

Dislocation Dynamics as Gradient Descent in a Space of Currents

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Abstract Recent progress in continuum dislocation dynamics (CDD) has been achieved through the construction of a local density approximation for the dislocation energy and the derivation of constitutive laws for the average dislocation velocity by means of variational methods from irreversible thermodynamics. Individual dislocations are driven by the Peach–Koehler-force which is likewise derived from a variational principle. This poses the question if we may expect that the averaged dislocation state expressed through the CDD density variables is driven by a variational gradient of the average energy, as is assumed in irreversible thermodynamics. In the current contribution we do not answer this questions, but rather present the mathematical framework within which the evolution of discrete dislocations is literally understood as a gradient descent. The suggested framework is that of de Rham currents and differential forms. We briefly sketch why we believe the results to be useful for formulating CDD theory as a gradient flow.

1 Introduction

During the last two decades crystal plasticity revealed itself as an area which poses great challenges in the discrete to continuum transition from individual dislocations to continuum dislocation formulations. One important line among others in this field is the program of continuum dislocation dynamics (CDD) pursued by the author and co-workers [12]. The original problem solved by CDD is the definition of sufficiently rich dislocation density measures capable of describing the evolution of a dislocation system in a kinematically closed form [14]. At least for single glide situations we regard this problem as solved since the introduction of a hierarchy of dislocation alignment tensors and their evolution equations [10] – even though the latter require closure assumptions in order to arrive at useful crystal plasticity theories [23]. But

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the achieved kinematic consistency has to be accompanied by a kinetic theory in order turn CDD into a crystal plasticity materials law.

Regarding a kinetic closure we currently regard energetic approaches as most promising. The energetic approach assumes that the energy of a dislocation system may be expressed by an energy functional depending on the CDD density variables. The evolution of the density variables, which are naturally formulated in terms of an average dislocation speed, are then derived in the spirit of irreversible thermodynamics from a variational derivative of the energy with respect to the evolution of the CDD variables [11]. This reasoning has been substantiated by the derivation of a local density approximation for the dislocation energy in terms of CDD variables, which (the derivation) bears strong analogies to quantum mechanics [26]. In the current contribution we are interested in the complementary question to energetic modelling in CDD, namely how the single dislocation evolution presents itself as a gradient descent.

Dislocations are well known to move in response to the so-called Peach–Koehler force. The Peach–Koehler force on dislocations is a prototypical configurational force *ante verbum*. In the original paper, Peach and Koehler [25] derived the force as the negative variational derivative of the ‘interaction energy with [the] stress field’. The dislocation mobility turns this force per length into a dislocation (segment) velocity. This means that discrete dislocation simulations, which employ the Peach–Koehler force, perform a gradient descent in energy space of some form. With regard to constitutive modeling in CDD this raises two questions: (i) What is a proper mathematical space in which the motion due to the Peach–Koehler force on single dislocations may actually be viewed as a ‘gradient descent’? – Where we expect the (variational) gradient to be obtained from a Gâteaux differential. (ii) Can we expect the gradient structure of the evolution equation to be conserved upon (ensemble) averaging? In the current contribution we focus on the first question (i) and only briefly discuss how the answer to the first question may affect reasoning on the second one.

The paper is structured as follows: in Sect. 2 we introduce the notions of (vector valued) differential forms and currents. In Sect. 3 we describe the differential calculus on currents from the perspective of variational theory. Subsequently, we briefly discuss the energetics of dislocations in Sect. 4. The key result is obtained in Sect. 5 where we introduce a metric structure which turns the equation of overdamped dislocation motion into a gradient descent in a space of one-dimensional vector valued currents. Finally we briefly summarize the results and give a cursory outlook on challenges in kinetic modeling of CDD in Sect. 6.

2 Mathematical Preliminaries

We focus on the case of interacting dislocation lines in an infinite crystal and employ the assumptions of small deformations and linear elasticity. Despite our restriction to small deformations, we will distinguish upper and lower indices in the sequel.

Consequently, we usually employ the original Einstein summation convention, where automatic contraction is restricted to pairs of like upper and lower indices. We think it is important to distinguish vector spaces and their dual spaces in the current context both locally and globally – even if the standard metric is available for mutual identification. As will be discussed in Sect. 5, we regard the viscous drag of dislocation motion as the origin of a *physical* metric of dislocation theory, which supersedes the standard metric.

In the current Section we introduce differential forms, vector valued differential forms, currents, and vector valued currents in a very condensed way, which, hopefully allows the reader to follow the subsequent theory. For thorough introductions to differential forms we refer to standard text books, e.g. [5, 21]. More details on vector valued differential forms may be found in [9, 15]. For the notion of currents we recommend [2], for their application to dislocations and the vector valued case we refer to [9, 13]. Note that we leave out all functional analytic or measure theoretic complexities.

Basic notation and differential forms

As we deal with small deformation theory, we regard the crystal as a Euclidean manifold with standard coordinates x^1, x^2, x^3 . The according basis vectors of the tangent space are denoted with ∂_i and the dual basis one-forms of the co-tangent space are denoted with dx^i . Differential forms are purely covariant and fully antisymmetric tensors, which are non-trivial in the three-dimensional case only for degrees 0,1,2, and 3. The wedge-product \wedge is used to combine two differential forms of order p and q to a differential form of order $p + q$. For details on the calculus of differential forms see [5, 21] and many other introductory book in differential geometry. We just recall a few salient features of and operators defined on differential forms. One important feature is that differential p -forms may be integrated over p -dimensional oriented submanifolds S^p ,

$$\int_{S^p} \alpha^p, \quad (1)$$

without assigning a standard ‘volume (surface or line) element’ to the submanifold. Furthermore, the exterior derivative d is defined independent of both Riemannian metrics and connections and maps differential p -forms to differential $p + 1$ -forms. The generalized Stokes theorem on differential forms reads

$$\int_{S^{p+1}} d\alpha^p = \int_{\partial S^{p+1}} \alpha^p. \quad (2)$$

The interior multiplication $\iota_X \alpha^p$ with a vector field X turns a differential p -form into a differential $(p - 1)$ -form. The Lie-derivative \mathcal{L}_X along a vector field X , which keeps the degree of a differential form fixed, is defined by Cartan’s *magic formula*,

$$\mathcal{L}_X \alpha = \iota_X d\alpha + d\iota_X \alpha. \quad (3)$$

Vector valued differential forms

In general, vector valued differential forms take values in some vector bundle (which includes, e.g., tensor bundles) over the crystal manifold [17]. In the current paper this will be either the tangent bundle or the co-tangent bundle (see [9, 15] for more detailed introductions of this special case). In the sequel we will reserve the term vector valued differential form usually for those taking values in the tangent bundle while we speak of one-form valued differential forms in the latter case. In local coordinates a vector valued p -form is of the form

$$P = \frac{1}{p!} P_{i_1 \dots i_p}{}^j dx^{i_1} \wedge \dots \wedge dx^{i_p} \otimes \partial_j, \quad (4)$$

while a one-form valued p -form appears as

$$Q = \frac{1}{p!} Q_{i_1 \dots i_p} dx^{i_1} \wedge \dots \wedge dx^{i_p} \otimes dx^j. \quad (5)$$

Vector valued differential forms (in the general sense) only allow for an integral calculus if the vector bundle is a trivial bundle and a trivialization is fixed. However, we do not explicitly integrate vector valued differential forms in the sequel, but restrict integration to differential forms arising from a generalized *dotted* wedge product $\hat{\wedge}$, taking a vector valued and a one-form valued form (or vice versa) to a usual differential form through¹

$$P^p \hat{\wedge} Q^q := \frac{1}{p!q!} P_{i_1 \dots i_p}{}^j Q_{i_{p+1} \dots i_{p+q} j} dx^{i_1} \wedge \dots \wedge dx^{i_p} \wedge dx^{i_{p+1}} \wedge \dots \wedge dx^{i_{p+q}} \quad (6)$$

$$Q^q \hat{\wedge} P^p := (-1)^{pq} P^p \hat{\wedge} Q^q. \quad (7)$$

The generalization of the exterior derivative to vector valued differential forms requires the consideration of a connection ∇ on the vector bundle and is denoted with d^∇ . In the Euclidean case, the connection is of course the standard connection with vanishing connection coefficients. The generalized exterior derivative of vector valued and one-form valued differential forms satisfies the product rule

$$d(P^p \hat{\wedge} Q) = d^\nabla P^p \hat{\wedge} Q + (-1)^p P^p \hat{\wedge} d^\nabla Q. \quad (8)$$

The interior multiplication ι_X applies in the usual fashion to the differential form part of the vector and one-form valued differential forms. We define a generalized Lie-derivative on vector and one-form valued differential forms through [9]

$$\mathcal{L}_X^\nabla = \iota_X d^\nabla \alpha + d^\nabla \iota_X \alpha. \quad (9)$$

¹Note that in [9] there is a mistake in the anti-symmetry condition below, where the exponent of -1 is erroneously given as p and not pq .

Currents

Currents are defined as linear functional on spaces of differential forms. In this work we deal with the basic definition according to de Rham [2], where the arguments of currents are C^∞ differential forms with compact support. De Rham developed the notion of currents from electrodynamics at the prototype of a current carrying wire. Such wire may be described as an electrical current (singularly) concentrated on a one-dimensional manifold. Even though such objects are often described by integrals over Dirac delta distributions, it is advantageous to regard singularities along submanifolds as objects of their own right. Currents which are non-trivial only for differential forms of a given degree p are called p -dimensional currents. This obviously includes p -dimensional submanifolds S^p which map smooth differential p -forms α^p onto their integral over the submanifold. We denote the current induced by such submanifold with γ_{S^p} , which is defined by

$$\gamma_{S^p} [\alpha^p] := \int_{S^p} \alpha^p. \quad (10)$$

Note that we mark the application of a functional to differential forms with brackets $[\cdot]$. Delta distributions at a point r are in this sense 0-dimensional currents assigning to a function f its value at r , i.e.,

$$\gamma_r [f] := f(r). \quad (11)$$

If the underlying space M is n -dimensional, p -dimensional currents are likewise said to be of degree $n - p$. The rationale for this notion is that $n - p$ -dimensional differential forms β^{n-p} define linear functionals on differential p forms as follows,

$$\gamma_{\beta^{n-p}} [\alpha^p] := \int_M \beta^{n-p} \wedge \alpha^p. \quad (12)$$

The above examples of currents motivate the following transfer of operations from manifolds or differential forms to currents. Stokes' theorem (2) immediately yields the notion of the boundary of a current ∂ , which is defined through

$$\partial \gamma [\alpha] := \gamma [d\alpha]. \quad (13)$$

The product rule of the exterior differential derivative yields the closely connected definition

$$d\gamma [\alpha^p] := (-1)^{p+1} \gamma [d\alpha^p]. \quad (14)$$

The interior multiplication with a vector field X is defined as

$$\iota_X \gamma [\alpha^p] := (-1)^{p+1} \gamma [\iota_X \alpha^p]. \quad (15)$$

Finally, the Lie derivative of a current in the direction of a vector field is

$$\mathcal{L}_X \gamma [\alpha^p] := -\gamma [\mathcal{L}_X \alpha^p]. \quad (16)$$

Currents from moving submanifolds

The Lie derivative of currents plays a special role for currents derived from moving submanifolds. It seems that the following transport theorem (e.g. found in [5, 21]) lacks a common denomination and is occasionally ‘rediscovered’ [4]. It may be viewed as a generalization of the Reynolds transport theorem to differential forms. We directly introduce it in the language of currents. Let $N(t)$ be a moving submanifold, where the motion of every point is described by a vector field $v(t)$ along the manifold. Let moreover $\gamma_{N(t)}$ denote the induced current on smooth differential forms, then the time derivative of the current is given by

$$\partial_t \gamma_{N(t)} = -\mathcal{L}_{v(t)} \gamma_{N(t)}. \quad (17)$$

Vector valued currents

We regard vector valued currents as linear functionals acting on one-form valued differential forms and vice versa. For example, a dislocation line c defines a vector valued (because of the Burgers vector b) one-dimensional current γ_{c^b} acting on one-form-valued one-forms $L = L_{ji} dx^j \otimes dx^i$ through

$$\gamma_{c^b} [L] = \int_c L_{ij} b^j dx^i. \quad (18)$$

The generalized operations on vector valued differential forms transfer to vector valued currents in full analogy to their original definition on currents, when replacing the exterior derivative with the connection dependent exterior derivative, that is

$$d^\nabla \gamma [P^p] := (-1)^{p+1} \gamma [d^\nabla P^p], \quad (19)$$

$$\iota_X \gamma [P^p] := (-1)^{p+1} \gamma [\iota_X P^p], \quad (20)$$

$$\mathcal{L}_X^\nabla \gamma [\alpha^p] := -\gamma [\mathcal{L}_X^\nabla \alpha^p]. \quad (21)$$

Vector valued currents from moving submanifolds

As a generalization of the second last paragraph imagine a moving submanifold to which a vector field is appended. A motion of such a current consists additionally to the spatial vector field v , which moves the base manifold, also of a variation \dot{X} of the vector field X . The latter variation may be split in the sense of a co-variant time derivative, $\dot{X} = X_t + \nabla_v X$, where X_t is the variation of the vector field keeping N fixed, while $\nabla_v X$ is understood as the covariant derivative of X along the motion path of each point moving with the flow of v . The according time derivative of the

induced current was found in [9] as

$$\partial_t \gamma_{N^b} = -\mathcal{L}_v^\nabla \gamma_{N^x} + \gamma_{N^{\dot{x}}} \quad (22)$$

Double forms

In order to deal with interacting dislocations we work with the interaction energy of two dislocations. The interaction energy will be discussed in detail below. At this point we only note for motivational purposes, that the interaction energy is obtained as a double integral over the two dislocation lines. In the terminology employed here, the kernel of the double integral is a one-form valued double differential form on the product space of the crystal manifold with itself. When dealing with double forms on $M \times M$ we distinguish the coordinates on the first and second copy of M as x^i and \bar{x}^i . For the first manifold we use the notations introduced above, while for the latter we employ the vector basis $\bar{\partial}_i$ and the co-vector basis $d\bar{x}^i$. In local coordinates a double (p, q) -form reads

$$\mathcal{D}^{p,q} = \frac{1}{p!q!} D_{i_1 \dots i_p | j_1 \dots j_q} dx^{i_1} \wedge \dots \wedge dx^{i_p} d\bar{x}^{j_1} \wedge \dots \wedge d\bar{x}^{j_q}. \quad (23)$$

Vector and one-form valued double forms are defined accordingly.

Double currents

Double currents are linear functionals on spaces of double differential forms. Of specific importance are products of single currents. Note that the double form $\mathcal{D}^{p,q}$ may (with interchangeable perspective) be viewed as a differential p -form on M taking values in the vector space (consequently a trivial vector bundle) of q -forms on M . If a fixed q -dimensional current γ^q is applied to the resulting q -form at every x this yields a real number, and henceforth this composition defines a (real-valued) differential p -form D^p . For this operation we introduce the following notation

$$D^p (\gamma^q) := \gamma^q [\mathcal{D}^{p,q}]. \quad (24)$$

Likewise a p -dimensional current produces a q -form, which we write as

$$D^q (\gamma^p) := \gamma^p [\mathcal{D}^{p,q}]. \quad (25)$$

The resulting differential p - or q -form, respectively, may again be used as argument for a p - or q -dimensional current. We define this composition of two currents as their product

$$\gamma^q \gamma^p [\mathcal{D}^{p,q}] := \gamma^q [D^q (\gamma^p)] = \gamma^p [D^p (\gamma^q)]. \quad (26)$$

The product is commutative, that is $\gamma^p \gamma^q = \gamma^q \gamma^p$ and it defines a double current on M . The generalization to vector and one-form valued double currents is obvious.

3 Variational Methods and the Lie-Derivative of Currents

We discuss the case that a current γ_N is induced by a submanifold N of the crystal manifold M . A variation of the submanifold N is assumed to be given by a (variational) vector field \tilde{v} along the manifold. This likewise induces a variation of the induced current, which is according to the transport theorem (17) given by

$$\tilde{\gamma}_N = -\mathcal{L}_{\tilde{v}}\gamma_N. \quad (27)$$

It seems worth noting that $\tilde{\gamma}_N$ is a tangent vector at γ_N to the space of currents. We now regard a functional $F^\phi[\gamma_N]$ on currents which is induced by a differential form ϕ whose degree equals the dimension of N , such that

$$F^\phi[\gamma_N] = \int_N \phi = \gamma_N[\phi]. \quad (28)$$

The Gâteaux differential dF^ϕ (at ‘point’ N) is a linear operator mapping tangent vectors $\tilde{\gamma}_N$ to scalars. It is defined by

$$dF^\phi[\tilde{\gamma}_N] = \lim_{t \rightarrow 0} \frac{F^\phi[\gamma_{N_t(\tilde{v})}] - F^\phi[\gamma_N]}{t}, \quad (29)$$

where $N_t(\tilde{v})$ is the manifold which results from letting each point of N move with the flow of \tilde{v} for time t . In other words the variational derivative was already given in the transport theorem (17), such that

$$dF^\phi[\tilde{\gamma}_N] = -\mathcal{L}_{\tilde{v}}\gamma_N[\phi] = \gamma_N[\mathcal{L}_{\tilde{v}}\phi]. \quad (30)$$

For the vector valued case we work with the induced current γ_{N^x} of a submanifold N with an appended vector field X . The functional F^P shall be induced by an according differential form P which takes values in the dual space to the vector bundle of X , such that

$$F^P[\gamma_{N^x}] = \gamma_{N^x}[P] = \int_N P \wedge X. \quad (31)$$

From the transport theorem for vector valued currents we obtain

$$dF^P[\tilde{\gamma}_{N^x}] = -\mathcal{L}_{\tilde{v}}^\nabla \gamma_{N^x}[P] + \gamma_{N^x}[P] \quad (32)$$

where the variational current $\tilde{\gamma}_{N^x}$ is induced by the spatial variation \tilde{v} and the variation of the vector field $\tilde{X} = \tilde{X}_t + \nabla_{\tilde{v}}X$.

4 Energetics of Dislocation

As we work consistently with vector valued differential forms, we adopt the understanding of [15, 18] that the stress tensor σ is most naturally viewed as a one-form valued two form

$$\sigma = \frac{1}{2} \sigma_{ijk} dx^i \wedge dx^j \otimes dx^k. \quad (33)$$

The components of the usual (fully covariant) stress tensor may be obtained (for once employing the modified Einstein summation convention) through $\sigma_{ij} = \frac{1}{2} \varepsilon_{ikl} \sigma_{klj}$. The latter relation may be reversed to $\sigma_{ijk} = \varepsilon_{ijl} \sigma_{lk}$. We disregard the possibility of body forces in the sequel, such that the stress tensor is solenoidal, which means it is closed in differential form formalism, that is $d^\nabla \sigma = 0$.

The interaction energy $E^{\text{cr}} [\gamma_{c^b}]$ is considered as a functional on vector valued currents in the sense of the last Section. The interaction energy of a dislocation with a stress field is usually given in terms of the work done to create the according loop within the stress field. Let S denote a surface swept by the dislocation to create the loop $c = \partial S$. The work done in creating the loop is then taken to be given by the integral of the scalar product of the stress vector on the surface with the Burgers vector b . In the language of currents this is the application of the vector valued current induced by the swept surface combined with the Burgers vector S^b to the stress form, i.e.,

$$E^{\text{cr}} [\gamma_{c^b}] = \gamma_{S^b} [\sigma] = \int_S \frac{1}{2} \sigma_{ijk} b^k dx^i \wedge dx^j. \quad (34)$$

Obviously, this definition only makes sense if this integral does not depend on the specific surface S whose boundary is the dislocation line c . We will briefly discuss this independence in Sect. 5.

Interaction energy

In this Section we define the interaction energy of two dislocations via a double integral over the dislocation lines. The integral kernel in this is in the current terminology a (each time) one-form valued $(1, 1)$ form

$$\mathcal{E} = E_{ik|jl} dx^k \otimes dx^i d\bar{x}^l \otimes d\bar{x}^j. \quad (35)$$

The total interaction energy $E [\gamma_{c_1^b}, \gamma_{c_2^b}]$ of two dislocations c_1^b and c_2^b may then be defined in terms of a double current as

$$E [\gamma_{c_1^b}, \gamma_{c_2^b}] := \gamma_{c_1^b} \gamma_{c_2^b} [\mathcal{E}] = \int_{c_1} \int_{c_2} E_{ik|jl} b_1^k b_2^l dx^i d\bar{x}^j. \quad (36)$$

Explicit expressions for the interaction kernel are known since decades for isotropic elasticity in an infinite medium, e.g. [3, 6, 8]. But only recently, Lazar and Kirchner [19] presented a closed form expression for the case of anisotropic elasticity, which reads (once again applying the modified Einstein convention)

$$E_{ik|jl} = \varepsilon_{jmn} C_{lnpq} \varepsilon_{qri} C_{stkr} F_{imps}^0, \quad (37)$$

where the fourth rank tensor F_{imps}^0 derives as a convolution of the elastic greens function tensor $G_{ps,tm}^0$ and the Greens function of the Laplace operator G^Δ as

$$F_{imps}^0 = -G_{ps,tm}^0 * G^\Delta. \quad (38)$$

Very recently Lazar and co-workers [20] were able to derive an analogous formula for gradient elasticity, where only the Green functions have to be exchanged for those of the underlying gradient elasticity theory. This is possibly the most elegant way of dealing with the problem of self-energies which are not defined in the classical case where the integrand is singular on the dislocation line. With this in mind we will not go in any detail about the modeling of self energies and shall keep the double integral formulation also for a single dislocation, such that we formally write

$$E^{\text{self}} [\gamma_{c^b}] = \frac{1}{2} E [\gamma_{c^b}, \gamma_{c^b}], \quad (39)$$

where the factor 1/2 corrects for double counting.

5 Variational Calculus Applied to Dislocation Energies

As a first application of the general variational formulas presented above we check the independence of the energy of creation $E^{\text{cr}} [\gamma_{c^b}]$ from the chosen surface S with $\partial S = c$. Locally, the value of the energy of creation is independent of the surface S , if the Gâteaux differential vanishes for any variational vector field \tilde{v}_0 , which vanishes along the boundary line, $\tilde{v}_0 \circ c = 0$, thus maintaining $\partial S = c$. We denote the according tangent vector in the space of currents with $\tilde{\gamma}_{S^b}^0$. The independence of the energy from the specific surface is a consequence of the solenoidality of the stress tensor, as we find

$$d_{S^b} E^{\text{cr}} [\tilde{\gamma}_{S^b}^0] = \int_S \mathcal{L}_{\tilde{v}_0}^\nabla \sigma \dot{\lambda} b \quad (40)$$

$$= \int_S d^\nabla \iota_{\tilde{v}_0} \sigma \dot{\lambda} b + \iota_{\tilde{v}_0} d^\nabla \sigma \dot{\lambda} b \quad (41)$$

$$= \int_S d (\iota_{\tilde{v}_0} \sigma \dot{\lambda} b) \quad (42)$$

$$= \int_c \iota_{\tilde{v}_0} \sigma \wedge b = 0. \quad (43)$$

In the above calculation we employed the product rule (8), the constancy of the Burgers vector ($\dot{b} = 0$), and the boundary condition $\tilde{v}_0 \circ c = 0$. All neighboring surfaces to S thus yield the same result for the creation energy and this consequently applies to all surfaces with the same boundary line which may be obtained from S by a continuous deformation *within* the crystal. Two surface with the same boundary line may for example *not* be continuously (without tearing) transformed into each other if the volume surrounded by them contains holes or inclusions. If we exclude the possibility of holes in the matrix² there is a potential one-form valued one-form (called the stress function tensor of first kind [19]) $\phi = \phi_{ij} dx^i \otimes dx^j$ available such that $\sigma = d^\nabla \phi$. The exterior differential turns into a curl-relation in classical vector calculus. Using this potential we may directly turn the surface integral for the creation energy into a line integral along the dislocation by Stokes theorem (using $\nabla b = 0$)

$$E^{\text{cr}}[\gamma_{c^b}] = \int_S d^\nabla \phi \wedge b = \int_{\partial S} \phi \wedge b = \gamma_{c^b}[\phi]. \quad (44)$$

This formulation is well suited to inspect the result of varying the position of the dislocation c , as opposed to varying the position of the surface S . In this case we obtain the Gâteaux differential with regard to a vector field \tilde{v} *along the curve*, and find

$$d_{c^b} E^{\text{cr}}[\tilde{\gamma}_{c^b}] = \int_c \mathcal{L}_{\tilde{v}}^\nabla \phi \wedge b \quad (45)$$

$$= \int_c d^\nabla \iota_{\tilde{v}} \phi \wedge b + \iota_{\tilde{v}} d^\nabla \phi \wedge b \quad (46)$$

$$= \int_c \iota_{\tilde{v}} \sigma \wedge b. \quad (47)$$

We expect this differential to be related to the Peach-Koehler force. To see this we write the one-form in the last integral in index notation and express it through the classical stress tensor $\tilde{v}^i \sigma_{ijk} b^k dx^j = \tilde{v}^i \varepsilon_{ijl} \sigma_{lk} b^k dx^j$. When the curve is parametrized by arc length s and if t denotes the unit tangent to the curve we easily find that

$$d_{c^b} E^{\text{cr}}[\tilde{\gamma}_{c^b}] = \int_c \tilde{v}^i \varepsilon_{ijl} \sigma_{lk} b^k t^j ds = - \int_c \tilde{v}^i F_i(t, b) ds, \quad (48)$$

²Regions without holes are called non-periphRACTIC by Gurtin [7], a term which goes back to Maxwell [22]. In terms of modern topology this means that the second Betti number is zero, such that all closed two-forms are exact, saying that they may be obtained from some one-form (a potential) by exterior differentiation.

with the well-known Peach–Koehler force $F_i(t, b) = \epsilon_{ilj} \sigma_{lk} b^k t^j$. We thus found the Peach–Koehler force as a representation of the negative Gâteaux differential on the space of currents. This comes of course at no surprise, because the Peach–Koehler force has been derived as a variational derivative of the interaction energy with the stress field from the outset [25].

However, the abstract Gâteaux differential is essential to understand how, and with regard to which Riemannian metric on the space of currents, classical equations of motion for dislocations actually define a gradient descent. We note that a gradient is a tangent vector as opposed to the differential which is a co-tangent vector. A Riemannian metric defines a linear way of mapping tangent vectors to co-vectors and vice versa. The gradient of a function, as opposed to its differential, will thus depend on the given Riemannian metric. The appropriate metric will as usual in the theory of gradient flow in dissipative systems be defined from the viscosity.³ In linear overdamped dislocation theory (as usually assumed in discrete dislocation simulations) the dislocation velocity v is obtained from the Peach–Koehler force by a mobility tensor M^{ij} as $v = M^{ij} F_j \partial_i$. Note that the mobility tensor depends on the Burgers vector, $M = M(b)$, though we will usually not state this explicitly. The velocity field then defines a tangent vector $-\mathcal{L}_v \gamma_{c^b}$ to the space of currents at γ_{c^b} , such that altogether we map the Gâteaux differential $d_{c^b} E^{\text{cr}}$ to a tangent (velocity) vector to the space of currents. Note that such a map would be defined through any non-linear mobility law as well. However, in the linear case, and if M is additionally positive definite, the so obtained evolution law may be understood as a gradient descent in the space of currents.⁴ The Riemannian metric is defined by the viscosity tensor B_{ij} , which is the inverse of the mobility tensor M_{ij} , i.e., $B_{ik} M^{kj} = \delta_i^j$ and $M^{ik} B_{kj} = \delta_i^j$. We note that this implies $F_i = B_{ij} v^j$ for the velocity defined by the linear mobility law. The viscosity tensor defines a Riemannian metric on the tangent space of dislocations with Burgers vector b as follows

$$g_B(-\mathcal{L}_v \gamma_{c^b}, -\mathcal{L}_w \gamma_{c^b}) = \int_c v^i B_{ij}(b) w^j ds. \quad (49)$$

With regard to the viscosity metric the gradient of the creation energy $\text{grad}_{c^b}^B E^{\text{cr}}$ at γ_{c^b} is defined as the tangent vector satisfying

$$g_B(\text{grad}_{c^b}^B E^{\text{cr}}, -\mathcal{L}_w \gamma_{c^b}) = d_{c^b} E^{\text{cr}}[-\mathcal{L}_w \gamma_{c^b}]. \quad (50)$$

³Compare [24], where Felix Otto puts it as follows: ‘The merit of the right gradient flow formulation of a dissipative evolution equation is that it separates energetics and kinetics. The energetics endow the state space M with a functional E , the kinetics endow the state space with a Riemannian geometry via the metric tensor g .’

⁴If the mobility is for instance taken to be zero in the climb-direction, M^{ij} is not positive definite. In this case the tangent space to dislocations is restricted to variations within the glide plane, such that only the in-plane component of the Peach–Koehler force matters. If one then assumes M to be positive definite for vectors in the glide plane, all the following ideas remain valid.

By inserting $v^i = M^{ij} F_j$ into (49) we immediately verify that

$$-\text{grad}_{c^b}^B E^{\text{cr}} = -\mathcal{L}_{M^{ij} F_j \partial_i} \gamma_{c^b}, \quad (51)$$

and consequently

$$\partial_t \gamma_{c^b} = -\text{grad}_{c^b}^B E^{\text{cr}}. \quad (52)$$

From the fact that dislocations evolve by a gradient descent with respect to the metric g_B we also obtain the usual interpretation of the evolution of the energy. The energy will never increase, the decrease in energy is entirely dissipative, and it is quadratic in (dislocation) velocity and force,

$$\partial_t E^{\text{cr}} [\gamma_{c^b}] = -g_B (\text{grad}_{c^b}^B E^{\text{cr}}, \text{grad}_{c^b}^B E^{\text{cr}}) \quad (53)$$

$$= -\int_c v^i B_{ij} v^j ds \quad (54)$$

$$= -\int_c v^i F_i ds. \quad (55)$$

Dislocation ensembles as interacting particle systems

The derivation of the Peach–Koehler force and the understanding of the usual equation of motion of dislocation lines as a steepest gradient descent in a space of currents is naturally transferred to the case of dislocations interacting by the interaction energy $E [c_1^b, c_2^b]$, if the Lie-derivative operation is applied to the according coordinates. That is, for two interacting dislocations, we obtain their evolution as

$$\partial_t \gamma_{c_i^b} = -\text{grad}_{c_i^b}^B E [\gamma_{c_1^b}, \gamma_{c_2^b}], \quad \text{for } i = 1, 2. \quad (56)$$

We see that in this abstract form we may view a dislocation ensemble of N dislocations with total energy

$$E^{\text{tot}} = \sum_{i=1}^N E^{\text{cr}} [\gamma_{c_i^b}] + \frac{1}{2} \sum_{i=1}^N \sum_{j=1}^N E [\gamma_{c_i^b}, \gamma_{c_j^b}], \quad (57)$$

as an interacting ‘particle’ system, where each particle follows a steepest descent with regard to the viscosity metric g_B ,

$$\partial_t \gamma_{c_i^b} = -\text{grad}_{c_i^b}^B E^{\text{tot}} = -\text{grad}_{c_i^b}^B E^{\text{cr}} - \sum_{j=1}^N \text{grad}_{c_i^b}^B E [\gamma_{c_i^b}, \gamma_{c_j^b}]. \quad (58)$$

6 Summary and Outlook

In the current work we took an abstract approach to dislocation systems, which is designed for averaging static and dynamic dislocation systems. We consider dislocations as linear functionals on spaces of differential forms, i.e., as vector valued de Rham currents. A transport theorem for moving manifolds provided us with descriptions of tangent vectors to the space of currents and differentials of functions on the space of currents. Tangent vectors at a current are induced Lie-derivatives of the current in the direction of vector fields along the dislocation line. We showed that the Peach–Koehler force is a representation of the negative Gâteaux differential of the energy function on the space of currents. Moreover, the overdamped linear viscous drag law for dislocations as employed in discrete dislocation dynamics simulations was identified as a gradient flow on the space of currents with regard to a Riemannian metric induced by the viscosity tensor.

The interpretation of the dislocation evolution in terms of a gradient descent may not be very surprising. We motivated the current investigation from the underlying question, if the variational methods applied to a recently derived local density approximation for continuous dislocation systems may be justified from averaging the discrete case. This question is still open and far beyond the scope of this paper. But we may sketch in which sense we think the results of the current work will help understanding the variational approach to constitutive modeling in CDD as a gradient flow on spaces of differential forms. Like in the discrete case, the salient question in the continuum case is the definition of the right Riemannian metric on the density spaces [24]. For particle systems underlying porous media equations, the distance induced by the appropriate Riemannian metric is known as the Wasserstein distance (which actually goes back to Kantorovich [16]). The Wasserstein distance between two (normed) densities may be interpreted as the minimum energy needed to shift either of the density distributions into the other. The Wasserstein distance is closely related to the conservation law for densities ρ of point particles, i.e., for evolution equations of the form $\partial_t \rho = -\operatorname{div}(\rho v)$ [1]. If the densities are considered as differential three-forms $\omega = \rho dV$, where dV is the standard volume element, this evolution equation has the form of a Lie-derivative $\partial_t \omega = -\mathcal{L}_v \omega$. We note that the general theory of currents developed in this paper yields that tangent vectors to point particles interpreted as zero-dimensional currents γ_p are likewise of the form $-\mathcal{L}_v \gamma_p$, in full analogy to the finding for moving dislocations. We may therefore hope to generalize the concept of viscous Riemannian metrics and the Wasserstein distance to the evolution equations of the CDD density variables which have the structure of generalized conservation laws [10] deriving from Lie-derivatives in the discrete case.

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