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A Threshold Dislocation Dynamics Method

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Abstract. The Merriman-Bence-Osher threshold dynamics method is an efficient algorithm to simulate the motion by mean curvature. It has the advantages of being easy to implement and with high efficiency. In this paper, we propose a threshold dynamics method for dislocation dynamics in a slip plane, in which the spatial operator is essentially an anisotropic fractional Laplacian. We show that this threshold dislocation dynamics method is able to give two correct leading orders in dislocation velocity, including both the $\mathcal{O}(\log\varepsilon)$ local curvature force and the $\mathcal{O}(1)$ nonlocal force due to the long-range stress field generated by the dislocations as well as the force due to the applied stress, where ε is the dislocation core size, if the time step is set to be $\Delta t=\varepsilon$. This generalizes the available result of threshold dynamics with the corresponding fractional Laplacian, which is on the leading order $\mathcal{O}(\log\Delta t)$ local curvature velocity under the isotropic kernel. We also propose a numerical method based on spatial variable stretching to correct the mobility and to rescale the velocity for efficient and accurate simulations, which can be applied generally to any threshold dynamics method. We validate the proposed threshold dislocation dynamics method by numerical simulations of various motions and interaction of dislocations.

AMS subject classifications: 65R20, 65N12, 74A50, 35R11

Key words: Dislocation dynamics, threshold dynamics method, nonlocal velocity, anisotropic mobility, variable stretching.

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1 Introduction

Mean curvature flow describes the motion of a co-dimension one object normal to itself with velocity equal to its mean curvature. Merriman, Bence and Osher (MBO) developed an efficient threshold dynamics method to simulate the motion by mean curvature [24, 25]. In this method, two simple steps alternates: a convolution with diffusion kernel and a thresholding step. The MBO threshold method has the advantages of being easy to implement and with high efficiency. The MBO threshold dynamics method has been further developed with some efficient implementations and generalization to multiphase interfaces [11,30,31,33] as well as convergence analysis [3,14,23,34]. Esedoglu and Otto developed a threshold dynamics method for dynamics of networks with arbitrary surface tensions [13]. Elsey and Esedoglu generalized the threshold dynamics method to anisotropic mean curvature motion by replacing the isotropic Gaussian kernel in the convolution step of the original algorithm with more general, anisotropic kernels [10]. Convergence of nonlocal threshold dynamics corresponding to the fractional Laplacian was proved by Caffarelli and Souganidis in [4]. The threshold dynamics method was also extended to Willmore flow and some high-order geometric flow problems [12], [20], wetting of fluids on rough surfaces [44], image segmentation [37], topology optimization for fluids [6, 21], and reconstructing surface from point clouds [36], etc.

Dislocation dynamics simulation is an important tool for the study of plastic deformation in crystalline materials [2, 5, 17, 22, 29, 40], in which the motion and interaction of dislocations (line defects) are simulated. The driving force on dislocations is nonlocal, which is due to the stress field generated by all the dislocations. This is unlike the motion by curvature, which depends only on the local profile of the curve. The driving force on dislocations consists of both the nonlocal $\mathcal{O}(1)$ force and the local $\mathcal{O}(\log\varepsilon)$ curvature force, where ε is the dislocation core size, and both are important in the dynamics of dislocations. This force on dislocations is in general anisotropic depending on the orientation of the dislocations. The Peierls-Nabarro model [1, 27, 28, 35] is a hybrid model that incorporates atomic-size dislocation core into the continuum framework. Computational models for dislocation structure and dynamics of curved dislocations based on the Peierls-Nabarro models and generalizations have been developed [26, 32, 38, 39, 42, 43, 45, 47]. Velocities of straight dislocations with the applied stress under the setting of fractional Laplacian equation (a simplified Peierls-Nabarro model) have been analyzed [7, 8].

In this paper, we propose an efficient threshold dynamics method for dislocation dynamics in a slip plane, based on the Peierls-Nabarro model for curved dislocations in [38, 42]. In the convolution step, the dislocation stress field kernel, which is essentially an anisotropic fractional Laplacian kernel, is used instead of the isotropic diffusion kernel in a standard threshold dynamics method. We show that this proposed threshold dislocation dynamics method gives correct dislocation velocity as compared with the discrete dislocation dynamics method. More precisely, we show that the threshold dislocation dynamics method gives both the correct $\mathcal{O}(\log\varepsilon)$ local curvature force and the correct $\mathcal{O}(1)$ nonlocal force due to the long-range stress field generated by the dislocations as