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Simulating Dislocation Densities with Finite Element Analysis

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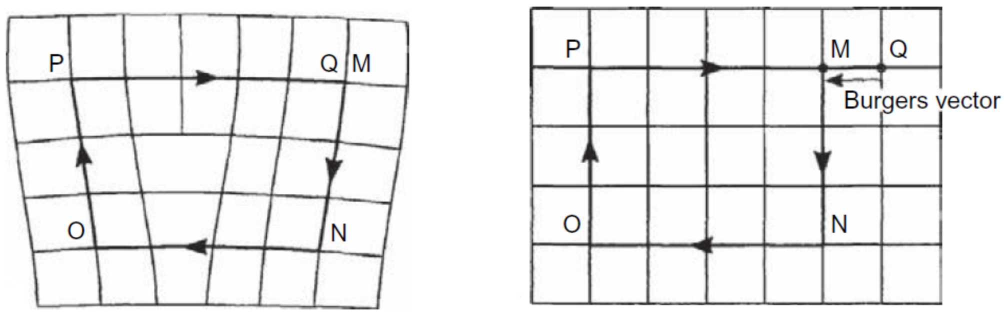
Abstract

A one-dimensional set of nonlinear time-dependent partial differential equations developed by Acharya (2010) is studied to observe how differing levels of applied strain affect dislocation walls. The framework of this model consists of a convective and diffusive term which is used to develop a linear system of equations to test two methods of the finite element method. The linear system of partial differential equations is used to determine whether the standard or Discontinuous Galerkin method will be used. The Discontinuous Galerkin method is implemented to discretize the continuum model and the results of simulations involving zero and non-zero applied strain are computed. The evolution in time of functions for plastic deformation, dislocation density, and internal shear stress are plotted and discussed.

1 Introduction

The study of crystalline materials has applications in aerospace, automotive, and nuclear engineering fields in order to achieve the optimal design of components. Crystalline structures include all materials that contain uniform planes of atoms that repeat themselves periodically in three directions. This description also applies to pure metals because they contain a simple, uniform atomic structure. The structures of pure metals can be compared to more complex metallic alloys that contain atoms derived from other metals to alter the properties of the structure. Dislocations in crystalline structures may have a positive or negative effect on the strength, corrosion resistance, or fracture resistance of materials. Dislocations are linear defects in crystals and their motion cause plastic deformation. Linear defects consist of edge and screw dislocations, which disturb the lattice of the material. Edge dislocations consist of an additional half-plane of atoms shown in Figure 2. Screw dislocations, shown in Figure 1, are where atoms are rearranged in a helical pattern like that of a spiral staircase.

The Burgers circuit is an atom to atom rectangular loop traced around the dislocation core, $\vec{t}$. After following the same path in the perfect crystal, we see a gap that defines the Burgers vector, $\vec{b}$. For an edge dislocation, $\vec{b} \perp \vec{t}$ and for a screw dislocation, $\vec{b} \parallel \vec{t}$. The Burgers vector is characterized by the dislocation in a lattice and plastic deformation is defined as the movement of these dislocations throughout the material.



(a) (b)

Figure 1: (a) shows a Burgers circuit being formed around the dislocation core, which is repeated in figure (b). The Burgers vector(QM) is formed to compensate for the gap. Image courtesy of Hull and Bacon (2011)

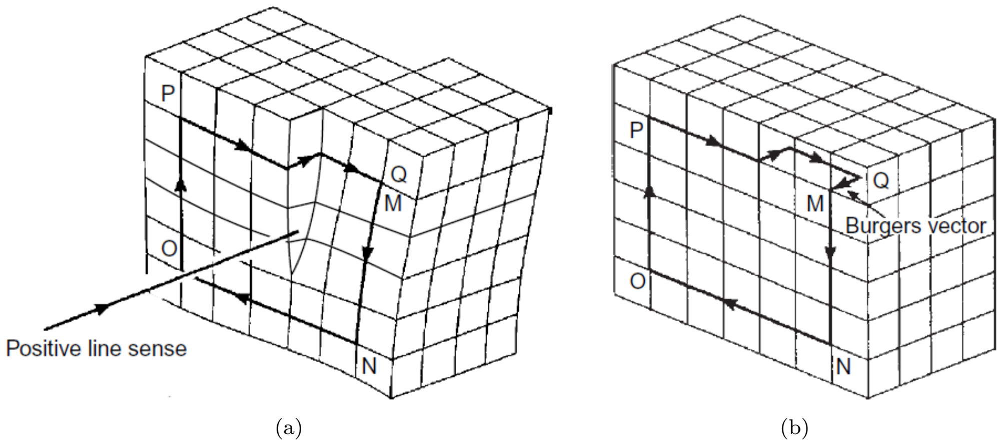


Figure 2: Burgers vector (QM) in (b) is perpendicular to the positive line sense or dislocation line in (a). Image courtesy of Hull and Bacon (2011)

Dislocation walls are regions within a material where dislocation dipoles are collected. All of these dislocations are close to one another and their dislocation lines are parallel. In a study of fatigue , Ahmed et al. (1997) studies a physical sample of copper to study how cyclic deformation can affect the material. In this study, dislocation walls containing edge dislocations are observed to form at regular spacings in the material due to plastic strain in Figure 3. There are two types of strain that can affect a material, elastic and plastic strain. Elastic strain is a component of applied strain which does not permanently alter the lattice. Once the material reaches its elastic limit, once unloaded, the material will experience physical changes throughout the lattice.

The primary focus of this paper is to analyze the behavior of few dislocations explicitly by numerically approximating a PDE-based model developed by Acharya (2010).

This model is described by a nonlinear system of equations driven by an applied strain, for which we do not have an exact solution. An approximate solution must be computed using some numerical method. There are convective and diffusive terms within this model, so as a first attempt to select a method for computation, we test two methods using a simple linear convection-diffusion equation. Linear models provide the advantage of allowing the error convergence rate to be easily computed.

To solve PDEs numerically, we use a computational tool called the Finite Element Method(FEM). This involves defining a mesh and a finite dimensional space of functions, used to represent the solution.

We simulate our linear convection-diffusion model using two different methods of Finite Element Analysis(FEA), the standard FEM and the Discontinuous Galerkin (DG) method. Upon simulating the models using the DG method, we see enhanced stability in our solutions.

The organization of the paper is as follows: Related work in the study of crystal materials is discussed in section 2. The mathematical features of the nonlinear one-dimensional continuum model are described in section 3. The preliminary FEM testing and convergence trials for verification of the linear model are implemented in section 4. Finally, after having selected the DG model, the setup and results of the simulations for the nonlinear model are described in section 5. This is followed by the discussion of results and conclusion.

The overarching goal of this study is to model and analyze the formation of patterns, such as persistent-slip bands, in cyclic deformation of metals (Ahmed et al. (1997)). We plan to model such behavior in three-dimensions in future, once a thorough understanding of the stability and efficiency of the numerical scheme has been developed in the one-dimensional framework.

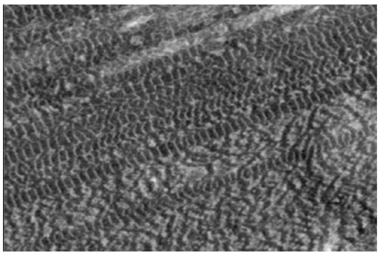
2 Related Work

Acharya (2010) developed a one-dimensional model of Field Dislocation Mechanics to study the movements of one or more screw dislocation walls. Screw dislocation walls and the governing equations surrounding them are frequently discussed in other literature, such as Roy and Acharya (2005). We reference Acharya (2010) for the non-monotone stress and elastic strain relationship which is pivotal to our work.

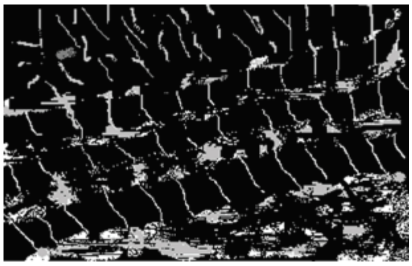
A model developed by Acharya (2010) is used in Das and Acharya (2013) to explore a one-dimensional model of screw dislocation walls, a reduction of a previous three-dimensional system of PDEs developed for Field Dislocation Mechanics. The finite difference method is used to solve the PDEs of this model. Within the results of the simulations, there is a spatially non-periodic and slow-evolving dislocation wall microstructure which is indistinguishable from equilibrium. While there is applied strain, the dislocation wall is capable of moving, as expected from the model.

Using similar nonlinear models to what is presented in this work, we will reproduce the results of this paper's simulations with a Discontinuous Galerkin FEM to examine the effects of stress and strain on dislocation walls.

A study conducted by Ahmed et al. (1997) studies how fatigue affects a copper sample when cyclic deformation is enacted upon the lattice. This cyclic deformation process results in a pattern that forms in the material which is viewed at a microscopic level.



(a) Patterns formed by cyclic strain.



(b) White lines represent the dislocation walls.

Figure 3: Images courtesy of Ahmed et al. (1997)

The white lines that form within the pattern represent dislocation walls which we will represent in our code as the dislocation density function α. This study serves as the motivation for the work of Das and Acharya (2013) and provides a clear interpretation of the dislocation densities discussed in this paper.

3 1D Continuum Model

Our model is capable of defining our time and length values into SI units, but we non-dimensionalize the model to simplify the process of modeling the system. Our nonlinear model uses the distance variable b, which is approximately $4.05e^{-10}m$ where b represents the magnitude of a Burgers vector. Time units are quantified as $\frac{bB}{c}$ where B represents the body under consideration, which converts to $2.47e^{5}N - \frac{s}{m^3}$. c is a spatially constant vector field, which converts to $2.3e^{1}0\frac{N}{m^2}$.

We use a non-dimensionalized model to simulate the evolution of dislocation density and plastic deformation when a shear strain is applied to a one-dimensional rod Figure 4.

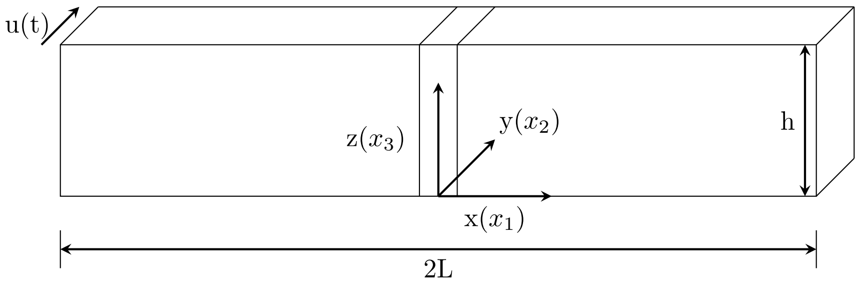


Figure 4: Schematic layout of a 3D cylinder with rectangular cross section and a screw dislocation wall. Image courtesy of Puri et al. (2021)

$$\partial_x \phi = \alpha \tag{1}$$

$$\partial_t \alpha = \partial_x \Big[\, |\alpha| \, \left(\tau + \frac{1}{4}\partial_x \alpha \right) \Big] \tag{2}$$

The domain is $(-L, L) \times (0, T)$ where α is set to 0 at the left and right boundaries of the system with Dirichlet boundary conditions. The subsection at the origin of the rod can represent a dislocation wall, a collection of screw dislocations dipoles within the lattice.

The function α represents the dislocation density, ϕ is the plastic deformation, and τ is the applied shear strain, which depends on the difference, γ_e, between the applied strain and the plastic deformation. We consider a periodically extended cubic stress function

$$\tau(\gamma_e) = \begin{cases} \frac{1}{2\left(\frac{\overline{\phi}}{2}\right)^2}\gamma_e \left(\gamma_e - \frac{\overline{\phi}}{2}\right)\left(\gamma_e - \overline{\phi}\right), & \gamma_e \in [0, \overline{\phi}) \\ \tau\left(\gamma_e - \overline{\phi}\left\lfloor \frac{\gamma_e}{\overline{\phi}} \right\rfloor\right), & \gamma_e \in R \setminus [0, \overline{\phi}), \end{cases} \tag{3}$$

where $\lfloor \cdot \rfloor$ is the floor function, which returns the largest integer less than or equal to its argument. $\gamma_e = g(t) - \phi$ and $\bar{\phi}$ is a dimensionless material constant.

In order to to define a single wall of dislocations, the initial conditions must be defined. The standard initial conditions are as follows:

$$\alpha(x, 0) = \frac{\bar{\phi}}{2}(1 - \tanh^2(x + 2)) \tag{4}$$

$$\phi(x, 0) = \frac{\bar{\phi}}{2}(1 - \tanh(x + 2)) \tag{5}$$

To separate the convective and diffusive terms, we can simplify (2) as

$$\partial_t \alpha = \partial_x \left(|\alpha| \tau \right) + \partial_x \left(\frac{|\alpha|}{4} \partial_x \alpha \right) \tag{6}$$

.

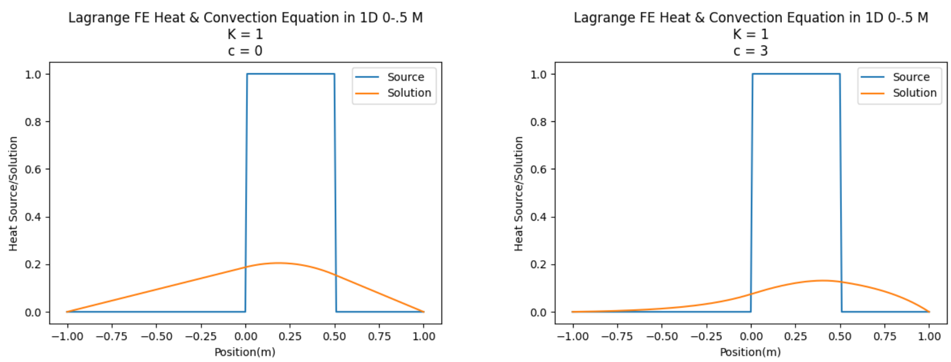
The non-linearity of this problem means it may not be possible to find an exact solution. Without an exact solution, we cannot determine the exact order of convergence for our methods. In order to test which FE method should be used to solve the previous set of equations, we will use a linear PDE which utilizes the previous model to simulate convection and diffusion of heat being applied to a one-dimensional rod.

$$\partial_x(cu) + \partial_x(K \partial_x u) = f \tag{7}$$

Let $\Omega = (-1, 1)$ where zero Dirichlet conditions are applied to the left and right boundaries. K represents the diffusivity of the material, replacing $\frac{|\alpha|}{4}$ in this case, c represents the convection coefficient, taking the role of τ in equation 5, and f is the heat source. Upon determining that DG methods are better than the standard method for this diffusion-convection model, we apply it to the nonlinear model for simulations.

4 Preliminary FE Method Testing

We begin our investigation of FE methods by evaluating two methods, the standard FEM and the DG method. When we test the standard method of FEA, we see increasing instability when the ratio between K and c decreases. Beginning with a larger ratios, we see the following results:

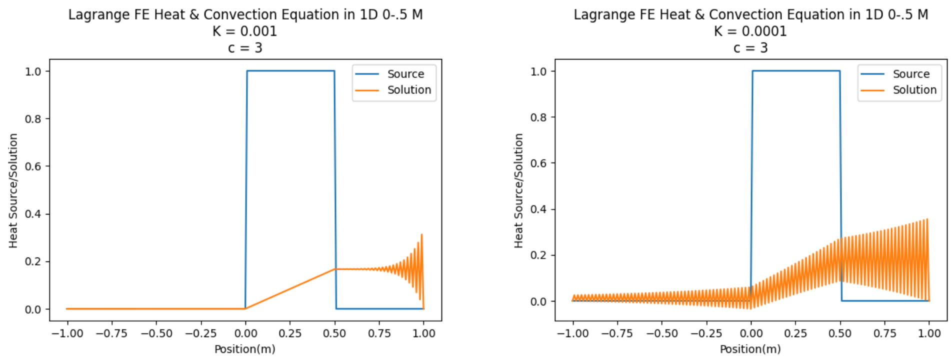


(a) pure diffusion

(b) diffusion-convection

Figure 5: Model for convection and diffusion. Diffusion with the Dirichlet boundary conditions cause the temperature of the rod to become zero at the boundary. Convection to the right changes the shape of the graph.

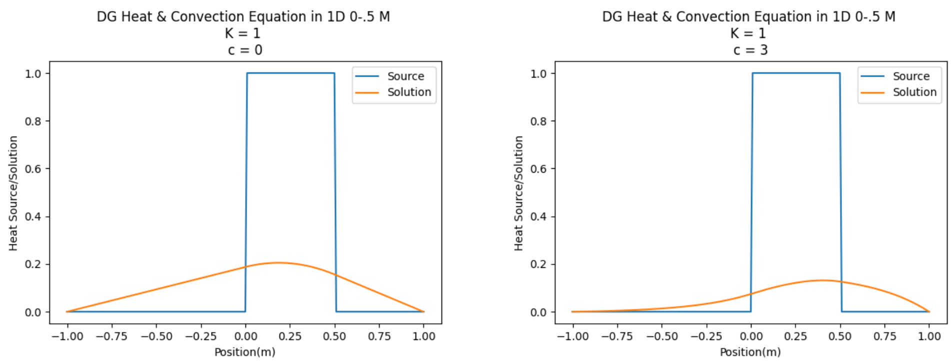
After increasing the ratio of K and c, we immediately see the onset of instability that occurs when using standard methods of FEA.



(a) K = 0.001 (b) K = 0.0001

Figure 6: Effect of increasing the ratio of K and c.

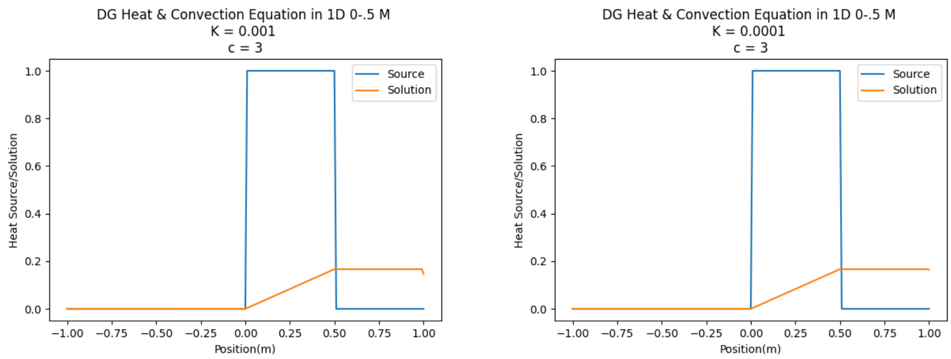
Once we apply the DG method to the model, we see that, like the standard FEM, the model behaves as expected with a high ratio between K and c.



(a) pure diffusion with DG (b) diffusion-convection with DG

Figure 7: Model for convection and diffusion using the DG method.

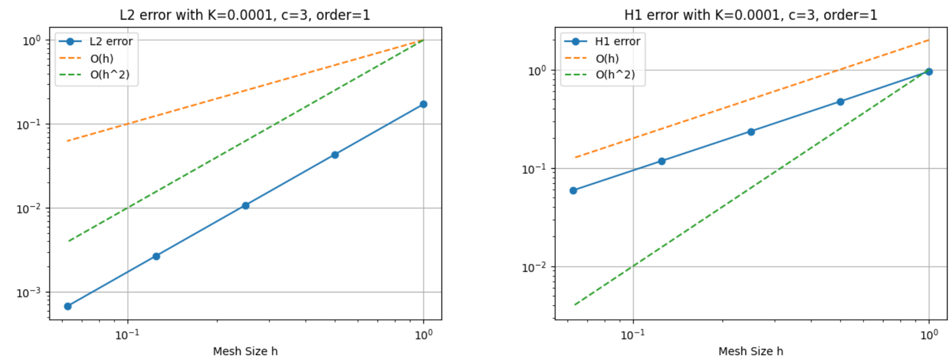
Even in cases of lower values, the DG method is successful in attaining pure convection with better stability than the standard FEM.



(a) K = 0.001 DG (b) K = 0.0001 DG

Figure 8: Implementing the same parameters for K and c using the DG results in a smooth solution.

When using FE methods to create simulations, we use convergence tests to determine whether this method is working as intended. Another advantage of using the linear model is that we can construct an exact solution corresponding to a source term with the method of manufactured solutions, thus allowing us to perform convergence trials.



(a) L2 norm (b) H1 norm

Figure 9: L2 and H1 errors

Convergence tests calculate how error changes as the mesh is refined. The L2 error integrates the squared difference of the exact and computed solution of the model and the H1 error takes the sum of the square of the function and the squared weak derivative of the function.

It is known that the correct convergence rate for this problem in H1 norm is $O(h^p)$ and $O(h^{(p+1)})$ for the L2 norm where p is the polynomial order of the functions in our finite dimensional space.

5 Results for Nonlinear Model

5.1 Problem Setup

The models will consider two cases of initial dislocation walls for α, one where we see a positive wall and negative wall and another case where we see two positive dislocation walls. We will modify (5) to achieve these models.

The first set of simulations will use an applied strain of g(t) = 0. The second set of experiments is similar to the first, with the only difference being that there will be an applied strain g(t) ramped to a small final value.

The initial conditions from (5) have been modified for the goal of our simulations. The initial conditions for the two opposite dislocation walls are represented by this function.

$$\alpha(x,0) = \begin{cases} \frac{\bar{\phi}}{2}(1-\tanh^2(x+5)), & x<0 \\ -\frac{\bar{\phi}}{2}(1-\tanh^2(x-5)), & x\geq 0 \end{cases} \tag{8}$$

$$\phi(x,0) = \begin{cases} -\frac{\bar{\phi}}{2}(1-\tanh(x+5)), & x<0 \\ \frac{\bar{\phi}}{2}(1-\tanh(x-5)), & x\geq 0 \end{cases} \tag{9}$$

The two dislocation walls of the same sign are represented by these initial conditions:

$$\alpha(x,0) = \begin{cases} \frac{\bar{\phi}}{2}(1-\tanh^2(x)), & x<0 \\ \frac{\bar{\phi}}{2}(1-\tanh^2(x-12)), & x\geq 0 \end{cases} \tag{10}$$

$$\phi(x,0) = \begin{cases} -\frac{\bar{\phi}}{2}(1-\tanh(x)), & x<0 \\ -\frac{\bar{\phi}}{2}(1-\tanh(x-12)), & x\geq 0 \end{cases} \tag{11}$$

The following parameters are used for all simulations: L = 50, $\bar{\phi}$ = 0.05, and p = 1. The domain(Ω) of our system is on the interval (-50, 50) We run our simulations for a time, T, of 5,000 with a time step of 5 and a mesh size of 0.1. Our mesh size and polynomial degree are chosen to achieve accuracy in the model. Whenever there is instability in the model, we decrease the time step. To maintain stability, the time step must be reduced if the mesh is refined or the polynomial order is increased.

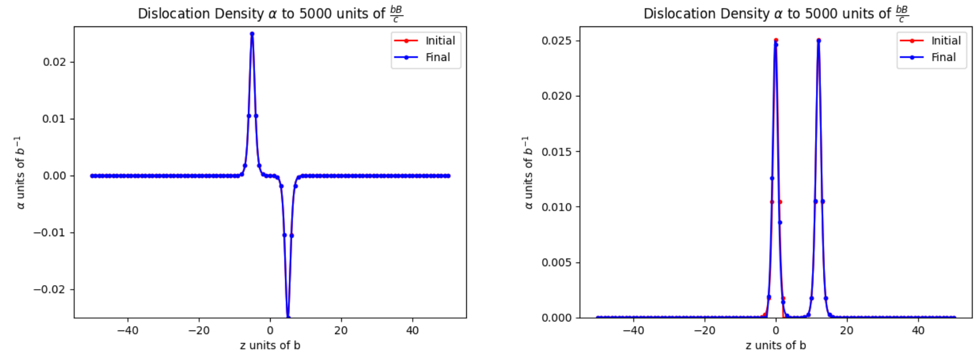
5.2 Time Stepping Methods

Explicit Runge-Kutta 4(RK4) is the optimal method for cases with smooth solutions, achieving high-order accuracy. It is the only method that achieves $O(h^{p+1})$ convergence. However, whenever our mesh size is reduced by $\frac{1}{2}$ we must change our time step by $\frac{1}{4}$ to maintain stability.

We will use the implicit-explicit (IMEX) time-stepping method which is a robust method that achieves the most accuracy for low-order, non-smooth solutions. Unlike RK4, reducing the mesh by $\frac{1}{2}$ results in having to reduce the time step by $\frac{1}{2}$. This allows us to reduce the mesh size as necessary without the need to reduce the time step by a large amount.

5.3 Simulations

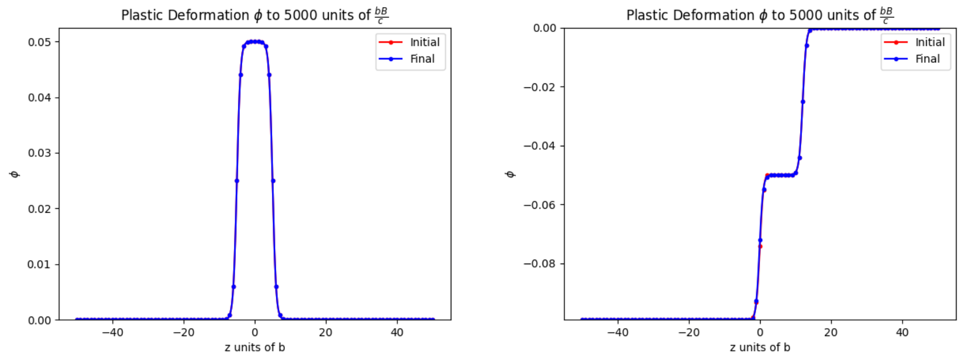
The pair of simulations in which there was no applied strain gathered the following results for the dislocation densities:



(a) g = 0 on two dislocation walls of opposite sign (b) g = 0 on two dislocation walls of the same sign

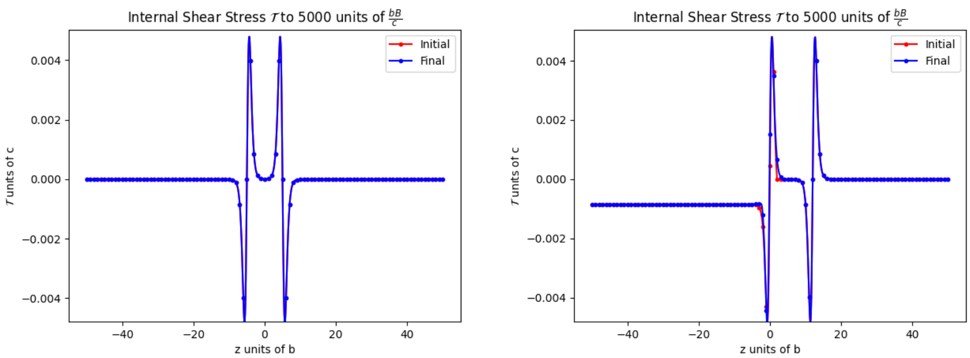
Figure 10: α plots for two screw dislocations with no applied strain

From these figures, it is clear that the absence of an applied strain the dislocation walls remain in equilibrium.



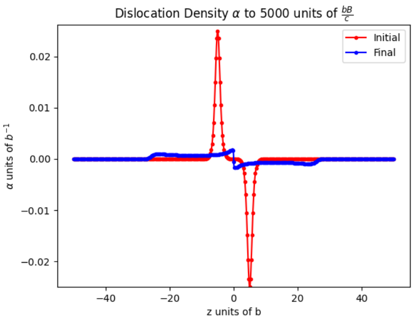
(a) g = 0 on two opposite dislocation walls (b) g = 0 on two dislocation walls of the same sign

As described in equation (2), α is the spatial derivative of ϕ, therefore the slopes of our ϕ plots are indicative of where α is located.

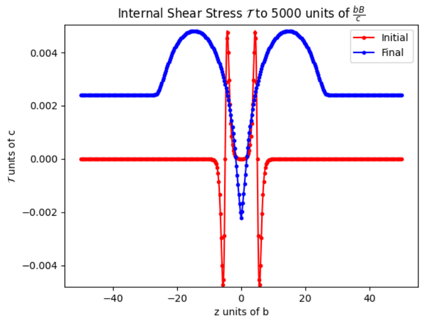


(c) g = 0 on two opposing dislocation walls (d) g = 0 on two dislocation walls of the same side

The following simulations allow us to see how dislocation densities are affected by an applied strain. When we apply a ramped strain on the system, we can see how the dislocations interact with one another. For the two opposing dislocation walls a strain $g(t) = 0.02(\frac{t}{T})$ is applied to illustrate the cancellation of the dislocation walls.

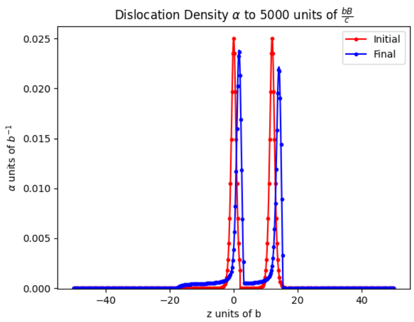


(e) α when $g(t) = 0.02$

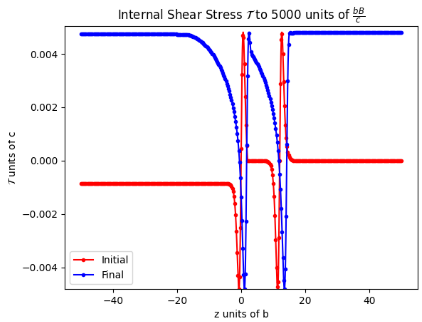


(f) τ when $g(t) = 0.02$

As expected, when two dislocation walls have opposite orientation, they will cancel out.



(g) α when $g(t) = 0.01$



(h) τ when $g(t) = 0.01$

Here, we see that the α plot results in little change in the system. There is some reduction in α, implying that the presence of applied strain causes changes in the system.

6 Discussion/Conclusion

The previous models were pivotal in understanding the way dislocation walls interact with one another. There may be a new drag model implemented with the simulations, which can determine how the simulations progress in time. The function α may also be used as a means to calculate shear stress using a new mathematical formula.

6.1 Conclusions about the Nonlinear Model

By observing the nonlinear model, we conclude that when there is no applied strain on a system, the dislocation tends to remain in equilibrium as intended by the design of Das and Acharya (2013). If two dislocation walls are of opposite signs, they will cancel out one another, as expected. When there is an applied strain, the dislocation densities of the same sign will be reduced by a small amount, but because the dislocation walls are not of opposite sign, they will not cancel one another out.

6.2 Conclusions about the FE Methods

By using the linear PDE as a test, we determined that the DG method would be better than the standard FE method for this model. However, studies could be implemented to test the standard FE method with the nonlinear model.

7 Acknowledgments

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