Bridging the Scales Between Discrete and Continuum Dislocation Models

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Abstract We prove the many-particle limit passage of interacting particle systems described by gradient flows. The limiting equation is a gradient flow which describes the evolution of the particle density. Our proof methods rely on variational techniques such as Γ-convergence of the particle configuration energies and stability of gradient flows. The interacting particle systems under consideration model the motion of dislocations in metals. Since the collective motion of dislocations is the main driving force of plastic deformation of metals, we aim to contribute with our analysis to the current understanding of plasticity.

1 Disagreeing Plasticity Models

A large field of ongoing research studies plastic deformation of metals. Plastic deformation is an irreversible process, in which permanent changes within the material result in a macroscopic change of shape. These permanent changes are the collective behaviour of curve-like defects in the atomic lattice of the metal. Such defects are called dislocations. It is typical for metals to contain *many* dislocations (as much as 1000 km of dislocation curve in a cubic millimetre [19, p. 20]). Because of this large amount of dislocations, there is a general belief that plasticity can be described in terms of upscaled quantities such as the dislocation density.

This belief has led to several *different* dislocation density models in the engineering literature, see for instance [1, 16, 17]. The discrepancies between these models arise from using different phenomenological closure assumptions. These assumptions are needed to bridge the gap between dislocations interacting on the micro-scale and their collective behaviour on the macro-scale. As a consequence of these different continuum models, it remains unclear to what extent they approximate discrete dislocation dynamics. This brings us to the main question:

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Which dislocation density models are the discrete-to-continuum limit of the dynamics of individual dislocations as the number of dislocations tends to infinity?

The main challenge in answering this question is to control the non-local and singular interactions between dislocations. Such interactions are not captured by similar discrete-to-continuum problems that are solved in, for example [6, 8, 18, 23, 27], because in those results the interactions are either local or bounded.

Instead, for non-local and singular interactions, different mathematical tools are needed to pass to the many-particle limit. Several such tools are developed, for instance, in [2, 11–15, 21]. We wish to expand this set of tools by connecting several more discrete dislocation models to their continuum counterparts, with the ultimate aim to validate the different models in the engineering literature. More precisely, we consider two scenarios for discrete dislocation dynamics: pile-ups of dislocation walls [25] in Sect. 2, and mixed positive and negative dislocations in two dimensions [16, 17] in Sect. 3.

2 Upscaling of Dislocation Walls

After introducing in Sect. 2.1 the model for the dynamics of dislocation walls, we describe in Sect. 2.2 the related upscaling results.

2.1 Pile-Up of Dislocation Walls

The idealised setting of dislocation walls (proposed in [20, 29]) allows to study a two-dimensional dislocation geometry by means of a one-dimensional problem. A dislocation wall is a vertically periodic arrangement of equidistant dislocations. We consider a pile-up of $n+1$ dislocation walls (based on the setting in [25]), which are trapped in a finite domain and subjected to a constant external force (see Fig. 1a).

The unknowns are the n horizontal positions of the dislocations walls given by

$$\Omega_n := \{x^n = (x_1^n, \dots, x_n^n) \in \mathbb{R}^n : 0 =: x_0 < x_1^n < \cdots < x_n^n \le L_n\}.$$

The energy related to a dislocation wall configuration is

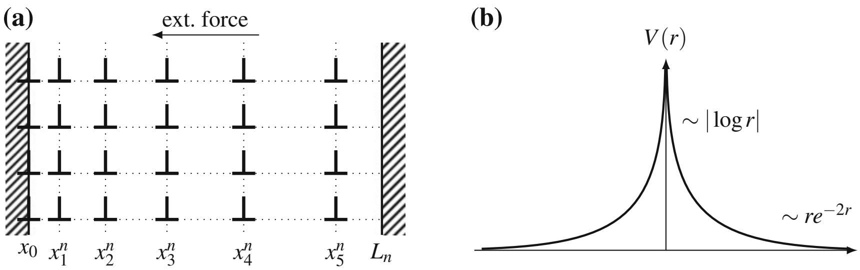

Fig. 1 **a** Pile-up of dislocations '⊥' arranged in wall structures. **b** Qualitative plot of the interaction potential V

$$E_n : \Omega_n \to [0,\infty], \qquad E_n = E_n^{\text{int}} + E_n^{\text{F}} + E_n^{\text{L}}, \tag{1}$$

$$E_n^{\text{int}}(x^n) = \frac{1}{n^2}\sum_{k=1}^{n}\sum_{j=0}^{n-k} \ell_n V\big(\ell_n(x_{j+k}^n - x_j^n)\big), \qquad E_n^{\text{F}}(x^n) = \frac{1}{n}\sum_{i=1}^{n} x_i^n,$$

$$E_n^{\text{L}}(x^n) = \chi_{\{x_n^n \le L_n/\ell_n\}} := \begin{cases} 0, & \text{if } x_n^n \le L_n/\ell_n, \\ \infty, & \text{otherwise.} \end{cases}$$

Here, V is the *interaction potential* between walls, which is illustrated in Fig. 1b and defined by

$$V : \mathbb{R} \to [0,\infty], \qquad V(r) := r \coth r - \log|2\sinh r|. \tag{2}$$

The parameters L_n and ℓ_n correspond to the two characteristic length scales in the pile-up problem. Relative to the vertical distance between two neighbouring dislocations within a wall, L_n is the distance between the barriers, and ℓ_n is the length scale at which the dislocation walls spread when the interaction energy is balanced with the external forcing term.

Regarding the dynamics, we follow the well-known linear drag law for modelling dislocation movement, which results in the following gradient flow

$$\begin{cases} \dfrac{d}{dt}x^n(t) = -n\nabla E_n\big(x^n(t)\big), & t > 0, \\ x^n(0) = x_{\text{init}}^n, \end{cases} \tag{3}$$

for some initial condition $x_{\text{init}}^n \in \Omega_n$. Since E_n is strictly convex and has compact level sets, the minimisation problem of E_n over Ω_n and the gradient flow (3) have unique solutions.

2.2 Discrete-to-continuum Limit

We are interested in the limits of n-indexed sequences of gradient flows (3). For brevity, we assume for the asymptotic behaviour of the parameters L_n and ℓ_n that $1 \lesssim \ell_n \lesssim n$ and $L_n \gtrsim \ell_n$ as $n \to \infty$. In [31, 32] any scaling regime for L_n and ℓ_n is considered. The main difference for $\ell_n \ll 1$ and $\ell_n \gg n$ is that the interaction energy E_n^{int} is scaled differently, and for $L_n \ll \ell_n$ that x^n is replaced by $L_n x^n / \ell_n$.

To give a meaning to the convergence of gradient flows, we first define notions of convergence for a sequence of n-tuples (x^n) via the embedding

$$\pi_n : \Omega_n \to \mathscr{P}([0,\infty)), \qquad \pi_n(x^n) := \frac{1}{n} \sum_{i=1}^{n} \delta_{x_i^n},$$

where $\mathscr{P}([0,\infty))$ is the space of probability measures. We consider convergence in either the narrow (or weak) topology

$$\pi_n(x^n) \rightharpoonup \mu \quad :\Longleftrightarrow \quad \forall\, \varphi \in C_c^\infty([0,\infty)) : \int \varphi \, d(\pi_n(x^n)) \to \int \varphi \, d\mu,$$

or with respect to the stronger 2-Wasserstein distance denoted by W_2 (see e.g. [4] for an introduction to the Wasserstein distance).

Our first main result (which is an extension of [15, Theorem 1]) gives a precise meaning to the convergence of the sequence of energies E_n

Theorem 1 (Γ-convergence [15, 32]) *Let $1 \lesssim \ell_n \lesssim n$ and $L_n/\ell_n \to \gamma \in (0,\infty]$ as $n \to \infty$. Then for all sequences (x^n) such that $x^n \in \Omega_n$ and $E_n(x^n)$ bounded, it holds that $(\pi_n(x^n))$ has a narrowly converging subsequence. Moreover, E_n Γ-converges with respect to the narrow topology to*

$$E : \mathscr{P}([0,\infty)) \to [0,\infty], \qquad E(\mu) := E^{int}(\mu) + \int_0^\infty x \, d\mu(x) + \chi_{\{\operatorname{supp} \mu \subset [0,\gamma]\}}, \tag{4}$$

where E^{int} depends on the asymptotic behaviour of ℓ_n (see Table 1).

We remark that we impose the conditions $1 \lesssim \ell_n \lesssim n$ and $L_n \gtrsim \ell_n$ for brevity, and that the full result can be found in [15, 32].

We briefly mention the main arguments in the proof of Theorem 1. Prokhorov's Theorem gives a convenient characterisation of pre-compactness in the narrow topology, which is easily seen to be satisfied if $E_n(x^n)$ is bounded uniformly in n.

We prove Γ-convergence by establishing its defining inequalities

Table 1 Dependence of E^{int}, the interaction part of the limit energy (4), on the asymptotic behaviour of ℓ_n

Regime	$E^{\text{int}}(\mu)$
$\ell_n \to \ell$	$\frac{\ell}{2}\int_0^\infty \int_0^\infty V(\ell(x-y))\,d\mu(y)\,d\mu(x)$
$1 \ll \ell_n \ll n$	$\begin{cases} \left(\int_0^\infty V\right)\int_0^\infty \rho^2, & \text{if } d\mu(x) = \rho(x)dx, \\ \infty, & \text{otherwise} \end{cases}$
$\frac{\ell_n}{n} \to \alpha$	$\begin{cases} \alpha \int_0^\infty V_{\text{eff}}\left(\frac{\alpha}{\rho(x)}\right)\rho(x)\,dx, & \text{if } d\mu(x) = \rho(x)dx, \\ \infty, & \text{otherwise} \end{cases}$

We define $V_{\text{eff}}(r) := \sum_{k=1}^\infty V(kr)$

$$\forall\, \mu \in \mathscr{P}([0,\infty))\ \forall\, x^n \in \Omega_n \text{ such that } \pi_n(x^n) \rightharpoonup \mu : \qquad \liminf_{n\to\infty} E_n(x^n) \geq E(\mu), \tag{5a}$$

$$\forall\, \mu \in \mathscr{P}([0,\infty))\ \exists\, y^n \in \Omega_n \text{ such that } \pi_n(y^n) \rightharpoonup \mu : \qquad \limsup_{n\to\infty} E_n(y^n) \leq E(\mu). \tag{5b}$$

The main challenge in proving these inequalities is in controlling the interaction term E_n^{int} (1). The limsup-inequality (5b) is established by choosing the wall positions y_i^n to be 'locally equi-spaced', by which the high values of V around its singularity are avoided as much as possible.

For proving the liminf-inequality (5a), the scaling regime of ℓ_n is crucial. If $\ell_n \to \ell \in (0,\infty)$, then $\ell_n V(\ell_n \cdot) \to \ell V(\ell \cdot)$, and the basic properties of the narrow convergence of $\pi_n(x^n)$ are enough to show (5a). However, if $\ell_n \to \infty$, then $\ell_n V(\ell_n \cdot) \rightharpoonup (\int_{\mathbb{R}} V)\delta_0$ in the narrow topology, which is too weak for concluding (5a) with the basic properties of the narrow convergence of $\pi_n(x^n)$. Instead, the convexity of V on the positive half-line is exploited to prove (5a). When $\ell_n \to \infty$ fast enough as $n \to \infty$ (i.e. $\ell_n \sim n$), then part of the discreteness of E_n remains visible in the continuum limit through V_{eff} (see Table 1).

As a direct consequence of Theorem 1, the minimisers of E_n converge in the narrow topology to a minimiser of E. Moreover, Theorem 1 is crucial for the proof of the convergence of the gradient flows defined in (3). While Fig. 2 gives an intuitive meaning to the convergence concept for gradient flows, Theorem 2 states the precise notion of convergence.

Theorem 2 (Convergence of gradient flows [31]) *Let $\mu_{init} \in \mathscr{P}([0,\infty))$. Then for any $x_{init}^n \in \Omega_n$ such that $W_2(\pi_n(x_{init}^n), \mu_{init}) \to 0$ as $n \to \infty$, it holds for the solutions $x^n(t)$ and $\mu(t)$ to the gradient flows of E_n and E, respectively, that $W_2(\pi_n(x^n(t)), \mu(t)) \to 0$ pointwise as $n \to \infty$ for all $t > 0$.*

Instead of giving the definition of 'the gradient flow of E' in terms of an evolution variational inequality (cf. [4]), we list in (6) the formally derived evolution equations

$$
\begin{tikzcd}
x^n_{\text{init}} \arrow[r, "\text{gradient flow of } E_n \text{ (3)}"] \arrow[d, "n \to \infty"] & x^n(t) \arrow[d, "n \to \infty"] \\
\mu_{\text{init}} \arrow[r, "\text{gradient flow of } E \text{ (6)}"] & \mu(t)
\end{tikzcd}
$$

Fig. 2 The gradient flows of E_n converge to the gradient flow of E if this diagram commutes for all $x^n_{\text{init}} \in \Omega_n$ such that $\pi_n(x^n_{\text{init}}) \rightharpoonup \mu_{\text{init}}$

from these inequalities. These equations are equipped with an initial condition and zero-flux boundary conditions at both sides of the domain.

$$\frac{\partial}{\partial t}\rho_t = \big(\rho_t + \rho_t(\ell V(\ell\,\cdot) * \rho_t)'\big)' \qquad \text{if } \ell_n \to \ell, \tag{6a}$$

$$\frac{\partial}{\partial t}\rho_t = \Big(\rho_t + \Big[\int_{\mathbb{R}} V\Big]\rho_t\rho_t'\Big)' \qquad \text{if } 1 \ll \ell_n \ll n, \tag{6b}$$

$$\frac{\partial}{\partial t}\rho_t = \Big(\rho_t + \frac{\alpha^3}{\rho_t^2}V_{\text{eff}}''\Big(\frac{\alpha}{\rho_t}\Big)\rho_t'\Big)' \qquad \text{if } \frac{\ell_n}{n} \to \alpha. \tag{6c}$$

The proof of Theorem 2 relies, in addition to Theorem 1, on the convexity of E_n and E, which are the main conditions under which the general theory [5, Theorem 6.1] concerning the convergence of gradient flows applies. In addition to these conditions, it is also required that there exists a sequence (y^n) as in (5b) for which $\pi_n(y^n)$ converges in the 2-Wasserstein distance.

While Theorems 1 and 2 connect different continuum dislocation density models, they do not quantify how well any of the continuum models approximate the discrete model for a *fixed* number of dislocations. We plan to face this challenge in the near future.

3 Upscaling of Mixed Positive and Negative Dislocations

In Sect. 3.1 we describe the scenario of mixed positive and negative dislocations, which is closely related to [16, 17]. Section 3.2 treats the upscaling of the related energy functionals, and Sect. 3.3 concerns evolutionary convergence of the related gradient flows. The proofs of these results are documented in [30, Chaps. 5 and 8], which is intended to be submitted for publication with A. Garroni, M.A. Peletier, and L. Scardia.

3.1 Setting

In contrast to the dislocation walls in Fig. 1a, we now consider a finite number $n \in \mathbb{N}$ of dislocations without any imposed configuration. In this setting, a dislocation is characterised by its position $x_i^n \in \mathbb{R}^2$ (we do not consider barriers) and its *orientation* $b_i^n = \pm 1$. The result of dislocations having a different orientation is that dislocations with opposite orientation interact with *opposite* force with respect to two dislocations with the same orientation.

The naive approach for defining an interaction energy is to consider

$$\tilde{E}_n(\,\cdot\,; b^n) : (\mathbb{R}^2)^n \to \overline{\mathbb{R}}, \qquad \tilde{E}_n(x^n; b^n) := \frac{1}{2n^2} \sum_{i=1}^{n} \sum_{\substack{j=1 \\ j \neq i}}^{n} b_i^n b_j^n V(x_i^n - x_j^n),$$

where V is the interaction potential in two dimensions given by

$$V : \mathbb{R}^2 \to (-\infty, \infty], \qquad V(r) := \frac{r_1^2}{|r|^2} - \log |r|. \tag{7}$$

The problem with this approach is that $\tilde{E}_n$ is unbounded from below. In fact, any small energy value can be obtained by taking two dislocations of opposite orientation close enough. Therefore, variational techniques are not suited for the upscaling of $\tilde{E}_n$.

We solve this problem by introducing an approximation to the energy $\tilde{E}_n$. The usual approximation in the literature consists of regularising the singularity in V. In contrast to choosing a specific regularisation, which is commonly done (for instance, the different regularisations used in [3, 7, 9, 22, 24]), we consider a large class of regularisations (specified below). For any such regularisation V_n of V, we consider the energy

$$E_n(\,\cdot\,; b^n) : (\mathbb{R}^2)^n \to \mathbb{R}, \qquad E_n(x^n; b^n) := \frac{1}{2n^2} \sum_{i=1}^{n} \sum_{j=1}^{n} b_i^n b_j^n V_n(x_i^n - x_j^n). \tag{8}$$

3.2 Γ-Convergence

We follow a similar program as in Sect. 2.2. To any given $x^n \in (\mathbb{R}^2)^n$ and $b^n \in \{-1, 1\}^n$, we associate the signed finite Borel measure $\kappa_n := \frac{1}{n} \sum_{i=1}^{n} b_i \delta_{x_i^n}$. In terms of κ_n, the energy in (8) reads

$$E_n(x^n; b^n) = \frac{1}{2} \int V_n * \kappa_n \, d\kappa_n,$$

which we denote by $E_n(\kappa_n)$. We use the following modified version of the narrow topology:

$$\kappa_n \overset{c}{\rightharpoonup} \kappa \quad :\Longleftrightarrow \quad \begin{cases} \kappa_n \rightharpoonup \kappa, \text{ and} \\ \bigcup_{n=1}^{\infty} \operatorname{supp} \kappa_n \text{ is bounded.} \end{cases} \tag{9}$$

The additional condition concerning the support of κ_n is artificial. It allows us to focus on the collective behaviour of the non-local dislocation interaction while side-stepping technical difficulties when dislocations spread infinitely far.

We motivate the Γ-convergence theorem below in terms of the main assumptions that we put on V_n. We observe [30, Proposition 5.3.1] that V can be split as

$$V = W * W + V_0$$

for some $W \in L^1(\mathbb{R}^2)$ and $V_0 \in C(\mathbb{R}^2)$. Then, we define

$$V_n := W_n * W_n + V_0^n \tag{10}$$

for some $W_n \to W$ in $L^1(\mathbb{R}^2)$ and $V_0^n \to V_0$ in $L^\infty_{\text{loc}}(\mathbb{R}^2)$ as $n \to \infty$, such that V_n converges uniformly to V in any annulus centred around 0. These are the core assumptions which we need on V_n. For the precise assumptions on V_n we refer to [30]. The main gain of the structure of V_n as in (10) is that the energy can be written as

$$E_n(\kappa_n) = \int_{\mathbb{R}^2} (W_n * \kappa_n)^2 + \int V_0^n * \kappa_n \, d\kappa_n,$$

which is crucial for our proof of the following theorem:

Theorem 3 (Γ-convergence [30]) *If $V_n(0)/n \to 0$ as $n \to \infty$, then E_n Γ-converges with respect to the modified narrow topology (9) to*

$$E : \left\{\kappa \in \mathscr{M}(\mathbb{R}^2) : \|\kappa\|_{TV} \leq 1\right\} \to [0, \infty], \qquad E(\kappa) := \int V * \kappa \, d\kappa. \tag{11}$$

Here, $\mathscr{M}(\mathbb{R}^2)$ is the space of finite Borel measures on $\mathbb{R}^2$. The condition $V_n(0)/n \to 0$ as $n \to \infty$ ensures that the energy contribution of the self-interactions (i.e. $i = j$ in (8)) vanishes in the limit. Regarding the case in which $V_n(0) \gtrsim n$, the only known Γ-convergence result of E_n is proved in [10, 14] for a specific regularisation V_n.

3.3 Convergence of Gradient Flows

A special feature of (edge) dislocations is that they move horizontally. Together with the linear drag law, their motion is described by the following gradient flow:

$$\begin{cases} \dfrac{dx}{dt}(t) = -nP\nabla E_n(x(t); b), \quad t \in (0, T], \\ x(0) = x_{\text{init}}, \end{cases} \tag{12}$$

where $P \in R^{2n \times 2n}$ is the diagonal projection matrix characterised by its diagonal given by $(1, 0, 1, 0, \ldots, 1, 0)$. As a consequence of the horizontal movement, the vertical coordinates of the dislocation positions can be considered as parameters.

Next we focus our attention on positive dislocations only, i.e. $b_i^n = 1$ for all $i = 1, \ldots, n$. Consequently, we characterise their positions by the probability measure $\mu_n := \frac{1}{n} \sum_{i=1}^n \delta_{x_i^n}$, and we use the restriction of the energy functionals E_n (8) and E (11) to $\mathscr{P}(\mathbb{R}^2)$ without changing notation.

Conjecture 1 (Convergence of gradient flows [30]) *Let $\mu_{init} \in \mathscr{P}(\mathbb{R}^2)$ be such that $E(\mu_{init}) < \infty$ and* supp *μ_{init} bounded. If $V_n(0)/n \to 0$, then for any recovery sequence μ_{init}^n (in the sense of* (5b)*) converging to μ_{init} as $n \to \infty$, it holds for the solutions $\mu_n(t)$ to* (12) *that there exists a solution $\mu(t)$ to the gradient flow of E such that, along a subsequence, $\mu_n(t) \overset{c}{\rightharpoonup} \mu(t)$ pointwise as $n \to \infty$ for all $t \in [0, T]$.*

Up to a few technical conjectures, the proof of Conjecture 1 is complete. It relies on the framework developed in [26, 28]. Other than Γ-convergence, an important requirement of this framework is that a similar liminf-inequality to (5a) holds for the *slope* of the energy, which is a generalisation for the length of the gradient for functionals defined on metric spaces. To prove this inequality, we require more regularity on $\partial_1 V_n$. Again, we refer to [30] for the details.

The gradient flow of E is characterised in terms of an energy-dissipation inequality, which we can formally write as

$$\frac{d}{dt}\mu = \partial_1(\mu \partial_1 V * \mu), \qquad \text{in } \mathscr{D}'\big(\mathbb{R}^2 \times (0, T)\big),$$

where ∂_1 denotes differentiation in the horizontal direction.

In future work, we aim to complete the proof of Conjecture 1, and extend it to mixed positive and negative dislocations. The challenge for proving this extension is to control the singularity in V, which may require us to put more restrictions on the regularisation V_n.

4 Implications for Plasticity Models

With the three theorems above and Conjecture 1 we have partially answered our main question in Sect. 1 about connecting discrete dislocation models with continuum dislocation models for several scenarios. Here, we elaborate on the implications of our results to existing dislocation density models.

The main result of [15] is that the local arrangement of dislocations, measured in terms of the parameter ℓ_n, can drastically change the pile-up profile of the dislocation density in equilibrium. Theorems 1 and 2 give a precise meaning to the extension of this statement to finite domains and to the dynamics of dislocation walls. As a result, it seems that an accurate two-dimensional model for the dislocation density should depend on more detailed information on the local arrangement of dislocations. Highly speculating, such a model may unite the currently available dislocation density models.

Theorem 3 and Conjecture 1 are closely related to the setting in [16, 17]. These theorems are consistent with the continuum model in [16], but only if the regularisation of the interaction potential converges *slowly* enough as $n \to \infty$. This is surprising, because the derivation of the continuum model in [16] does not rely on any regularisation. This suggests that the regularisation in the discrete model should converge, instead, *fast* enough to obtain the continuum gradient flow proposed in [16]. In the near future we aim to shed more light on this peculiar observation.

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