Delta A \to 0} \left( \frac{\Delta b_r}{\Delta A} \right)_{\Delta A \gg l^2} \) |

| Local quantity | \( s = \frac{dF}{dA} \) | \( a = \frac{d b_r}{dA} \) |

The definitions of the traction and the dislocation vectors as differential quotients are only valid, if the (infinitesimal) area element is much bigger than the mean atomic spacing – the lattice constant \( a \) – and the mean dislocation spacing \( l \), respectively (figures in table 1). The other way round, a material point in the continuum sense averages over many atoms, dislocations and other possible microstructural features [1].

3.2. Evaluation of balance laws on the tetrahedral volume element
The well-known balance of forces (1), applied on an infinitesimal, tetrahedron-shaped volume element implicates the introduction of the stress tensor [4, 5]. By exploiting the conservation of Burgers’ vector in a similar way, the dislocation (density) tensor can be identified (table 2).
The elementary tetrahedron is obtained by cutting an elementary cube with faces perpendicular to the Cartesian coordinate axes. This results in a new cut face with an area $dA$ and with an arbitrary outward unit normal $n = n_a e_a$ (figures in table 2), where Einstein’s summation convention is to be applied. The other three faces have the area elements $dA_a = n_a dA$ and the normals $-e_x, -e_y$ and $-e_z$. As they point in negative coordinate direction, the corresponding tractions $s_a$ and closure failures $a_a$ have a minus sign, too [5].

Table 2. Evaluation of balance laws on an elementary tetrahedral volume element.

| Tetrahedron element | with tractions: | with closure failures: |
|---------------------|-----------------|-----------------------|
|                       | $dF + \sum_{a=x} dF_a = 0$ | $db + \sum_{a=x} db_a = 0$ |
| Global balance      | $s dA + (-s_a dA_a) = 0$ | $a dA + (-a_a dA_a) = 0$ |
| with local quantities | $s dA - s_a n_a dA = 0$ | $a dA - a_a n_a dA = 0$ |
| (cf. table 1)       | $s dA = (s_a \otimes e_a) \cdot n dA$ | $a dA = (a_a \otimes e_a) \cdot n dA$ |
| Local mapping       | $s(r, n) = \sigma(r) \cdot n$ | $a(r, n) = \alpha(r) \cdot n$ |

The transition from the global balances to the local mappings in table 2 is demonstrated on the stresses: the composition $s_a n_a = s_x n_x + s_y n_y + s_z n_z$ may be re-written into the symbolic expression $(s_a \otimes e_a) \cdot n$, which reveals the second-order tensor

$$\sigma = s_a \otimes e_a$$

analogous to

$$\alpha = a_a \otimes e_a \quad \text{1} \quad \text{1}$$

Obviously, it suffices to know the traction/dislocation vectors with respect to three orthogonal faces in order to construct the corresponding second-order tensors [1]. Furthermore, both traction and dislocation vector depend on the cutting plane defined by the unit normal $n$. In the context of CDT it is natural to choose the crystal’s slip planes as cut faces in order to obtain the resultant Burgers vector for the different slip systems. However, as $\alpha$ is a second-order tensor, $n$ does not necessarily need to be a slip plane normal but may be related to any cut face.

The analogy can even be extended to local conservation laws: as will become clear in section 4, the dislocation density tensor is divergence-free, i.e. $\alpha \cdot \nabla = 0$. In the absence of inertia and body forces the local balance of linear momentum leads to the same condition for the stress tensor, i.e. $\sigma \cdot \nabla = 0 \quad \text{2}$

1 Note that the sequence is not unique here. Likewise, $s_a n_a = n_a s_a = n_a \cdot (e_a \otimes s_a)$ could have been chosen. However, in the context of right differential operators, the normal is to stand right of the second-order tensor.

2 Here, the right-divergence is applied. In the literature the left-divergence can be found as well [1]. Then, the corresponding stress and dislocation density tensors defined by equations (2) need to be transposed.
4. The analogy between Kelvin’s circulation and the resultant Burgers vector

In order to answer the question under which circumstances a solid body (e.g. an aircraft) within some fluid (e.g. air) is able to ascend, Kelvin introduced a scalar quantity called circulation. Consider some fluid flow prescribed by the velocity field \( \mathbf{v}(\mathbf{r}) \) and let \( C \) stand for the contour of some vortex tube with the cross-sectional area \( \Delta A \) (figure 2).\(^3\) Now the circulation is defined as:

\[
\Gamma := \oint_C \mathbf{v} \cdot d\mathbf{r} \quad \text{(3)}
\]

\[
\Gamma = - \int_A (\nabla \times \mathbf{v}) \cdot \mathbf{n} \, dA = \int_A (\nabla \times \mathbf{\Omega}) \cdot \mathbf{n} \, dA = \int_A \mathbf{\Omega} \cdot \mathbf{n} \, dA . \quad \text{(4)}
\]

Here, Stokes’ theorem was used to transform the path integral into the surface integral. Thereby, the derived vectorial quantity \( \mathbf{\Omega} = -\nabla \times \mathbf{v} \) appeared. It is called vorticity (or vortex vector) and represents the curl of the velocity. A solid body within a fluid experiences a static lift (Archimedes’ Principle). If the fluid (or the solid body) is in motion and the circulation around this body does not vanish, the body additionally experiences a dynamic lift \([6]\) (cf. table 3).

\[\text{Figure 2. Vortex tube within a fluid (left) and dislocation ensemble (right) in a solid body: the lines with tangent } t \text{ depict vortex and dislocation lines, respectively.}\]

In order to answer the question how the internal state (i.e. the dislocation configuration) of a body is related to the plastic deformation of this body, Kröner introduced the resultant Burgers vector. It may be thought of as an average value summing up the elementary Burgers vectors \( b \) from all dislocations of some dislocation ensemble (figure 2). Hence, a dislocation ensemble is characterized by a constant resultant Burgers vector. Now consider some plastic flow prescribed by the plastic distortion field \( \beta_p(\mathbf{r}) \) and let \( C \) stand for the contour of some dislocation ensemble with the cross-sectional area \( \Delta A \) (figure 2). Then the resultant Burgers vector is defined as \([7]\):

\[
\mathbf{b}_r := \oint_C \mathbf{\beta}_p \cdot d\mathbf{r} \quad \text{(5)}
\]

\[
\mathbf{b}_r = - \int_A (\mathbf{\beta}_p \times \nabla) \cdot \mathbf{n} \, dA = \int_A (\nabla \times \mathbf{\beta}_p^T)^T \cdot \mathbf{n} \, dA = \int_A \mathbf{\alpha} \cdot \mathbf{n} \, dA . \quad \text{(6)}
\]

Here again, Stokes’ theorem was used to transform the path integral into the surface integral. Thereby, the derived tensorial quantity \( \mathbf{\alpha} = -\mathbf{\beta}_p \times \nabla \) appeared. It is called Nye-Kröner-Bilby dislocation density tensor and represents the curl of the plastic distortion \([1]\). As a consequence of definition (5), \( \mathbf{\alpha} \) is an average quantity containing only information about Geometrically Necessary Dislocations (GNDs). Furthermore, as a curl field, \( \mathbf{\alpha} \) is divergence-free.

\(^3\) A vortex tube is the surface in the continuum formed by all vortex lines passing through a given closed curve in the continuum \([6]\).
The striking analogy between derivations (4) and (6) is obvious and there are manifold further aspects of it. The correspondence between vortices and dislocations has already been investigated thoroughly for the classical (local) continuum theory of dislocations [8]. Furthermore, a one-to-one relationship between a screw dislocation in gradient elasticity and a smoothed vortex in fluid mechanics has been shown before, including a tabular review of the corresponding field quantities [9]. The present study both reviews some of these results and further enriches the analogy with some more nuances, see table 3. Vortices within a flowing fluid induce discontinuities in the velocity field and vice versa. Likewise, dislocations within a deforming solid induce discontinuities in the plastic distortion field and vice versa. Furthermore, in both cases the relations are of pure kinematical nature, i.e. they are valid for any admissible motion (including deformation) of a fluid and solid continuum, respectively. Moreover, there is a continuity condition (zero divergence) both for $\Omega$ and $\varphi$: similar to dislocation lines, vortex lines must form closed loops (or junctions) [8]. In other words: both dislocations and vortices cannot end inside a continuous body [9]. Moreover, vortex line tangents can be post-processed from a given vorticity field $\varphi(x)$, cf. table 3. Then, the underlying network of dislocation ensembles could be revealed as post-processing step. This would be an alternative to tracking the motion of individual dislocation lines, which results in high numerical costs [3].

5. Further properties of the dislocation density tensor

Despite the analogies presented in sections 3 and 4 there are also important differences. As a consequence of the balance of angular momentum the stress tensor is symmetric [4]. The dislocation density tensor is unsymmetric, which will be illustrated now. In general, according to equation (6), $\varphi$ has the following coefficients with respect to a Cartesian coordinate system:

$$\varphi = -\varphi_{ab} \times \nabla = -\frac{\partial \beta_{ab}}{\partial x_c} \epsilon_{bed} \varphi_a \otimes \varphi_d = \beta_{ab,c} \epsilon_{bed} \varphi_a \otimes \varphi_d = \alpha_{ad} \varphi_a \otimes \varphi_d,$$  \hspace{1cm} (7)

with the permutation symbol $\epsilon_{bed} = (\varphi_b \times \varphi_c) \cdot \varphi_d$. The coefficient matrix takes thus the form:

$$[\alpha_{ad}] = \begin{bmatrix} \alpha_{xx} & \alpha_{xy} & \alpha_{xz} \\ \alpha_{yx} & \alpha_{yy} & \alpha_{yz} \\ \alpha_{zx} & \alpha_{zy} & \alpha_{zz} \end{bmatrix} = \begin{bmatrix} \beta_{xx,x} & \beta_{xx,y} & \beta_{xx,z} \\ \beta_{yy,x} & \beta_{yy,y} & \beta_{yy,z} \\ \beta_{zz,x} & \beta_{zz,y} & \beta_{zz,z} \end{bmatrix}.$$

The elements on the principal and secondary diagonal represent the screw character ($a = d$) and the edge character ($a \neq d$) of the dislocation ensemble [7].

Table 3. Confrontation of analogous quantities of a flowing fluid and a dislocated solid.

| Flowing fluid [6] | Continuously dislocated solid |
|-------------------|------------------------------|
| Integral quantity | $\Gamma = \oint C \cdot \nabla \cdot \varphi$ dA |
| Significance      | $\Gamma = 0$ : static lift only |
|                   | $\Gamma \neq 0$ : dynamic lift |
|                   | $\varphi = -\varphi_{ab} \times \nabla$ |
| Significance      | $\varphi = 0 \ \forall \ x$ : curl-free flow |
|                   | $\varphi = \alpha_{ab} \times \nabla$ |
| Tangent lines     | $\varphi \times T = 0$ : vortex line $t$ |
|                   | $\varphi \times T = 0$ : dislocation line tangent $t$ |
When the plastic distortion field only depends on a single coordinate $x$, $y$ or $z$, the corresponding column in the coefficient matrix of $\mathbf{\alpha}$ is zero (table 4).

**Table 4.** Special dislocation states for different dependencies of $\mathbf{\beta}_p(x,y)$.

| $\mathbf{\beta}_p = \mathbf{\beta}_p(x)$ | $\mathbf{\beta}_p = \mathbf{\beta}_p(y)$ | $\mathbf{\beta}_p = \mathbf{\beta}_p(z)$ |
|-----------------|-----------------|-----------------|
| $[\alpha_{ab}] = \begin{bmatrix} 0 & -\beta_{px,z}^p & \beta_{px,y}^p \\ 0 & -\beta_{py,z}^p & \beta_{py,y}^p \\ 0 & -\beta_{pz,z}^p & \beta_{pz,y}^p \end{bmatrix}$ | $[\beta_{xz,y}^p \beta_{xx,y}^p 0] \begin{bmatrix} -\beta_{xx,y}^p & \beta_{xx,z}^p & 0 \\ -\beta_{yy,z}^p & \beta_{yy,y}^p & 0 \\ \beta_{zx,y}^p & \beta_{zx,z}^p & 0 \end{bmatrix}$ | $[\beta_{xy,y}^p \beta_{xx,y}^p 0] \begin{bmatrix} 0 & -\beta_{xx,y}^p & \beta_{xx,z}^p \\ 0 & \beta_{yy,z}^p & \beta_{yy,y}^p \\ -\beta_{zx,y}^p & -\beta_{zx,z}^p & 0 \end{bmatrix}$ |

Plane plastic distortions $\mathbf{\beta}_p = \beta_{xx}^p(x,y)e_x \otimes e_x + \beta_{yy}^p(x,y)e_y \otimes e_y + \beta_{yz}^p(x,y)e_y \otimes e_x + \beta_{zy}^p(x,y)e_y \otimes e_y$ result in $\mathbf{\alpha}(x,y)$ with

$$[\alpha_{ad}] = \begin{bmatrix} 0 & 0 & \beta_{xy,y}^p - \beta_{xx,y}^p \\ 0 & 0 & \beta_{yy,y}^p - \beta_{xx,y}^p \\ 0 & 0 & 0 \end{bmatrix}.$$  

Choosing a cut face with normal $n = e_z$, the corresponding resultant Burgers vector and thus also the dislocation vector have only two (plane) components:

$$\mathbf{\alpha}(x,y,n = e_z) = \mathbf{\alpha}(x,y) \cdot e_z = (\beta_{xy,x} - \beta_{xx,x})e_x + (\beta_{yy,y} - \beta_{xx,y})e_y. \quad (10)$$

Moreover, certain decompositions known from the stress tensor are not possible. In general, a geometrical dislocation state is neither a symmetric nor a pure spherical tensor. This shall be demonstrated now: Starting from the definition

$$\mathbf{\alpha} = (\nabla \times \mathbf{\beta}_p^T)^T = -\mathbf{\beta}_p \times \nabla = -\mathbf{\beta}_p \cdot I \times I \cdot \nabla = \mathbf{\beta}_p \cdot \epsilon \cdot \nabla, \quad (11)$$

and considering that $\mathbf{\beta}_p$ is unsymmetric and $\epsilon$ is totally skew-symmetric, it follows immediately:

$$\mathbf{\alpha} \neq \mathbf{\alpha}^T \quad \text{and} \quad \mathbf{\alpha} \neq \mathbf{\alpha} I = \mathbf{\alpha}.$$  

(12)

This has the following consequence: for an unsymmetric dislocation density tensor, there is no orthonormal coordinate system where $[\alpha_{ad}]$ is a diagonal matrix. Physically speaking, there is in general no cut surface where all dislocations piercing the surface appear as screw dislocations. This is evident since otherwise, a dislocation ensemble with screw and edge character could be transformed into screw character only by rotating the coordinate system.

However, there is indeed a special case where $\mathbf{\alpha}$ can be symmetric or even spherical. If the plastic distortion tensor is skew-symmetric, a vector may be assigned in the following way:

$$\mathbf{\beta}_p = -\mathbf{\beta}_p^T \rightarrow \mathbf{\beta}_p = \theta \cdot \epsilon \cdot \nabla.$$  

(13)

Physically speaking, there is only a plastic rotation now but no plastic strain. The rotation vector $\theta$ contains both the rotation angle and the axis. Substituting relation (13) into definition (11), Nye’s famous formula is obtained:

$$\mathbf{\alpha} = \theta \cdot \epsilon \cdot \nabla = \nabla \otimes \theta - (\nabla \cdot \theta) I = \mathbf{\alpha}.$$  

(14)

Obviously, $\mathbf{\alpha}$ is symmetric or even spherical if the rotation gradient $(\nabla \otimes \theta)^T$ is symmetric or spherical, respectively. This case is of practical relevance, because relation (14) is often used to approximate $\mathbf{\alpha}$ from experimental orientation data by methods such as electron backscatter diffraction. Some more properties of $\mathbf{\alpha}$ under special slip conditions can be found elsewhere [10].
6. Conclusions and outlook

In this study, analogies between different branches of continuum mechanics were presented. To be precise, traction vector and dislocation vector can be obtained by a similar physical limiting process such that the continuum hypothesis is preserved. Moreover, similar conservation laws of forces and Burgers vectors may be evaluated on an elementary tetrahedron leading to the introduction of the second-order stress tensor and dislocation density tensor, respectively. Thus, a new way is shown how to motivate the dislocation density tensor. In addition, the quantity vorticity known from fluid mechanics has an analogous significance as the resultant Burgers vector for a continuously dislocated solid. Both quantities may be used to obtain further knowledge about the fluid’s flow characteristics and the microstructural state of the solid.

Going beyond the pure mathematical analogy it might be even possible to consider vortices within flowing fluids as a (temporary) microstructure. Indeed, the vorticity vector may be considered as a measure of the defect concentration within a fluid – its vortex density – in total accordance with the dislocation density tensor [8]. It is well-known that macroscopic properties of solids (e.g. hardening) emerge from the collective self-organization of crystal defects during the plastic deformation. Here, dislocation cell patterns are observed often. Analogously, the famous Bénard cells can emerge in the velocity field of fluids under some external thermal load. Furthermore, both dislocations and vortices may form wall structures [8]. Nevertheless, there is an important difference: as the plastic behavior of solids depends on the defect state, the dislocation density tensor enters constitutive equations in CDT. The counterpart in fluid mechanics, the vorticity, cannot enter constitutive equations since it is neither a state nor an objective quantity.

Maybe the presented analogies can help to transfer knowledge between the field theories. There is also a far reaching correspondence between the continuum theory of dislocations and the one of electromagnetism (Maxwell’s field theory) [11, 12]. From an even wider perspective, such analogies might be helpful to identify fundamental symmetries leading to unified physical theories.

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