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A single theory for some quasi-static, supersonic, atomic, and tectonic scale applications of dislocations

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ABSTRACT

We describe a model based on continuum mechanics that reduces the study of a significant class of problems of discrete dislocation dynamics to questions of the modern theory of continuum plasticity. As applications, we explore the questions of the existence of a Peierls stress in a continuum theory, dislocation annihilation, dislocation dissociation, finite-speed-of-propagation effects of elastic waves vis-a-vis dynamic dislocation fields, supersonic dislocation motion, and short-slip duration in rupture dynamics.

1. Introduction

This paper explores some qualitative aspects of Field Dislocation Mechanics (FDM), a nonlinear, partial differential equation (pde)-based model of the mechanics of dislocations. The physical phenomena explored correspond to behavior of individual or a collection of few dislocations. In particular, we analyze phenomena complementary to what can be dealt with by the Discrete Dislocation Dynamics methodology in a fundamental manner. Specifically, we explore

- Peierls' stress effects in a translationally-invariant continuum theory like FDM.
- Dislocation annihilation and dissociation as consequences of fundamental kinematics and energetics and not targeted constitutive rules for the phenomena.
- Dislocation dynamics in the presence of significant effects of material inertia, including finite-speed-of-propagation effects of elastic waves and dislocation motion past sonic speeds.
- Dislocation dynamics with nonlinear elasticity.
- Short-slip duration in rupture dynamics.

The question of the possibility of a Peierls-like threshold for onset of dislocation motion in a translationally-invariant, time-dependent continuum theory was discussed by Acharya (2010). The classical, static, argument going back to Peierls

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(1940) relies crucially on the fact that such a threshold is directly related to changes in the total potential energy of the body induced by changes in position of the dislocation (naturally, then, viewed as a rigid object or profile). Since in a homogeneous infinite continuum the total potential energy remains invariant due to changes in position of the rigid dislocation profile, the conclusion is that there cannot be a Peierls stress in a translationally-invariant continuum theory; breaking translational invariance, possibly by modeling the effects of an atomic lattice (as was done by Peierls, 1940; Nabarro, 1947) or by introducing a heterogeneous medium, can introduce a Peierls stress. However, questions of stability of equilibria under perturbations of loading in a time-dependent model of dislocation mechanics with a significantly different notion of a driving force (that includes self-stress effects) can be quite different, in particular whether an unloaded equilibrium dislocation profile can serve as a traveling wave profile under a continuous spectrum of finite loads tending to zero – and, if not, is there an interval of loads about zero for which different equilibrium profiles can be attained parametrized by the load. Such questions have to do intimately with changes in 'shape' of the dislocation profile. In this paper we computationally explore this question – as a point of principle, most of all – for three natural models that the structure of FDM makes available. These correspond to a *non-local Ginzburg Landau* model, a *non-local level set* model and what may be termed as a *generalized, non-local Burgers model*. In Sections 4 and 7.1 we describe these models and results in detail. Despite the great utility of analysis of traveling waves, our results point definitely in the direction of avoiding an over-reliance on characteristics of traveling wave solutions in making general statements about the non-existence of certain types of predictions related to the representation of physical phenomena characterized by fronts. After all, there is no reason why a traveling front necessarily has to be perfectly rigid during motion, making an infinite-dimensional object (a profile allowed us to change shape, while still remaining localized) into one of dimension 1. A physical example related to this paper is the onset of motion of screw dislocations in some BCC materials. There, it is understood that the dislocation core is spread out on multiple planes and the core has to be compacted further into a preferred slip plane before gross motion can ensue; once motion stops, the multiple-plane equilibrium configuration is regained. In a qualitative sense, we demonstrate such features, including differences between dynamic and equilibrium shapes in Section 7.

With respect to dislocation annihilation, since the fundamental statement of evolution in FDM is a conservation law for Burgers vector content of the dislocation density field, the density field evolves by tensorial addition rules resulting in natural accumulation or annihilation of non-singular localizations of net positive and negative Burgers vector when physically expected. We demonstrate such results in Section 7.4.

The discussion of the possible dissociation of a dislocation of a certain Burgers vector strength into two whose strengths vectorially sum up to that of the original one is a text-book example of the phenomenology of dislocations related to the energy-decreasing feature of dislocation mechanics. Due to the treatment of a dislocation core as either a formless or a rigid singularity in classical versions of any sort of dislocation dynamics, dissociation cannot be a prediction. The field setting is ideally suited for such explorations as we demonstrate in Section 7.1.7.

As for dislocation dynamics with material inertia, it is physically natural that a moving dislocation induces elastic stress-waves that cannot transmit the stress signal instantaneously to all parts of the body. This fact is naturally encoded in FDM and our simulations, without extra effort or computational expense beyond solving standard elastodynamics equations. As discussed in Gurrutxaga-Lerma et al. (2013), when time intervals of observation are small (as in very high rate deformations) this time delay in stress signal transmission due to stress-wave propagation can be of importance, and merely correcting for individual dislocation motion laws in DD simulations by added-mass effects, while utilizing the static stress fields of dislocations, is not sufficient; instead, dislocation stress fields utilizing the full dynamic Green's function have to be utilized and this becomes a significantly onerous task, especially with an increase in number of segments. We demonstrate the efficacy of FDM in dealing with such problems in Section 8.3. In addition, we show that there is no conceptual or practical problem within FDM in dealing with dislocation motion past linear-elastic sonic speeds (in appropriate circumstances) as observed in the molecular dynamics (MD) experiments of Gumbsch and Gao (1999), or in dealing with nonlinear elasticity, with beneficial effect related to matching trends of dislocation velocity vs. applied loading to MD results.

Finally, we make a successful first attempt at modeling the observed phenomenon of short-slip duration in earthquake rupture as well as the more conventional crack-like slip response obtained from slip-weakening cohesive zone models of rupture dynamics. These features are obtained without sophisticated constitutive modifications of velocity-weakening or rate-and-state friction type, but simply by invoking a requirement of damage of elastic modulus at a point on propagation of the rupture front past it.

In this work we utilize an ansatz to produce an exact, reduced, plane model of FDM. Our model is built on the previous work of Acharya (2010) where a 1-D FDM model was derived and further explored numerically in Das et al. (2013). The 1-D model, taking the form of a nonlinear Hamilton–Jacobi equation, governs the evolution of plastic shear strain in a 1-D bar. Mathematical analysis of traveling waves in the model for the scalar case was performed in Acharya et al. (2010); global existence and uniqueness for the 1-D space $\times$ time system was analyzed in Acharya and Tartar (2011). Our work generalizes the 1-D model to plane strain where edge dislocations exist and glide horizontally along a prescribed plastic layer. The plastic evolution is governed by a similar 1-D model as derived in Acharya (2010), but now nonlocal if viewed solely as an equation in terms of the plastic strain, with the 3-d dissipation maintained non-negative without approximation. This results in a useful model that is amenable to reasonably efficient and accurate numerical simulation.

The rest of the paper is organized as follows: in Section 2 we settle on notational conventions. In Section 3 we briefly recall the full 3-D FDM theory in the geometrically linear framework. We describe the derivation of the 2-d model in Section 4. The numerical schemes utilized in the paper are described in Section 5. Equilibrium aspects of the system are discussed in