Simulating Dislocation Densities with Finite Element Analysis

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Why Simulations?

- This project is on building mathematical simulation tools.
- We need accurate and fast simulation tools.
- Ex. Sleipner A:
  - A major oil platform collapsed due to inaccurate FEA
  - Shear stresses were underestimated
  - Total loss: $ 700 M

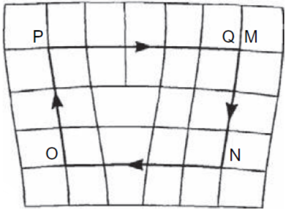
Why Simulations?

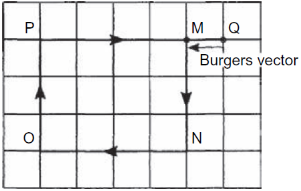
- In this project, we will build simulation tools for dislocation mechanics

What are dislocations?

- Any defect in a perfect crystal lattice caused by atoms being out of place
  - A perfect crystal lattice is any structure consisting of uniform planes of atoms
- Dislocations can be good or bad
  - Intentionally used to strengthen materials
  - Can also cause catastrophic failures in material structures
- Dislocations in pictures . . .

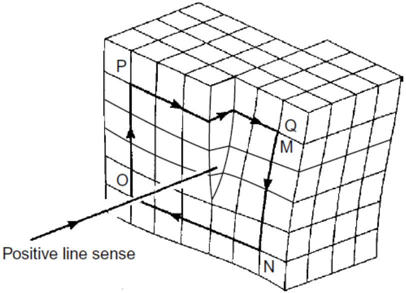
Edge Dislocations



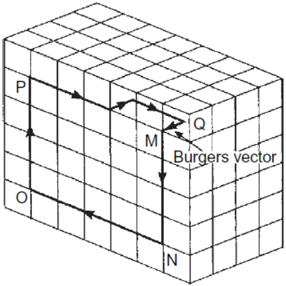


- Edge dislocations consist of an additional half-plane of atoms in a lattice

Screw Dislocations



(a)



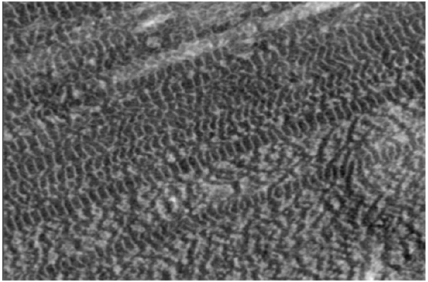
(b)

- In a screw dislocation, the lattice plane shifts and causes the atomic structure to take a helical shape

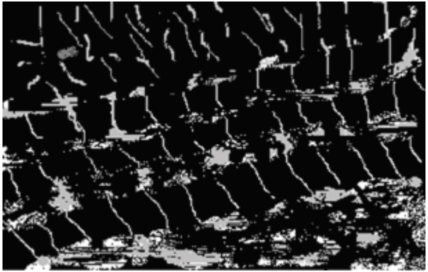
Ahmed et al. Copper Experiments

- Copper samples are taken and cyclically hardened to examine how fatigue affects the material
- Cyclic strain causes a pattern to appear in the microstructure of the copper lattice
- Dislocation walls are represented within the patterns formed as a result of the cyclic hardening

Microscopic Copper Dislocation Walls



(a) Patterns formed by cyclic strain.



(b) White lines represent the dislocation walls.

- Our model represents a dislocation wall by a dislocation density function α.

Model Features

- Study continuum models which examine dislocation densities
- PDEs involving deformation encapsulate models which include diffusive and convective terms
- Simulate solutions of the nonlinear PDE using the FEM

Nonlinear System of Time-Dependent PDEs

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

$$\partial_t \alpha = \partial_x \left(|\alpha| \tau \right) + \partial_x \left(\frac{|\alpha|}{4} \partial_x \alpha \right) \tag{2}$$

Functions to be found:

- α - dislocation density
- ϕ - plastic deformation

Known data:

- $g(t)$ - applied strain
- τ - internal shear stress (known function: $g - \phi$)
- Boundary conditions: α is set to 0 at the left and right boundaries

Linear PDE

Recall:

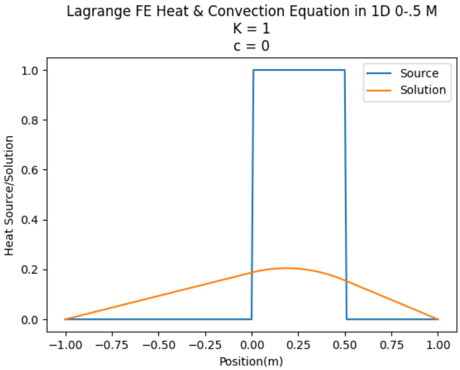
$$\partial_t \alpha = \partial_x \left(|\alpha| \tau \right) + \partial_x \left(\frac{|\alpha|}{4} \partial_x \alpha \right)$$

Simpler:

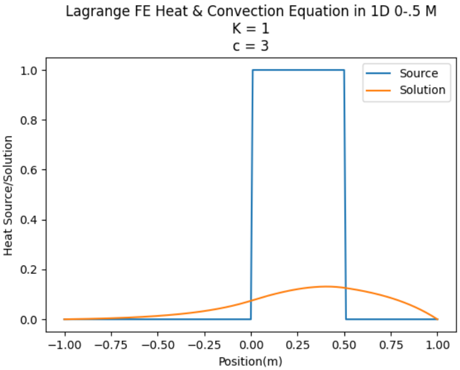
$$f = \partial_x (c u) + \partial_x (K \partial_x u) \quad (3)$$

- $\Omega = (-1, 1)$ where zero Dirichlet conditions are applied to the left and right boundaries
- c represents the convection coefficient
- K represents the diffusivity of the material
- We use a mathematical tool to verify exact solutions

Convective and Diffusive Solutions from Standard FEM

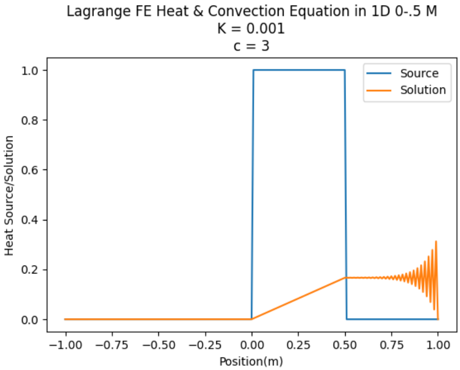


(a) diffusion - K=1

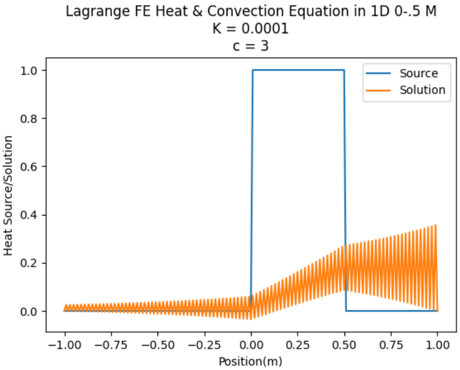


(b) diffusion-convection - c=3

Failure of Standard FEM for Small Diffusion



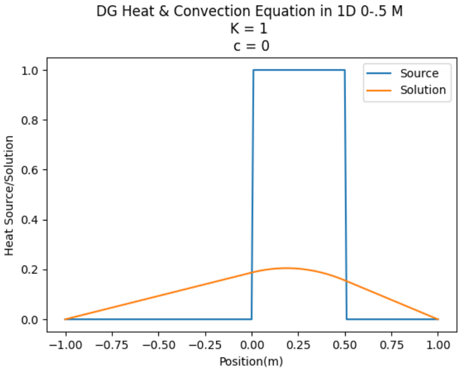
(a) K = 0.001



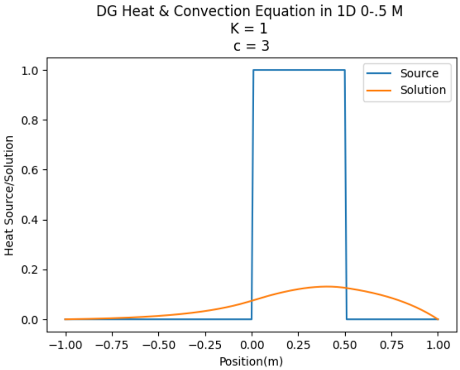
(b) K = 0.0001

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

Convective and Diffusive solutions from DG FEM

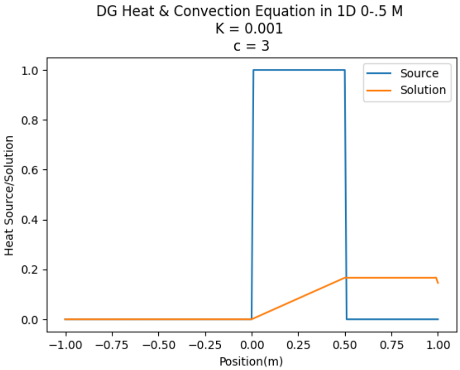


(a) K = 1 DG

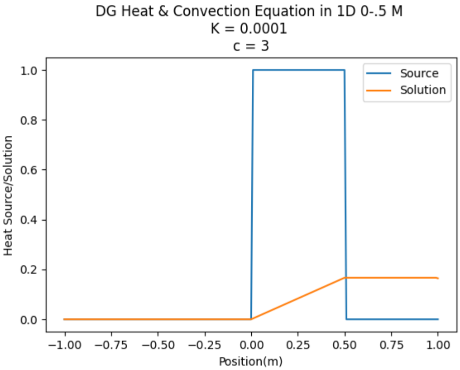


(b) c = 3 DG

DG Method Stability



(a) K = 0.001 DG

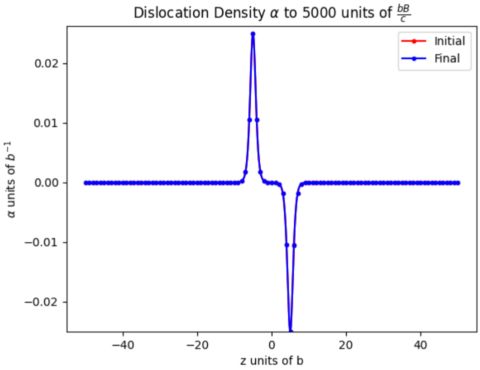


(b) K = 0.0001 DG

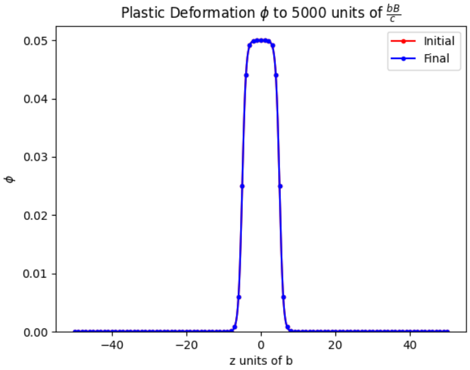
Problem Setup

- We define the sign of a dislocation wall as the sign of its dislocations.
- Consider two dislocation walls of opposite and the same sign.
- Observe dislocation walls of zero applied strain and a small final value for applied strain.
- $g(t)$ represents the applied strain.

Opposite Dislocation Walls: No Applied Strain



(a) Dislocation Density α



(b) Plastic Deformation ϕ

Opposite Dislocation Walls: No Applied Strain

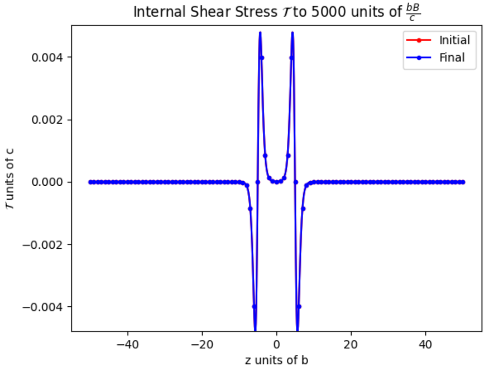
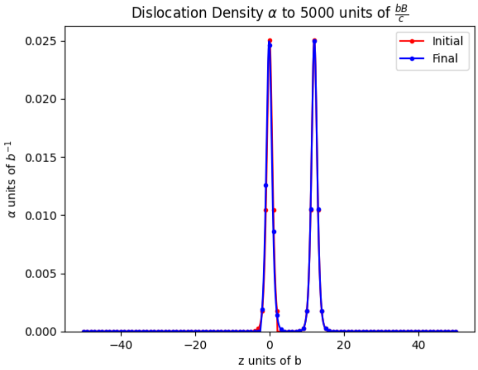
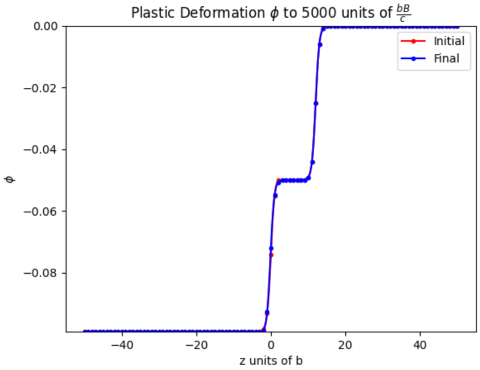


Figure: Internal shear stress under no strain

Adjacent Dislocation Walls: No Applied Strain



(a) Dislocation Density α



(b) Plastic Deformation ϕ

Adjacent Dislocation Walls: No Applied Strain

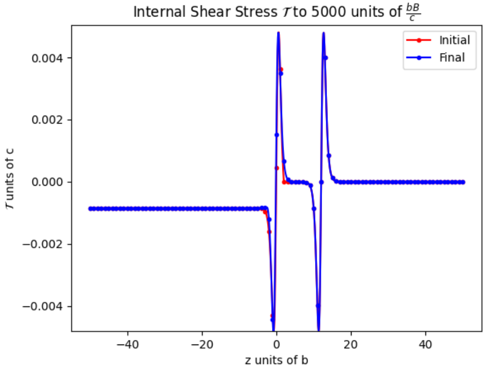


Figure: Internal shear stress under no strain

Opposite Dislocation Walls: Ramped Applied Strain

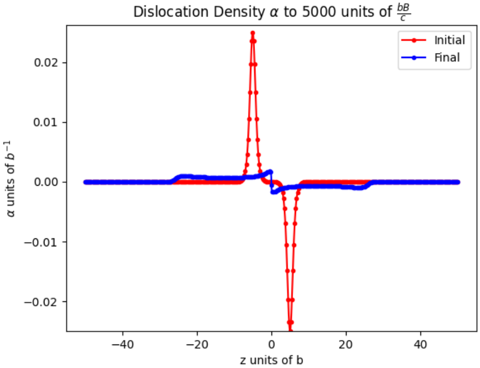


Figure: α when g(t) = 0.02

Opposite Dislocation Walls: Internal Shear Stress

- Internal shear stress increases and decreases as the dislocation walls cancel
- Video Progression

Adjacent Dislocation Walls: Ramped Applied Strain

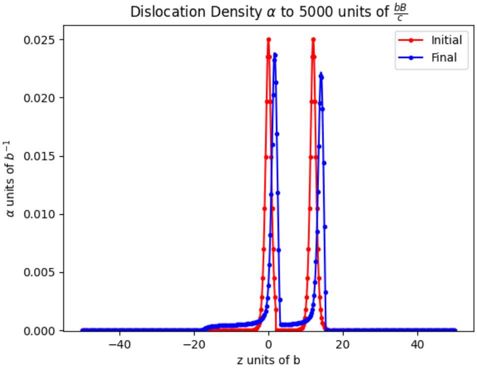


Figure: α when g(t) = 0.01

Adjacent Dislocation Walls: Internal Shear Stress

- Internal shear stress simply increases within the system as there is little change in α
- Video Progression

Discussion & Conclusions

- DG FEM was determined to be better than standard FEM.
- Applying DG FEM to the nonlinear model outputs the expected results.
- The results of these simulations imply that two nearby dislocation walls with opposite sign will tend to attract and cancel under applied strain.
- Even under applied strain, the adjacent dislocation walls didn't seem to cancel.

What's Next?

- Implement a new drag model with the nonlinear model.
- Simulate a different mathematical model that computes shear stress from α.

Impact on Community

- Better analysis of material deformations
- Production of more durable materials
- Safer living conditions for citizens

References

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[2] Ahmed, Jobayer and Roberts, Steve and Wilkinson, Angus J
Characterizing dislocation structures in bulk fatigued copper single crystals using electron channeling contrast imaging (ECCI)
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