Introduction

A dislocation is a crystal defect which corresponds to a discontinuity in the crystalline structure organization. This concept has been introduced by Polanyi and Tammann in 1914 as the main explanation of the microscopic scale of plastic deformation. A dislocation creates around it a perturbation that can be seen as an elastic field. Under an external strain, a dislocation moves according to its Burgers vector which characterizes the intensity and the direction of the defect displacement (see Birk and Lothe [4] for an introduction to dislocations).

Presentation of the 1-D Groma-Balogh model

Here, we are interested in the dynamics of dislocations densities.

(a) We consider dislocation densities that are 1-periodic in x1 and x2.
(b) We consider edge dislocations that move in the direction of the Burgers vector \( \mathbf{b} = (1, 0) \).
(c) The dislocation densities only depend on the variable \( x = x_1 + x_2 \).

Assume (a)-(b)-(c), the 2-D model of [3] reduces to the system of coupled 1-D non-local transport equations (see [1])

\[
\begin{cases}
\frac{\partial \rho}{\partial t} = -\nabla \cdot \left( \rho \mathbf{v} \right) + \int_0^1 \left( \rho \mathbf{v} (x, \tau) - \rho \mathbf{v} (x, t) \right) d\tau \text{ on } \mathbb{R} \times (0, T) \\
\rho(x, t) = \rho_0(x) \text{ on } \mathbb{R} \times (0, T)
\end{cases}
\]

(1)

Where \( \rho_\mathbf{v} \) are the unknown scales such that \( \rho_\mathbf{v} \) represents the plastic deformation.
Their space derivatives \( D\rho = \frac{\partial \rho}{\partial x} \geq 0 \) are the dislocations densities.
The function \( L(t) \) represents the exterior shear stress field.
The initial conditions for the system (1) are defined as follows:

\[ \rho(x, 0) = \rho_0(x) + \rho_c^0(x) \text{ on } \mathbb{R} \]

(2)

Where \( \rho_c^0 \) are 1-periodic and Lipschitz continuous.
The constant \( \mathbf{v}_0 \) is a given constant which is the total density of type \( \mathbf{v}_0 \), i.e. we suppose that initially, we have the same total density of type \( \mathbf{v}_0 \).

Theoretical Results

Theorem 0.1 (Existence and uniqueness for the non-local problem) Suppose that \( \rho_c^0 \in \mathcal{L}(\mathbb{R}) \) satisfying (2) for some \( \rho_0 \in \mathbb{R} \), \( L \in L^{1, \infty} (\mathbb{R}^2) \). Then, for all \( T > 0 \), the system (1)-(2) admits a unique viscosity solution \( \rho = (\rho_\mathbf{v}, \rho_c) \). Moreover, this solution is locally Lipschitz continuous in space and time.

Error estimate of Crandall-Lions type

Theorem 0.2 (Discrete-continuous error estimate) Assume that \( \Delta x = \Delta t \leq 1 \), \( L \in L^{1, \infty}(\mathbb{R}^2) \) and with the CFL condition \( \left( \frac{T}{\sqrt{\gamma}} \right)^2 \leq \frac{\Delta t}{\Delta x} \).

Then there exists a constant \( K > 0 \) depending only on \( \| \rho_c^0 \|_{L^2(\mathbb{R})}, \max_{x \in \mathbb{R}^2} |D\rho_0|_{L^\infty(\mathbb{R})} \) and \( |L(x, y)| \) such that the error estimate between the solution \( \rho \) of the continuous system (1)-(2) and the discrete solution \( \rho \) of the finite difference scheme (1)-(2) is given by

\[
\max_{k \leq \ell \leq \ell+1} \sup_{\Omega_k} |\rho_k - \rho_{k+1}| \leq K \left( T + T \right)^{1/2} \Delta x^{1/2}
\]

for all \( T \geq 0 \).

provided \( K \left( T + T \right) \leq 1 \).

Numerical results

1-Numerical error estimate

Here, we show a numerical test in order to confirm our error estimate for local system.

- Let us fix \( L(t) = 0 \) (even if it is not physically relevant).
- Let us choose the following initial conditions:
  \[ \rho_c^0(x) = |x - 1/2| + 1/2 \text{ and } \rho_c^0(x) = |x - 1| + 1 \text{ on } [0, 1] \text{ (and extend it by periodicity on } \mathbb{R} \).

The figure shows the behaviour of the \( L^n \)-error versus the discretization parameter \( \Delta x \) in the log-log coordinates. The regression slope is close to 0.7 and the ideal regression is \( \frac{1}{2} \). Hence, the behaviour of this error confirms coherent with our result.

2-Dislocations densities dynamics

In this paragraph, we are interested by the evolution of dislocations densities for the 1-D Groma-Balogh model (1)-(2) under the uniformly applied shear stress \( L(t) = 3 \).

In this simulation, we choose an example of initially concentrated dislocation densities, i.e. where dislocation densities are initially periodic and equal to zero on some sub-interval of \([0,1]\).

This initial condition means that there exist some regions without dislocations and others with concentrated dislocations.

The scheme

We want to approximate the solution of (1)-(2). Given a mesh size \( \Delta x, \Delta t \), we define

\[ \Omega = \{ \Delta x, \Delta t \} \quad \mathbb{O} = \{ 0, \ldots, |\Delta x| N \} \]

- The discrete running point is \((x_k, t_m)\) with \( x_k = x_n \Delta x \), \( t_m = m \Delta t \).
- The approximation of the solution \( \rho \) at the node \((x_k, t_m)\) is written inﬁnitely as \( \rho_\mathbf{v}(x_k, t_m) = \rho_{\mathbf{v}}^m \).

Now, we will introduce the numerical monotone scheme:

\[ v_{n+1}^m = v_{n+1}^m + \Delta t C^m_{n+1} \left( v_n^m + \mathbf{v}_0(x_n) \right) \]

(3)

where

\[ C^m_{n+1} (v_n^m) = \begin{cases} E^m ((P, Q)) = \min ((P, 0), (Q, 0))^2 & \text{if } C^m_{n+1} (v_n^m) \geq 0 \\ E^m ((P, Q)) = \min ((P, 0), (Q, 0))^2 & \text{if } C^m_{n+1} (v_n^m) \leq 0 
\end{cases}

\]

and the non-local term \( v_{n+1}^m \) is given by

\[ v_{n+1}^m (x_n) = L_n + \sum_{k=1}^{N} \Delta x (v_{n+1}^m (x_k) - v_{n+1}^m (x_{k-1})) \]

(4)

where \( N \) is the integer part of \( 1/\Delta x \), \( E^m \) are the approximations of the Ensmen norm proposed by Osher and Sethian [4]

\[ E^m ((P, Q)) = \frac{\min ((P, 0)^2 + \min (Q, 0)^2)}{ \max ((P, 0)^2 + \min (Q, 0)^2)} \]

(5)

and \( C^m_{n+1} \), \( D^m_{n+1} \), \( C^m_{n+1} \), \( D^m_{n+1} \), \( C^m_{n+1} \), \( D^m_{n+1} \) are the discrete gradients for all \( n \in \{0, \ldots, N\} \), \( k \in \mathbb{Z} \) and \( l \in \{1, \ldots, \} \).

\[ D^m_{n+1} (v_n) = \frac{v_{n+1}^m - v_{n+1}^m}{\Delta x} \]

(6)

The initial conditions for the scheme are defined as follows:

\[ v_{0}^{m_{0}} (x_n) = \rho_{\mathbf{v}}^0 (x_n) \]

(7)

where \( \rho_{\mathbf{v}}^0 (x_n) \) is an approximation of \( \rho_{\mathbf{v}}^0 (x_n) \).

The figure shows the behaviour of the \( L^n \)-error versus the discretization parameter \( \Delta x \) in the log-log coordinates. The regression slope is close to 0.7 and the ideal regression is \( \frac{1}{2} \). Hence, the behaviour of this error confirms coherent with our result.

References


https://cermics.enpc.fr/~elhahj