A Non-Local Transport Equation modelling Dislocations Dynamics

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Outline

Dislocations are lines defects in a crystal material (Hirth & Lothe, 1992).

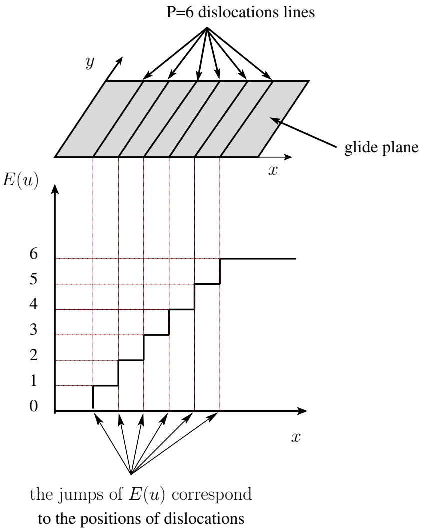

Figure: Representation of dislocations with the function $E(u)$

$$
\begin{cases}
\dfrac{\partial u}{\partial t}(x,t) = c[u](x,t)\,\dfrac{\partial u}{\partial x}(x,t) \quad \text{in } \mathbb{R}\times(0,+\infty) \\[2ex]
c[u](x,t) = c^{\text{ext}}(x) + \displaystyle\int_{\mathbb{R}} c^0(x')E\left((u(x-x',t)\right)\,dx' \\[2ex]
u(x,0) = u^0(x) \quad \text{in } \mathbb{R}
\end{cases}
\tag{1}
$$

where E is the floor function.

Dislocations move with a non-local velocity $c[u]$. It is the sum of two terms:

- c^{ext} represents the exterior stress created by obstacles (such as precipitates, other defects, ...).
- The second term is non-local and represents the elastic interior stress created by all the dislocations in the material.

First Main Result

We make the following assumptions for the exterior stress c^{ext} and the kernel c^0:

$$\begin{cases} c^{\text{ext}} \in W^{1,\infty}(\mathbb{R}) \quad \text{such that} \quad c^{\text{ext}}(x+1) = c^{\text{ext}}(x) \quad \text{in } \mathbb{R}, \\ c^0 \in C_0^\infty(\mathbb{R}) \quad \text{such that} \quad c^0(x) = c^0(-x) \text{ and } \displaystyle\int_{\mathbb{R}} c^0(x)\, dx = 0\,. \end{cases} \tag{2}$$

We consider the initial condition $u^0 \in \mathrm{Lip}(\mathbb{R})$ such that for $x \in \mathbb{R}$

$$u^0(x+1) = u^0(x) + P \quad \text{and} \quad 0 < b_0 \leq \frac{\partial u^0}{\partial x} \leq B_0 < +\infty \quad a.e. \tag{3}$$

with b_0 and B_0 some constants and $P \in \mathbb{N} \setminus \{0\}$. A natural case to study the solutions of (1) is the continuous viscosity solutions (Barles, 1994).

Theorem 1

Under Assumptions (2) and (3), there exists a unique continuous viscosity solution $u \in W^{1,\infty}_{\text{loc}}(\mathbb{R} \times (0, +\infty))$ of (1) such that

$$u(x+1, t) = u(x, t) + P \quad \forall (x, t) \in \mathbb{R} \times (0, +\infty). \tag{4}$$

We prove the previous theorem in two steps.

1. First, we prove the result for a short time (Alvarez and *al.*, 2005; Ghorbel and *al.*, 2005) using a fixed point theorem.
   Given $T > 0$ and a function v satisfying (4), we consider the function $w = \phi(v)$ satisfying (4), solution of

$$\frac{\partial w}{\partial t}(x,t) = c[v](x,t)\,\frac{\partial w}{\partial x}(x,t) \quad \text{in } \mathbb{R} \times (0,+\infty). \tag{5}$$

   For T chosen sufficiently small, we prove that the map ϕ is a contraction in a well chosen space.

2. Secondly, we repeat this short time result on a sequence of time intervals of lengths T_n decreasing to zero, such that $\sum_{n\in\mathbb{N}} T_n = +\infty$.

Given a mesh size Δx, Δt and a lattice $I_d = \{(i\Delta x, n\Delta t);\ i \in \mathbb{Z},\ n \in \mathbb{N}\}$, (x_i, t_n) denotes the node $(i\Delta x, n\Delta t)$ and $v^n = (v_i^n)_i$ the values of the numerical approximation of the continuous solution $u(x_i, t_n)$.

$$v_i^0 = u^0(x_i), \quad v_i^{n+1} = v_i^n + \Delta t\, c_i(v^n) \times \begin{cases} \dfrac{v_{i+1}^n - v_i^n}{\Delta x} & \text{if } c_i(v^n) \geq 0 \\ \dfrac{v_i^n - v_{i-1}^n}{\Delta x} & \text{if } c_i(v^n) < 0 \end{cases} \tag{6}$$

We choose $\Delta x = \dfrac{1}{K}$, $K \in \mathbb{N} \setminus \{0\}$ because of the 1-periodicity in space. We denote $c_i^{\mathrm{ext}} = c^{\mathrm{ext}}(x_i)$ which satisfies $c_{i+K}^{\mathrm{ext}} = c_i^{\mathrm{ext}}$. The discrete velocity is

$$c_i(v^n) = c_i^{\mathrm{ext}} + \sum_{l \in \mathbb{Z}} c_l^0\, E(v_{i-l}^n)\, \Delta x \tag{7}$$

where

$$c_i^0 = \frac{1}{\Delta x} \int_{I_i} c^0(x)\, dx \quad \text{and} \quad I_i = \left[x_i - \frac{\Delta x}{2}, x_i + \frac{\Delta x}{2}\right]. \tag{8}$$

We assume the CFL (Courant, Friedrichs, Levy) condition. Then

Theorem 2

there exists two constants $T, C > 0$ such that

$$\sup_{i \in \mathbb{Z}} \left| u(i\Delta x, n\Delta t) - v_i^n \right| \leq C\sqrt{\Delta x} \quad \text{for all } n \leq \frac{T}{\Delta t}.$$

Main Idea of Proof of Theorem 2

We apply the technical reasoning of Alvarez and *al.*, 2005.

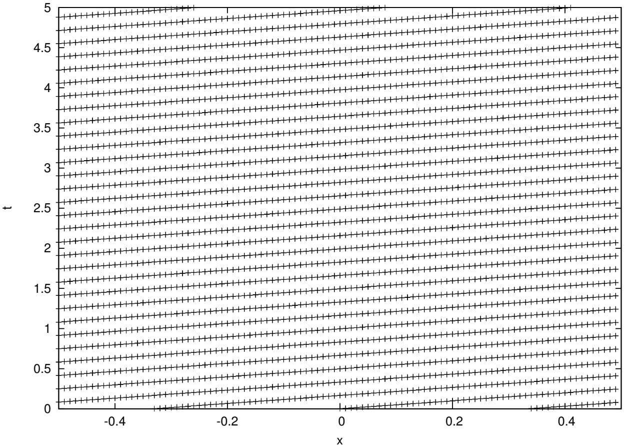

Figure: Linear: $\Delta x = 0.01$, $\Delta t = 2.438\ 10^{-3}$

Dynamics of several dislocations through obstacles

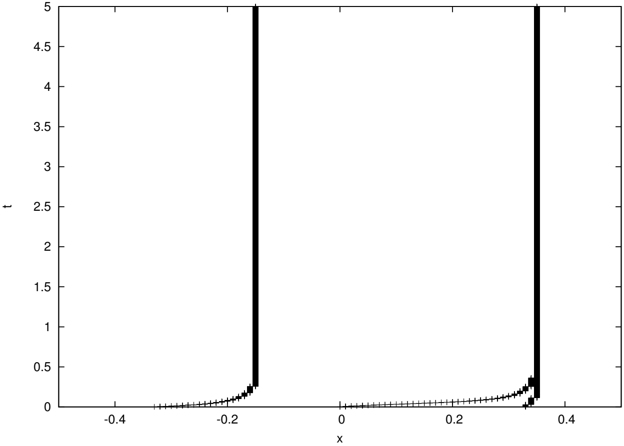

Figure: Trapping: $\Delta x = 0.01$, $\Delta t = 1.239\ 10^{-3}$

Dynamics of several dislocations through obstacles

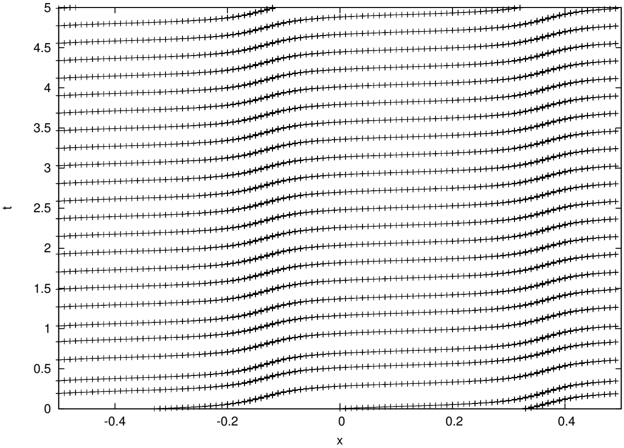

Figure: Pile-Up: $\Delta x = 0.01$, $\Delta t = 1.102\ 10^{-3}$

Dynamics of several dislocations through obstacles

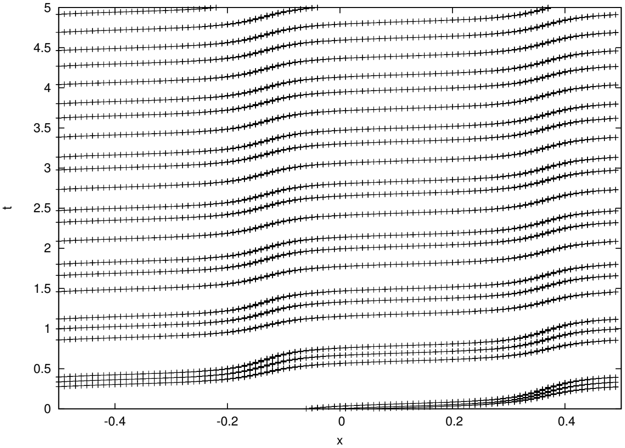

Figure: Pile-Up: $\Delta x = 0.01$, $\Delta t = 1.10219\ 10^{-3}$

Conclusion and Perspectives

- Homogenization of a large number of dislocations through obstacles.
- Friction of dislocations.
- Homogenization of walls of dislocations.
  Joint works with P. Hoch (CEA) and R. Monneau (Cermics).