Wellposedness and Convergent scheme for a non-local system modelling dislocations densities dynamics

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Introduction

A dislocation is a crystal defect which corresponds to a discontinuity in the crystalline structure organisation. This concept has been introduced by Polanyi, Taylor and Orowan in 1934 as the main explanation at the microscopic scale of plastic deformation. A dislocation creates around it a perturbation that can be seen as an elastic field. Under an exterior strain, a dislocation moves according to its Burgers vector which characterises the intensity and the direction of the defect displacement (see Hirth and Lothe [3] for an introduction to dislocations).

Presentation of the 1-D Groma-Balogh model

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

(a) We consider dislocation densities that are 1-periodic in x_1 and x_2.

(b) We consider edge dislocations that move in the direction of the Burgers vectors $\pm\vec{b} = (1, 0)$.

(c) The dislocations densities only depend on the variable $x = x_1 + x_2$.

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

$$\begin{cases} (\rho_+)_t = -\left(\rho_+ - \rho_- + L(t) + \displaystyle\int_0^1 (\rho_+(x,t) - \rho_-(x,t))\, dx\right) D\rho_+ \ \text{ on } \ \mathbb{R}\times(0,T) \\ (\rho_-)_t = \quad \left(\rho_+ - \rho_- + L(t) + \displaystyle\int_0^1 (\rho_+(x,t) - \rho_-(x,t))\, dx\right) D\rho_- \ \text{ on } \ \mathbb{R}\times(0,T) \end{cases} \tag{1}$$

- Where ρ_+, ρ_- are the unknown scalars such that $(\rho_+ - \rho_-)$ represents the plastic deformation.
- Their space derivatives $D\rho_\pm := \frac{\partial \rho_\pm}{\partial x} \geq 0$ 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:

$$\rho_\pm(x,0) = \rho^0_\pm(x) = P^0_\pm(x) + L_0 x \text{ on } \mathbb{R} \tag{2}$$

- Where $P^0_\pm$ are 1-periodic and Lipschitz continuous.
- The constant L_0 is a given constant which is the total density of type $\pm$, *i.e.* we suppose that initially, we have the same total density of type $+$ and $-$.

Theoretical Results

Theorem 0.1 (Existence and uniqueness for the non-local problem) *Suppose that $\rho^0_\pm \in \mathrm{Lip}(\mathbb{R})$ satisfying (2) for some $L_0 \in \mathbb{R}$, and $L \in W^{1,\infty}(\mathbb{R}^+)$. Then, for all $T > 0$, the system (1)-(2) admits a unique viscosity solution $\rho = (\rho_+, \rho_-)$. Moreover, this solution is locally Lipschitz continuous in space and time.*

The scheme

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

$$\Xi = \{i\Delta x,\ i \in \mathbb{Z}\} \quad \Xi_T = \Xi \times \{0, ..., (\Delta t)N_T\}.$$

- The discrete running point is (x_i, t_n) with $x_i = i(\Delta x),\ t_n = n(\Delta t)$.
- The approximation of the solution ρ_k at the node (x_i, t_n) is written indifferently as $v_k(x_i, t_n) = v^n_{k,i}$.

Now, we will introduce the numerical monotone scheme:

$$v^{n+1}_{k,i} = v^n_{k,i} + \Delta t C^\Delta_k[v](x_i,t_n) \begin{cases} E^+\left(D^+v^n_{k,i}, D^-v^n_{k,i}\right) & \text{if } C^\Delta_k[v](x_i,t_n) \geq 0 \\ E^-\left(D^+v^n_{k,i}, D^-v^n_{k,i}\right) & \text{if not} \end{cases} \qquad \forall k \in \{+,-\} \tag{3}$$

where

$$C^\Delta_k[v](x_i,t_n) = -k\left(v^n_{+,i} - v^n_{-,i} + a^\Delta[v](t_n)\right)$$

and the non-local term $a^\Delta[v](t_n)$ is given by

$$a^\Delta[v](t_n) = L(t_n) + \sum_{i=0}^{N_x - 1} \Delta x\,(v_+(x_i,t_n) - v_-(x_i,t_n)) \tag{4}$$

where N_x is the integer part of $1/\Delta x$. $E^\pm$ are the approximation of the Euclidean norm proposed by Osher and Sethian [4]:

$$E^+(P,Q) = \left(\max(P,0)^2 + \min(Q,0)^2\right)^{\frac{1}{2}}, \tag{5}$$

$$E^-(P,Q) = \left(\min(P,0)^2 + \max(Q,0)^2\right)^{\frac{1}{2}}$$

and $D^+v^n_{k,i},\ D^-v^n_{k,i}$ are the discrete gradients for all $n \in \{0, ..., N_T\},\ i \in \mathbb{Z}$ and $k \in \{+,-\}$:

$$D^+v^n_{k,i} = \frac{v^n_{k,i+1} - v^n_{k,i}}{\Delta x}, \tag{6}$$

$$D^-v^n_{k,i} = \frac{v^n_{k,i} - v^n_{k,i-1}}{\Delta x}.$$

The intial conditions for the scheme are defined as follows:

$$v^0_i = (v^0_{+,i}, v^0_{-,i}) = (\rho^0_+, \rho^0_-), \tag{7}$$

where $v^0_\pm(x_i)$ is an approximation of $\rho^0_\pm(x_i)$.

Error estimate of Crandall-Lions type

Theorem 0.2 (Discrete-continuous error estimate) *Assume that $\Delta x + \Delta t \leq 1$, $L \in W^{1,\infty}(\mathbb{R}^+)$ and with the CFL condition $\left(\Delta t \leq \frac{1}{4(\|P^0_+ - P^0_-\|_{L^\infty(\mathbb{R})}+1)}\Delta x\right)$.
Then there exists a constant $K > 0$ depending only on $\|P^0_+ - P^0_-\|_{L^\infty(\mathbb{R})}$, $\max_{k\in\{+,-\}}\|D\rho^0_k\|_{L^\infty(\mathbb{R})}$ and $\|L\|_{W^{1,\infty}(\mathbb{R}^+)}$ such that the error estimate between the solution ρ of the continuous system (1)-(2) and the discrete solution v of the finite difference scheme (7)-(3) is given by*

$$\max_{k\in\{+,-\}} \sup_{\Xi_T} |\rho_k - v_k| \leq K\left((T + \sqrt{T})\,(\Delta x + \Delta t)^{1/2}\right) \ \text{for all } T \geq 0.$$

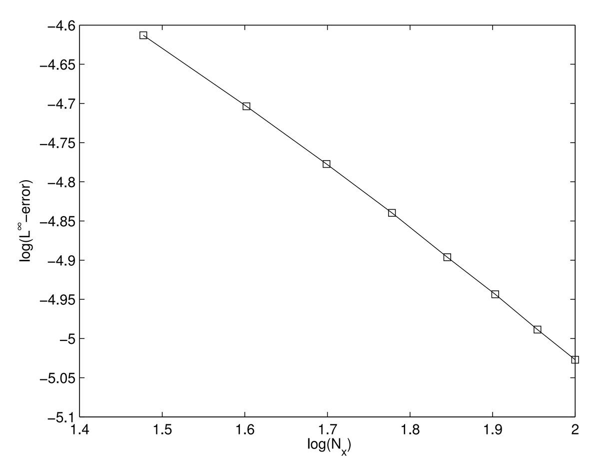
provided $K\left((T+\sqrt{T})(\Delta x + \Delta t)^{\frac{1}{2}}\right) \leq 1$.

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:
  $\rho^0_+(x) = -|x - 1/2| + 1/2$, and $\rho^0_-(x) = -|2x - 1| + 1$ on $[0, 1[$ (and extend it by periodicity on $\mathbb{R}$).

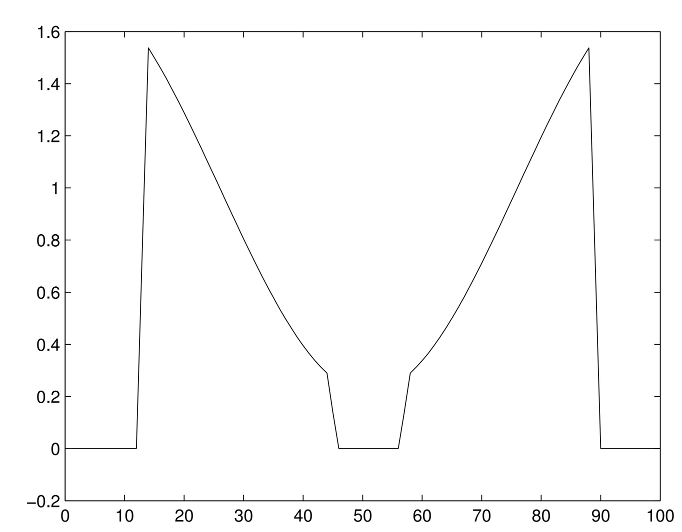


This figure shows the behaviour of the L^∞-error versus the discretization parameter Δx in the log-log coordinates. The regression slope is close to 0.7 and the ideal regression is $\frac{1}{2}$. Hence, the behaviour of this errors confirms coherant with our result.

2-Dislocations densities dynamics

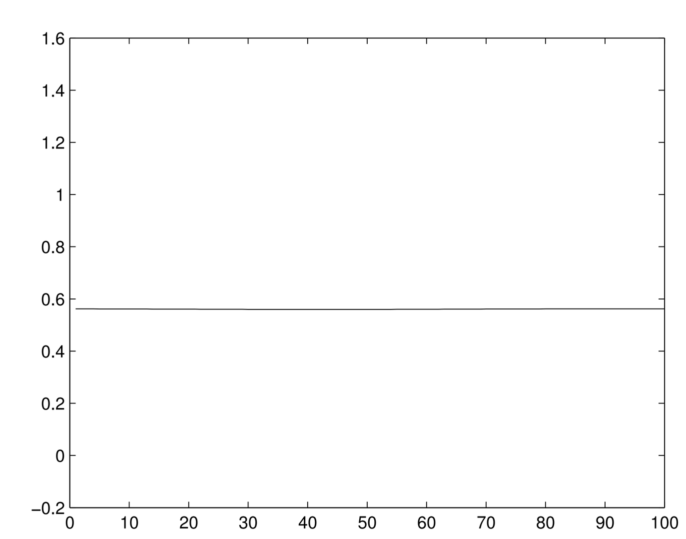
In this paragraph, we are interested by the evolution of dislocations densities for the 1-D Groma-Balogh model (1)-(2) under the uniformly applied shear stress $L(t) = 3t$.
In this simulation, we choose an example of initially concentrated dislocation densities, *i.e.* where dislocation densities are initially periodic and equal to zero on some sub-intervals of $[0, 1[$.

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



dislocations density $D\rho^0_+(\cdot)$

- Intuitively, dislocations are intended to be uniformly distributed in the whole crystal as shown in the (figure below) where finally a uniform distribution in all the crystal is observed, *i.e.* the density of dislocations becomes a constant.



We remark that when $L(t)$ is non-constant, our system behaves like a diffusion equation. But evidently when $L(t) = 0$, with the same initial condition, the system does not evolve.

References

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[a] http://cermics.enpc.fr/∼elhajj