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Coupled atomistic/discrete dislocation method in 3D Part II: Validation of the method

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ABSTRACT

A methodology for coupling a fully atomistic domain to a surrounding domain described by discrete dislocation plasticity, including the treatment of hybrid dislocation lines that span between the two domains, was presented in the first paper of this series (Anciaux et al., 2017). Here, key features of the methodology are assessed quantitatively within a quasi-static framework at 0 K. To avoid solving an expensive but standard complementary problem for the atomistic/continuum coupling of mechanical fields, which is not essential to the key features of the method, a simplified model for obtaining accurate stress and displacement fields is introduced and validated. The test problem consists of the bow-out of a single dislocation in a semi-periodic box under an applied shear stress, and excellent results are obtained in comparison to fully-atomistic solutions of the same problem.

1. Introduction

Predictive mathematical tools for modeling plasticity at different length scales began to develop in the beginning of the last century. The current theoretical frameworks can be broadly grouped into atomic, meso-, micro- and macroscale models, describing phenomena across scales from individual dislocation motion in nanometer specimens to accumulated plastic flow in large structures. Since plasticity is now established to be size-dependent, and since important controlling dislocation phenomena occur at the atomic scale, the understanding of macroscopic behavior can often require handling plasticity phenomena across several scales simultaneously.

The discrete dislocation dynamics (DDD) method has been developed to study metal plasticity at the micron scale by following the collective motion of complex dislocation arrays. The DDD method must be informed by rules/laws regarding dislocation mobility, dislocation reactions, and interactions of dislocations with metallurgical defects. These latter phenomena are atomistic in nature, and atomistic simulations can be used to provide the necessary input in many simple cases. However, dislocation nucleation and interactions with defects (surfaces, crack tips, voids, solutes, grain boundaries) involves inherently atomistic response that can be difficult to characterize at the level of discrete dislocation line defects. It is not possible, however, to treat mesoscale plasticity problems using purely atomistic methods, due to the computational cost. Thus, it is beneficial to have a methodology that directly couples evolving atomistic and discrete dislocation domains, such

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that atomistic behavior beyond the capabilities of the DDD method can be modeled explicitly in local regions, outside of which the plasticity evolves via the DDD rules. Atomistic/continuum coupling of mechanical fields wherein all inelastic phenomena are contained only in the atomistic domain has been achieved in many methods, starting with the Quasicontinuum method (Tadmor et al., 1996) and continue to evolve today (Amelang et al., 2015; Knap and Ortiz, 2001; Kochmann and Venturini, 2014; Shimokawa et al., 2004; Xiao and Belytschko, 2004). Extending the methods to handle dislocation plasticity in the continuum domain, and with nearly seamless passing of dislocations back and forth between atomistic and continuum domains, was achieved in the 2d plane strain limit by the Coupled Atomistic and Discrete Dislocations (CADD) method (Miller et al., 2004; Shilkrot et al., 2002a; 2004). In 2d, where the dislocation line direction is perpendicular to the plane of analysis, the individual dislocations are wholly contained within the atomistic domain or the DDD domain. While 3d methods can also handle dislocations solely in both domains, there has been no method for dealing with the full problem wherein individual dislocation lines exist in both domains simultaneously, so-called **hybrid dislocations**. Since many dislocation phenomena occur in 3d, the development of a full 3d CADD method provides powerful new capability for realistic multiscale simulation of dislocation plasticity.

In a companion paper (Anciaux et al., 2017), we have proposed such a 3d CADD method, denoted as CADD-3d. The transition region of a hybrid dislocation between atomistic and continuum-line representations is accomplished through a **template** imposed at the atomistic/continuum interface that enriches the continuum-line description with an atomistic description of the dislocation core structure. This template thus approximates the atomistic environment that the atomistic system would have if embedded in a fully atomistic domain, and thus minimizes coupling errors at the crucial core region of the dislocation as the line passes from one description to the other. An algorithm for the coupled evolution of such hybrid dislocations was also presented in detail. This enables the atomic region to experience accurate forces from the dislocation(s) spanning both domains.

In the present work, we aim to quantitatively assess this key concept of CADD-3d. More precisely, we are interested in the error in the evolution of the hybrid dislocation line, induced by the boundary condition on the atomistic problem which is enriched with the dislocation core template. Therefore we have selected a relatively simple quasi-static test problem which focuses on the main aspects by neglecting non-essential parts such as dynamics and external boundary conditions. One feature of fully 3d problems is the necessity of solving for the stress fields throughout the entire domain. This is normally accomplished using a computationally expensive finite-element solution to solve the complementary problem for the $\hat{\bullet}$ fields, as stated in Paper I. To avoid this part of the method for the time being, since this aspect of the problem is well-established conceptually, we introduce a simplified methodology that is valid in infinite domains and when the atomistic domain only contains dislocations (no other defects). In this limit, we compute the entire problem as if it is purely a DDD problem for all dislocation segments, including those in the atomistic domain, and compute the necessary stress fields on the true DDD segments and displacement fields on the atomistic boundary analytically via the $\tilde{\bullet}$ fields plus the superimposed stress field at infinity. We validate this simplified methodology independently of our CADD-3d test problem. We then apply the CADD-3d method to study the periodic bow-out of a single dislocation, for which reference solutions in essentially infinite domains can be obtained for both fully atomistic and fully DDD problems. This test problem allows us to isolate the modeling of the evolution of a hybrid dislocation and demonstrate minimal errors relative to the reference fully atomistic solution.

The remainder of this paper is organized as follows. In Section 2 we first state the governing equations of CADD-3d in a general quasi-static setting at 0 K. Subsequently the approximate problem is derived from the general formulation. We present a practical yet efficient alternating Schwarz-type solution procedure and highlight the advantages of the approximate formulation but also show its limitations by quantifying spurious effects on dislocations in the atomistic domain depending on the complexity of the linear elastic solution used to compute the dislocation fields of the atomic dislocation. In Section 3 we present the numerical validation of the method and discuss key features.

2. Coupled atomistic/discrete dislocations in 3D

2.1. General formulation

In paper I (Anciaux et al., 2017), we have presented the general algorithm for the coupling of an atomistic domain Ω_A to a continuum domain Ω_C described by discrete dislocation dynamics, for systems containing dislocations spanning both domains (hybrid dislocations formed by the intersection of the two lines γ_a and γ_c as shown in Fig. 1). The (artificial) interface between both subdomains is denoted as $\partial\Omega_I$. At any instant or increment of loading, the atomistic problem involves the interactions of atoms via interatomic potentials subjected to boundary conditions on a surrounding atomistic pad region $\Omega_P \subset \Omega_C$ whose atomic positions are dictated by the solution of the continuum dislocations problem. The associated continuum problem involves a small-strain elasticity solution of a discrete dislocation dynamics problem subjected to the displacement boundary conditions associated with atomic positions at the atomistic/continuum interface plus any boundary conditions applied on the external boundaries. For hybrid dislocations, the continuum displacement field in the pad region is enriched by the addition of a corrective displacement field $\Delta\tilde{\boldsymbol{u}}_{\text{corr}}(\boldsymbol{x}; \boldsymbol{b}, \vartheta_p)$ that approximates the true atomistic core structure of the hybrid dislocation at the interface with character angle ϑ_p and Burgers vector $\boldsymbol{b}$. An algorithm for the simultaneous evolution of both atomistic and continuum domains was then presented for the case of full quasi-dynamic coupling (quasi-static evolution of the dislocation dynamics problem).