A numerical study for the homogenization of one-dimensional models describing the motion of dislocations

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Abstract: In this paper we are interested in the collective motion of dislocations defects in crystals. Mathematically, we study the homogenisation of a non-local Hamilton-Jacobi equation. We prove some qualitative properties on the effective Hamiltonian and we provide a numerical scheme which is proved to be monotone under some suitable CFL conditions. Using this scheme, we compute numerically the effective Hamiltonian. Furthermore, we provide numerical computations of the effective Hamiltonian for several models corresponding to the dynamics of dislocations where no theoretical analysis is available.

Keywords: continuous viscosity solution; dislocations dynamics; eikonal equation; effective Hamiltonian; finite difference scheme; Hamilton-Jacobi equation; non-local equation; numerical homogenisation; Peach-Koehler force; transport equation.

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1 Introduction

In this paper we study the homogenisation of non-local Hamilton-Jacobi equations modelling dislocations dynamics, we propose a scheme and provide numerical simulations for several models.

1.1 Physical modelling of dislocations dynamics

In this work, we are interested in the collective behaviour of several dislocations moving in a crystal. Dislocations are defects present in real crystals and are at the origin of the plastic behaviour of metals, we refer to Hirth and Lothe (1992) for a physical description of dislocations.

In our work and in the simplest case, we consider a particular geometry of parallel dislocations lines moving in the same plane. This particular geometry can be modelled by the following 1D problem:

$$\begin{cases} \frac{\partial u}{\partial t}(x,t) = c[u](x,t) \left| \frac{\partial u}{\partial x}(x,t) \right| & \text{in } \mathbb{R} \times (0,+\infty) \\ c[u](x,t) = A + c^{1}(x) + c^{\text{int}}[u](x,t) \\ c^{\text{int}}[u](x,t) = \int_{\mathbb{R}} c^{0}(x') u(x - x',t) dx' \end{cases}$$
(1)

with initial condition

$$u(x,0) = u_0(x) \text{ on } \mathbb{R}.$$
(2)

For similar model, we refer to Ghorbel and Monneau (2006) and Imbert et al. (2006).

Here the positions x_i of the dislocations are defined by $u(x_i, t) = i$ for $i \in \mathbb{Z}$. These dislocations move with a velocity

 $\dot{x}_i(t) = -c[u](x_i(t), t)$

which corresponds to the equation (1) without absolute values on $\frac{\partial u}{\partial x}$.

In the regime that we are interested in, the velocity c[u] is proportional to the force acting on the dislocations. This velocity is then the sum of three contributions. The first one is the exterior applied stress $A \in \mathbb{R}$, assumed here to be constant. The second one is

the force c^1 created by the other defects in the crystal. The last one and the most original here is c^{int} which is the force created by all the elastic interactions between dislocations. This last contribution, in a simplified model, can be modelled by a convolution term as in the last line of equation (1).

Physically, each dislocation i can have a positive or negative Burgers vector, which corresponds to the sign of $\frac{\partial u}{\partial x}$ at the point x_i . Here in equation (1), we allow the annihilation of dislocations of opposite Burgers vectors. This is why we write equation (1) with the absolute value $|\frac{\partial u}{\partial x}|$. Here we see that the function u has no physical meaning in itself, but on the contrary what is physically meaningful is the set where u takes integer values in this model (see Figure 1).

Figure 1 Choice of representation



the function u takes integer values at the positions of dislocations

We will study problem (1) and similar equations in the framework of viscosity solutions. Let us recall that the notion of viscosity solution was first introduced by Crandall and Lions (1981) for first order Hamilton-Jacobi equations. For an introduction to this notion, see in particular the books of Barles (1994), and of Bardi and Capuzzo-Dolcetta (1997), and the User's guide of Crandall et al. (1992).

We assume that the kernel c^0 satisfies

$$c^{0}(x) = c^{0}(-x)$$
 and $\int_{\mathbb{R}} c^{0}(x) dx = 0.$ (3)

We also assume the periodicity and the regularity of the micro-stress c^1

$$c^{1}(x+1) = c^{1}(x)$$
 on \mathbb{R} , and c^{1} is a Lipschitz continuous function. (4)

1.2 Goal of the paper

We want to understand the properties of the solution of equation (1) for A = 0 at a large scale. Define

$$u^{\varepsilon}(x,t) = \varepsilon \, u\!\left(\frac{x}{\varepsilon}, \frac{t}{\varepsilon}\right)$$

where ε is the ratio between the mesoscopic scale and the microscopic scale associated to dislocations (like distances between obstacles to the motion of dislocations). Because we made a rescaling of the solution, the dislocations are now given by the values such that $u^{\varepsilon} = \varepsilon k$ for $k \in \mathbb{Z}$.

Homogenisation of Hamilton-Jacobi equations was studied by Lions et al. (1986) and this work was followed by a large literature on the subject, that would be difficult to cite here.

For this equation (see Imbert et al., 2006) and for a certain class of kernels c^0 , it is known that u^{ε} converges to u^0 , solution of

$$\frac{\partial u^0}{\partial t} = \overline{H}\left(I_1 u^0, \frac{\partial u^0}{\partial x}\right)$$

where I_1 is a non-local Levy operator, and \overline{H} is the effective Hamiltonian given by the following definition.

Definition 1.1 (*Effective Hamiltonian*): We assume (4). For $(A, p) \in \mathbb{R} \times \mathbb{R}$, the effective Hamiltonian $\overline{H}(A, p)$ is defined by

$$\overline{H}(A,p) = \lim_{t \to +\infty} \frac{w(x,t)}{t} \quad (\text{independent on } x)$$
(5)

where w solves the 'cell problem', i.e., w solves (1) with w(x, 0) = px.

The goal of the present paper is to compute numerically $\overline{H}(A, p)$ for equation (1) for specific kernels c^0 . In particular, we numerically check that the ergodicity property (5) holds for general kernels c^0 (like for instance for the Peierls-Nabarro model, see Subsection 5.2), even in the case where the equation has no comparison principle and it is even not clear if equation (5) holds theoretically. We also do some simulations for some similar equations or systems of equations. To this end, we implemented several numerical schemes.

1.3 Brief presentation of our results

We present here properties of the effective Hamiltonian and the scheme used to compute it numerically. We prove the following qualitative result on the effective Hamiltonian.

Theorem 1.2 (*Monotonicity of the effective Hamiltonian***):** For the choice $c^0 = -\delta_0 + J$ with δ_0 is the Dirac mass and $J \in C^{\infty}(\mathbb{R})$ is given by:

$$\begin{cases} J(-x) = J(x) \ge 0; \quad \int_{\mathbb{R}} J(x) \ dx = 1 \quad and \quad \int_{\mathbb{R}} |x|J(x) \ dx < +\infty \\ c_2 := \inf_{\delta \in [0,1)} \int_{\mathbb{R}} \min(J(z), J(z+\delta)) \ dz > 0. \end{cases}$$

$$\tag{6}$$

Then the effective Hamiltonian given in Definition 1.1 satisfies

- 1 $\overline{H}(A, p)$ is non-decreasing in A,
- 2 If $\int_{\mathbb{R}} c^1(x) dx = 0$ then $\overline{H}(0, p) = 0$ and $A\overline{H}(A, p)$ is non-decreasing in |p| and satisfies

$$|A| + \left(1 + \frac{2}{c_2}\right) |c^1|_{L^\infty(\mathbb{R})} \geq \operatorname{sgn}(A) \frac{\partial \overline{H}}{\partial |p|}(A,p) \geq 0.$$

Remark 1.3: This particular choice of *J*, as given in equation (6), is natural from the mathematical point of view but is also physically relevant because $J(x) = \frac{1}{|x|^2}$ for |x| large enough, is a good approximation of the physical kernel (see Alvarez et al., 2006).

We build a finite difference scheme of order one in space and time using an explicit Euler scheme in time and an upwind scheme in space. 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 $u(x_i, t_n)$. We then consider the following numerical scheme (without absolute values here, because we restrict our simulations to the case of increasing data):

$$v_i^0 = u_0(x_i), \quad v_i^{n+1} = v_i^n + \Delta t \, c_i(v^n) \times \begin{cases} D_x^+ v_i^n & \text{if } c_i(v^n) \ge 0\\ D_x^- v_i^n & \text{if } c_i(v^n) < 0 \end{cases}$$
(7)

with $D_x^- v_i^n = \frac{v_i^n - v_{i-1}^n}{\Delta x}$ and $D_x^+ v_i^n = \frac{v_{i+1}^n - v_i^n}{\Delta x}$. The discrete velocity is

$$c_i(v^n) = A + c^1(x_i) + c_i^{\text{int}}(v^n).$$
(8)

We approximate the non-local term $c^0 \star u$ by:

$$\begin{cases} c_i^{\text{int}}(v^n) = -v_i^n + \sum_{l \in \mathbb{Z}} J_l v_{i-l}^n \Delta x\\ J_i = \frac{1}{\Delta x} \int_{I_i} J(x) \, dx \quad \text{and} \quad I_i = \left[x_i - \frac{\Delta x}{2}, x_i + \frac{\Delta x}{2} \right]. \end{cases}$$
(9)

Several works have been done for the discretisation of more general first order Hamilton-Jacobi equations (even with boundary conditions). We refer in particular to the works of Abgrall (2003), Alvarez et al. (2005, 2006a, 2006b), Barles and Souganidis (1991), Crandall and Lions (1984), Falcone and Ferretti (2002) and Ghorbel and Monneau (2006).

For problem (7)–(9), we have the following result about monotonicity of the scheme for the special kernel $c^0 = -\delta_0 + J$.

Theorem 1.4 (Monotonicity of the scheme): We assume that

$$v_{i+1}^0 \ge v_i^0, \quad \forall \ i \in \mathbb{Z} \tag{10}$$

(respectively
$$w_{i+1}^0 \ge w_i^0, \quad \forall i \in \mathbb{Z}$$
). (11)

If the time step Δt satisfies

$$\Delta t \le \left(\sup_{j \in \mathbb{Z}} \frac{|c_{j+1}(v^k) - c_j(v^k)|}{\Delta x}\right)^{-1}, \quad \text{for } 0 \le k \le n$$
(12)

$$\left(\text{respectively }\Delta t \le \left(\sup_{j\in\mathbb{Z}} \frac{|c_{j+1}(w^k) - c_j(w^k)|}{\Delta x}\right)^{-1}, \text{ for } 0 \le k \le n\right),$$
(13)

then we have the monotonicity preservation:

$$v_{i+1}^k \ge v_i^k, \quad \forall \ i \in \mathbb{Z}, \quad \forall \ 0 \le k \le n+1$$
(14)

(respectively
$$w_{i+1}^k \ge w_i^k$$
, $\forall i \in \mathbb{Z}$, $\forall 0 \le k \le n+1$). (15)

Assume moreover that

$$v_i^0 \ge w_i^0, \quad \forall \ i \in \mathbb{Z}.$$
 (16)

Moreover, if the time step Δt satisfies

$$\Delta t \sup_{j \in \mathbb{Z}} \left\{ \max\left(\frac{v_{j+1}^k - v_j^k}{\Delta x}, \frac{w_{j+1}^k - w_j^k}{\Delta x}\right) \right\} \le \frac{1}{2} \quad \text{for } 0 \le k \le n$$
(17)

and

$$\frac{\Delta t}{\Delta x} \le \frac{1}{2} \left(\sup_{j \in \mathbb{Z}} \left\{ \max\left(|c_j(v^k)|, |c_j(w^k)| \right) \right\} \right)^{-1} \text{ for } 0 \le k \le n,$$
(18)

then

$$v_i^k \ge w_i^k, \quad \forall \ i \in \mathbb{Z} \quad \text{for } 0 \le k \le n+1.$$
 (19)

Remark 1.5: There would be no monotonicity of the scheme if *J* would be negative. We emphasise that, for instance, for the physical kernel of Peierls-Nabarro given in Hirth and Lothe (1992) (see also Subsection 5.2 of the present paper), we are not able to prove such monotonicity.

We use this scheme to compute numerically an approximation $\overline{H}^{num}(A,p)$ of $\overline{H}(A,p)$ and we numerically check that $\overline{H}^{num}(A,p)$ satisfies the monotonicity properties given in Theorem 1.2. We also compute the effective Hamiltonian for other similar equations (like for instance the case with Peierls-Nabarro kernel, see Subsection 5.2), and for some systems of equations (see Section 6).

There are very few works on numerics for homogenisation. Up to our knowledge, let us mention for first order Hamiltonians some works where are computed the effective Hamiltonian: Gomes and Oberman (2004), Qian (2003) and the work of Rorro (2006) using semi-Lagrangian schemes. Finally let us mention the work of Capuzzo-Dolcetta and Ishii (2001) where are given some a priori estimates on the rate of convergence for the homogenisation of Hamilton-Jacobi equation and the work of Camilli et al. (2006) where are given error estimates for a scheme approximating to the effective Hamiltonian.

1.4 Organisation of the paper

In Section 2, we give the proof of Theorem 1.2. In Section 3, we study the numerical scheme and prove Theorem 1.4. In Section 4, we give numerical simulations corresponding to the scheme of Theorem 1.4. In Section 5, we present numerical simulations for similar equations with for instance the Peierls-Nabarro kernel. In Section 6, we present numerical simulations for systems of equations for two types of dislocations. Finally in the Appendix we provide the proof of a technical (Lemma 2.1) and give a brief derivation of the kernel for walls of dislocations.

2 Qualitative properties of the effective Hamiltonian

Before proving Theorem 1.2, we need the following lemma whose proof is given in the Appendix.

Lemma 2.1 (*Coercivity of the convolution***):** Assume J satisfies (6), and $c^0 = -\delta_0 + J$. If $u \in C_b^0(\mathbb{R})$ is maximal at $Y \in \mathbb{R}$, minimal at $y \in \mathbb{R}$ and |Y - y| < 1, then

$$(c^{0} \star u)(Y) - (c^{0} \star u)(y) \le -c_{2}(u(Y) - u(y)),$$

where c_2 is given by equation (6).

To keep light notation in this section, we denote by M the operator defined by:

$$(Mv)(x) = (c^0 \star v)(x) = -v(x) + \int_{\mathbb{R}} J(z)v(x-z) \, dz.$$
⁽²⁰⁾

We also need the following result.

Lemma 2.2 (*Existence of sub and supercorrectors*): For any $p \in \mathbb{R}$ and $A \in \mathbb{R}$, there exist $\lambda \in \mathbb{R}$, a subcorrector $\underline{v}(x)$ and a supercorrector $\overline{v}(x)$ which are 1-periodic in x and satisfy

$$\begin{split} \lambda &\leq |p + \partial_x \underline{v}| (c^1 + A + M \underline{v}), \quad \text{with } p(p + \partial_x \underline{v}) \geq 0 \quad \text{on } \mathbb{R}, \\ \lambda &\geq |p + \partial_x \overline{v}| (c^1 + A + M \overline{v}), \quad \text{with } p(p + \partial_x \overline{v}) \geq 0 \quad \text{on } \mathbb{R} \end{split}$$

with

$$\max \underline{v} - \min \underline{v} \le \frac{2}{c_2} |c^1|_{L^{\infty}(\mathbb{R})} \quad \text{and} \quad \max \overline{v} - \min \overline{v} \le \frac{2}{c_2} |c^1|_{L^{\infty}(\mathbb{R})},$$

where c_2 is given by equation (6).

The proof of Lemma 2.2 is a slight adaptation of the work of Imbert et al. (2006). We give below a quick proof of this fact.

Sketch of the proof of Lemma 2.2: Let us work in the case p > 0 (the case p < 0 is similar, and for the case p = 0, we have $\lambda = 0$ with a corrector equal to zero).

Step 1

Using the theory developed in Imbert et al. (2006), let us consider (using the fact that $\int_{\mathbb{R}} |x| J(x) \, dx < +\infty$) for p > 0, the solution u of:

$$\begin{cases} u_t = |\partial_x u|(c^1 + A + M(u - p \cdot)) \\ u(x, t = 0) = px \end{cases}$$

then $\bar{\omega}(t) = \inf_{x} \partial_x u(t, x)$ formally satisfies:

$$\bar{\omega}_t \ge |\bar{\omega}|(\partial_x c^1 + M\bar{\omega}) \ge |\bar{\omega}|(\partial_x c^1) \text{ with } \bar{\omega}(0) = p > 0,$$

and therefore the lower-bound on the possible exponential decay of $\bar{\omega}$ implies that

 $\partial_x u \ge 0.$

This result can be justified rigorously using some classical viscosity arguments (as in Imbert et al., 2006). We also know that u(t, x) - px is 1-periodic in x. We already know by Imbert et al. (2006) that there exists a unique $\lambda \in \mathbb{R}$ such that $v(t, x) = u(t, x) - px - \lambda t$ is bounded. Moreover $\lambda = \overline{H}(A, p)$. Let us now define Y_t and y_t such that $M(t) := \max_x v(t, x) = v(t, Y_t)$ and $m(t) := \min_x v(t, x) = v(t, y_t)$ and $|Y_t - y_t| < 1$, we get formally

$$\lambda + M'(t) \le |p|(c^1(Y_t) + A + (Mv)(Y_t)), \lambda + m'(t) \ge |p|(c^1(y_t) + A + (Mv)(y_t))$$

which implies for $p \neq 0$ that $\omega(t) = M(t) - m(t)$ satisfies:

$$\omega'(t)/|p| - ((Mv)(Y_t) - (Mv)(y_t)) \le c^1(Y_t) - c^1(y_t).$$

Moreover, by Lemma 2.1, we get that

$$\omega'(t)/|p| + c_2\omega(t) \le c^1(Y_t) - c^1(y_t)$$
 with $\omega(0) = 0$

This inequality can be justified rigorously by routine viscosity arguments. We deduce that for every $t \geq 0$

$$\omega(t) = \max_{x} v(t, x) - \min_{x} v(t, x) \le \frac{2}{c_2} |c^1|_{L^{\infty}(\mathbb{R})}.$$

Step 2

Considering the semi-relaxed limits of $u(t, x) - px - \lambda t$ with the suppremum (resp. the infimum) in time, we build a subsolution \underline{v} (resp. a supersolution \overline{v}) of the following equation

$$\lambda = |p + \partial_x v|(c^1 + A + Mv)$$

which satisfies the expected properties, and this ends the proof of the Lemma. \Box

Proof of Theorem 1.2:

1 We first prove the monotonicity of $\overline{H}(A, p)$ in A. Let us consider $A_2 > A_1$, $\lambda_i = \overline{H}(A_i, p), i = 1, 2$ and a subcorrector \underline{v}_1 for (A, p) then we have

$$\lambda_1 \le |p + \partial_x \underline{v}_1| (c^1 + A_1 + M \underline{v}_1)$$

$$\le |p + \partial_x \underline{v}_1| (c^1 + A_2 + M \underline{v}_1).$$

This shows that $\underline{v}_1(x) + px + \lambda_1 t$ is a subsolution to the cell problem which implies that $\lambda_2 \ge \lambda_1$ i.e., $\overline{H}(A_2, p) \ge \overline{H}(A_1, p)$.

2 We now prove that $\overline{H}(0,p) = 0$ in the case $\int_{(0,1)} c^1 = 0$. Let us define v_0 as the periodic solution of

$$Mv_0 = -c^1 \quad \text{on } \mathbb{R} \tag{21}$$

such that $\int_{(0,1)} v_0 = 0$. We notice that v_0 is a corrector for the cell problem with $\lambda = 0 = \overline{H}(0, p)$.

3 Let us now show the monotonicity in |p| in the case $\int_{(0,1)} c^1 = 0$. Indeed, for $p_2 > p_1 > 0$ and A > 0 such that $\lambda_1 > 0$ with $\lambda_i = \overline{H}(A, p_i)$, i = 1, 2 (the other cases are similar), let us consider a subcorrector \underline{v}_1 satisfying:

$$0 < \lambda_1 \leq (p_1 + \partial_x \underline{v}_1) (c^1 + A + M \underline{v}_1) \text{ with } p_1 + \partial_x \underline{v}_1 \geq 0$$

and a supercorrector \bar{v}_1 satisfying

$$\lambda_1 \ge (p_1 + \partial_x \bar{v}_1)(c^1 + A + M\bar{v}_1)$$
 with $p_1 + \partial_x \bar{v}_1 \ge 0$.

From Lemma 2.2, we also know that we can bound these sub/supercorrectors by $\frac{2}{c_2}|c^1|_{L^{\infty}(\mathbb{R})}$. Therefore

$$0 \leq c^1 + A + M \underline{v}_1 \quad \text{and} \quad \left(1 + \frac{2}{c_2}\right) |c^1|_{L^{\infty(\mathbb{R})}} \geq c^1 + M \underline{v}_1.$$

Then

$$\lambda_1 \le \lambda_1 + (p_2 - p_1) \left(c^1 + A + M \underline{v}_1 \right) \le (p_2 + \partial_x \underline{v}_1) \left(c^1 + A + M \underline{v}_1 \right),$$

which implies that $\lambda_2 \ge \lambda_1 > 0$. Similarly, we have

$$\lambda_1 + \left(\left(1 + \frac{2}{c_2} \right) |c^1|_{L^{\infty}(\mathbb{R})} + A \right) (p_2 - p_1) \ge \lambda_1 + (p_2 - p_1)(c^1 + A + M\bar{v}_1) \\ \ge (p_2 + \partial_x \bar{v}_1)(c^1 + A + M\bar{v}_1),$$

which implies that $\lambda_2 \leq \lambda_1 + ((1 + \frac{2}{c_2})|c^1|_{L^{\infty}(\mathbb{R})} + A)(p_2 - p_1)$ and gives the result. \Box

3 Monotonicity of the scheme

In this section we prove Theorem 1.4. We will use the following result (consequence of Lemma 2.5.2 in Ghorbel and Monneau, 2006).

Lemma 3.1 (A monotonicity preserving scheme for prescribed velocity): Assume that

$$v_i^{n+1} = v_i^n + \frac{\Delta t}{\Delta x} c_i^n \times \begin{cases} v_{i+1}^n - v_i^n & \text{if } c_i^n \ge 0\\ v_i^n - v_{i-1}^n & \text{if } c_i^n < 0 \end{cases}$$

and

$$\Delta t \le \frac{1}{2} \left(\sup_{j \in \mathbb{Z}} \frac{|c_{j+1}^k - c_j^k|}{\Delta x} \right)^{-1} \quad \text{for } 0 \le k \le n.$$
(22)

If

$$v_{i+1}^0 \ge v_i^0, \quad \forall \ i \in \mathbb{Z},$$

then

$$v_{i+1}^k \ge v_i^k, \quad \forall i \in \mathbb{Z}, \quad \text{for } 0 \le k \le n+1.$$

Proof of Theorem 1.4: Let $(v_i^n)_{i \in \mathbb{Z}, n \in \mathbb{N}}$ and $(w_i^n)_{i \in \mathbb{Z}, n \in \mathbb{N}}$ be two discrete solutions such that v_i^0 and w_i^0 are non-decreasing in $i \in \mathbb{Z}$. We set $M^n(v) := \sup_{i \in \mathbb{Z}} \frac{v_{i+1}^n - v_i^n}{\Delta x}$ and $M^n(w) := \sup_{i \in \mathbb{Z}} \frac{w_{i+1}^n - w_i^n}{\Delta x}$. One writes the numerical scheme for v (and the same for w):

$$v_i^{n+1} = v_i^n + \frac{\Delta t}{\Delta x} c_i(v^n) \times \begin{cases} v_{i+1}^n - v_i^n & \text{if } c_i(v^n) \ge 0\\ v_i^n - v_{i-1}^n & \text{if } c_i(v^n) < 0 \end{cases}$$
(23)

with $c_i(v^n)$ defined in equations (8) and (9). Let us assume that $v_i^k \ge w_i^k$ for every $i \in \mathbb{Z}$ and every $0 \le k \le n$. We will prove that it is still true for k = n + 1.

Case 1: We assume that $c_i(v^n) \ge 0$ and $c_i(w^n) \ge 0$. We have

$$v_i^{n+1} - w_i^{n+1} = v_i^n - w_i^n + \frac{\Delta t}{\Delta x} (c_i(v^n) (v_{i+1}^n - v_i^n) - c_i(w^n) (w_{i+1}^n - w_i^n)).$$

One can add and substract $\frac{\Delta t}{\Delta x}c_i(w^n)(v_{i+1}^n-v_i^n)$ to obtain

$$\begin{aligned} v_i^{n+1} - w_i^{n+1} &= (v_i^n - w_i^n) \left(1 - \frac{\Delta t}{\Delta x} c_i(w^n) \right) + \frac{\Delta t}{\Delta x} c_i(w^n) (v_{i+1}^n - w_{i+1}^n) \\ &+ \frac{\Delta t}{\Delta x} (c_i(v^n) - c_i(w^n)) (v_{i+1}^n - v_i^n) \\ &\ge (v_i^n - w_i^n) \left(1 - \frac{\Delta t}{\Delta x} c_i(w^n) \right) + \frac{\Delta t}{\Delta x} (c_i(v^n) - c_i(w^n)) (v_{i+1}^n - v_i^n) \end{aligned}$$

where we have used the fact that $v_{i+1}^n \ge w_{i+1}^n$. Since

$$c_i(v^n) = A + c^1(x_i) - v_i^n + \sum_{j \in \mathbb{Z}} J_j v_{i-j}^n \Delta x,$$
(24)

the difference between the discrete velocities can be written as

$$c_i(v^n) - c_i(w^n) = -(v_i^n - w_i^n) + \sum_{j \in \mathbb{Z}} J_j(v_{i-j}^n - w_{i-j}^n) \,\Delta x, \tag{25}$$

and then we get (using $J_j \ge 0$ and $v_{i-j}^n - w_{i-j}^n \ge 0$):

$$v_{i}^{n+1} - w_{i}^{n+1} \ge (v_{i}^{n} - w_{i}^{n}) \left(1 - \frac{\Delta t}{\Delta x} c_{i}(w^{n}) \right) - \frac{\Delta t}{\Delta x} (v_{i}^{n} - w_{i}^{n}) (v_{i+1}^{n} - v_{i}^{n}) \\ \ge (v_{i}^{n} - w_{i}^{n}) \left(1 - \frac{\Delta t}{\Delta x} c_{i}(w^{n}) - M^{n}(u) \Delta t \right).$$
(26)

Therefore we have

$$v_{i}^{n+1} - w_{i}^{n+1} \ge (v_{i}^{n} - w_{i}^{n}) \left(1 - \frac{\Delta t}{\Delta x} c_{i}(w^{n}) - M^{n}(u) \Delta t \right).$$
⁽²⁷⁾

It is then sufficient to have the following two restrictions on the time step

$$\frac{\Delta t}{\Delta x} \leq \left(2\sup_{j\in\mathbb{Z}} |c_j(v^n)|\right)^{-1} \text{ and } M^n(u)\Delta t \leq \frac{1}{2},$$

to deduce, in this case, that the scheme is monotone.

Case 2: We assume that $c_i(v^n) \leq 0$ and $c_i(w^n) \leq 0$. We compute

$$v_i^{n+1} - w_i^{n+1} = v_i^n - w_i^n + \frac{\Delta t}{\Delta x}c_i(v^n)(v_i^n - v_{i-1}^n) - \frac{\Delta t}{\Delta x}c_i(w^n)(w_i^n - w_{i-1}^n).$$

One can add and substract $\frac{\Delta t}{\Delta x}c_i(v^n)(w_i^n-w_{i-1}^n)$ to obtain

$$v_i^{n+1} - w_i^{n+1} = (v_i^n - w_i^n) \left(1 + \frac{\Delta t}{\Delta x} c_i(v^n) \right) + \frac{\Delta t}{\Delta x} (c_i(v^n) - c_i(w^n))(w_i^n - w_{i-1}^n) \\ - \frac{\Delta t}{\Delta x} c_i(v^n)(v_{i-1}^n - w_{i-1}^n).$$

Since $c_i(v^n) < 0$ and $v_{i-1}^n \ge w_{i-1}^n$, we get:

$$v_i^{n+1} - w_i^{n+1} \ge (v_i^n - w_i^n) \left(1 + \frac{\Delta t}{\Delta x} c_i(v^n) \right) + \frac{\Delta t}{\Delta x} (c_i(v^n) - c_i(w^n)) (w_i^n - w_{i-1}^n)$$
$$\ge (v_i^n - w_i^n) \left(1 + \frac{\Delta t}{\Delta x} c_i(v^n) - M^n(w) \Delta t \right)$$
$$\ge 0,$$

 $\text{if } \tfrac{\Delta t}{\Delta x} \leq \left(2 \sup_{j \in \mathbb{Z}} |c_j(u^n)|\right)^{-1} \text{ and } M^n(v) \Delta t \leq \tfrac{1}{2}.$

Case 3: We assume that $c_i(v^n) \ge 0$ and $c_i(w^n) < 0$. We compute

$$v_i^{n+1} - w_i^{n+1} = v_i^n - w_i^n + \frac{\Delta t}{\Delta x} c_i(v^n) (v_{i+1}^n - v_i^n) - \frac{\Delta t}{\Delta x} c_i(w^n) (w_i^n - w_{i-1}^n)$$

$$\geq v_i^n - w_i^n$$

because $v_{i+1}^n - v_i^n \ge 0$ and $w_i^n - w_{i-1}^n \ge 0$. It is then sufficient to assume that

$$\Delta t \le \left(\sup_{j \in \mathbb{Z}} \frac{|c_{j+1}(v^k) - c_j(v^k)|}{\Delta x}\right)^{-1} \quad \text{for } 0 \le k \le n$$
(28)

and

$$\Delta t \le \left(\sup_{j \in \mathbb{Z}} \frac{|c_{j+1}(w^k) - c_j(w^k)|}{\Delta x}\right)^{-1} \quad \text{for } 0 \le k \le n$$
(29)

to guarantee the monotonicity of v and the monotonicity of w using Lemma 3.1.

Case 4: We assume that $c_i(v^n) < 0$ and $c_i(w^n) \ge 0$. We compute

$$v_i^{n+1} - w_i^{n+1} = v_i^n - w_i^n + \frac{\Delta t}{\Delta x} c_i(v^n)(v_i^n - v_{i-1}^n) - \frac{\Delta t}{\Delta x} c_i(w^n)(w_i^n - w_{i-1}^n).$$

But

$$0 > c_i(v^n) - c_i(w^n) = -(v_i^n - w_i^n) + \sum_l J_l(v_{i-l}^n - w_{i-l}^n)$$

$$\ge -(v_i^n - w_i^n)$$

and for general $c_+ \geq 0, \, c_- \leq 0$ and $a,b \geq 0$ we have

$$|c_{-}a - c_{+}b| \le \max(a, b)|c_{+} - c_{-}|$$

and then

$$\begin{aligned} |c_i(v^n)(v_i^n - v_{i-1}^n) - c_i(w^n)(w_i^n - w_{i-1}^n)| &\leq \Delta x \max(M^n(v), M^n(w)) \\ &\times |c_i(v^n) - c_i(w^n)| \\ &\leq \Delta x \max(M^n(v), M^n(w))(v_i^n - w_i^n). \end{aligned}$$

Therefore

$$v_i^{n+1} - w_i^n \ge (v_i^n - w_i^n)(1 - \Delta t \max(M^n(v), M^n(w)))$$

 $\ge 0,$

if we assume $\Delta t\max(M^n(v),M^n(w))\leq 1$ and equations (28)–(29).

4 Computation of the effective Hamiltonian for equation (1)

We recall here that the effective Hamiltonian is given in Definition 1.1. Numerically, we compute $\overline{H}(A, p)$ for

$$p = \frac{P}{Q}$$
 for a fixed $Q \in \mathbb{N} \setminus \{0\}$ and $P \in \mathbb{Z}$. (30)

Because p is given by equation (30), we know that the solution w of equation (1) with initial value w(x, 0) = px satisfies:

$$w(x+Q,t) = w(x,t) + P.$$

For this reason, numerically, we restrict the computation on the interval $\left[-\frac{Q}{2}, \frac{Q}{2}\right]$ with periodic boundary conditions for $\bar{w}(x,t) = w(x,t) - px$ and we write the equation for \bar{w} . In particular, we also choose Δx such that $\frac{Q}{\Delta x} \in \mathbb{N} \setminus \{0\}$.

We then use the numerical scheme of Theorem 1.4 with Δt satisfying the CFL conditions stated in Theorem 1.4, which guarantees the monotonicity of the scheme.

4.1 The method to compute the effective Hamiltonian

Here we describe two possible strategies to compute numerically the effective Hamiltonian $\overline{H}^{num}(A, p)$.

Method 1: Using the numerical solution w^n of equation (7), we take its values at two discrete times $t_1 > 0$ and $t_2 > 0$ at a discrete point x_{ref} and we define $\overline{H}^{\text{num}}(A, p) = \frac{v(x_{\text{ref}}, t_2) - v(x_{\text{ref}}, t_1)}{t_2 - t_1}$ for $t_2 - t_1$ large enough, which is difficult to fix in practice.

Method 2: We follow the position of a dislocation (as a marker) starting from a point x_{ref} at time t_1 and waiting until it passes a second time (in the 'periodic' interval [-Q/2, Q/2]) at the same point at time t_2 , and we define $\overline{H}^{num}(A, p) = \frac{|P|}{t_2 - t_1}$ with $p = \frac{P}{Q}$ (see Figure 2). Here $\frac{\overline{H}^{num}(A, p)}{p}$ can be interpreted as an effective velocity.

Figure 2 Tracking the trajectory of a dislocation until it comes back to the initial position



In practice we prefer to use the Method 2 in general, because, given a time t_1 large enough, it provides naturally a time t_2 . On the contrary, the result given by the Method 1 can be more sensitive to the choice of t_2 with respect to t_1 .

Figure	3	4	5	6	7	8	9
c^0	$-\delta_0 + J$	$-\delta_0 + J$					
p	0.3125	(0, 10)	$2.5/k, \ k =$	(-10, 10)	(-10, 10)	3	3
			1, 2, 3, 4				
A	(-10, 10)	B/k, k =	(0, 10)	(-10, 10)	(-10, 10)	2	2
		1, 2, 3, 4					
В	1	1	1	1	1	0	2
k	1	1	1	1	1	2	2
Q	10	10	10	10	10	1	1
Δx	0.01	0.01	0.01	0.01	0.01	0.01	0.01
Δt	$< 10^{-3}$	$< 10^{-3}$	$< 10^{-3}$	$< 10^{-3}$	$< 10^{-3}$	$2.49 \ 10^{-3}$	$1.24 \ 10^{-3}$
t_1	10	10	10	10	10	-	-

Figure 3 $\overline{H}^{num}(A,p)$ for p = 0.3125 and a monotone kernel $c^0 = -\delta_0 + J$

Figure	10	11	12	14	15	17
c^0	$-\delta_0 + J$	$-\delta_0 + J$	(36)	$-\delta_0 + J$	(36)	(39)
p	3	2.5/k, k =	1, 2, 5, 10	(0.1, 2)	1, 2, 3, 4	0.2, 0.4, 0.7
		1, 2, 3, 4				
A	2.5	(0, 10)	(0, 10)	(0, 10)	(0, 10)	(0, 10)
B	2	1	1	-	-	-
k	1	1	1	-	-	-
Q	1	10	10	10	10	10
Δx	0.01	0.01	0.01	0.01	0.01	0.01
Δt	$1.11 \ 10^{-3}$	$< 10^{-3}$	$< 10^{-3}$	$< 10^{-4}$	$< 10^{-4}$	$< 10^{-4}$
t_1	-	50	50	$1000\Delta t$	50	50



4.2 Results of the numerical simulations

Let us recall that the convolution is written as

$$c^{0} \star w = c^{0} \star (w - px)$$

= $-\bar{w} + J \star \bar{w}$
= $-\bar{w} + J^{*} \star \bar{w}$
[$-\frac{Q}{2}, \frac{Q}{2}$] (31)

with

$$J^*(x) = \sum_{k \in \mathbb{Z}} J(x+kQ).$$
(32)

For the present simulations we choose

$$J^*(x) = \frac{1}{Q} \quad \text{for } x \in \left[-\frac{Q}{2}, \frac{Q}{2}\right)$$
(33)

and

$$c^{1}(x) = B\sin(2\pi kx) \quad \text{with } k \in \mathbb{N} \setminus \{0\}.$$
(34)

For the simulations we have the following particular choices.

Figure 4 $\overline{H}^{num}(A, p)$ as a function of the density p for a monotone kernel $c^0 = -\delta_0 + J$



Figure 5 $\overline{H}^{num}(A, p)$ as a function of A and a monotone kernel $c^0 = -\delta_0 + J$



In Figure 3, we present the numerical effective Hamiltonian $\overline{H}^{num}(A, p)$ which is monotone in A as expected from the first property of Theorem 1.2. Moreover, this reveals the existence of a threshold effect, i.e., the effective Hamiltonian is zero on a whole interval of the parameter A. In addition, $\overline{H}^{num}(A, p)$ is antisymmetric in A because of the symmetries of c^1 . For $|A| \gg B = 1$, the effective Hamiltonian is linear

and can be approximated here by Ap which is the classical Orowan law (see Kratochvil et al., 2003). In addition, we note that $\overline{H}^{num}(A, p)$ behaves like the square-root function of A in a neighbourhood of the zero-plateau of \overline{H}^{num} . In Figure 4, the effective Hamiltonian $\overline{H}^{num}(A, p)$ is represented as a function of p for some values of A. We note here the monotonicity of \overline{H}^{num} with respect to p. For a large density of dislocations, the effective Hamiltonian \overline{H}^{num} is linear and can again be approximated by Ap.

Figure 6 Graph of $\overline{H}^{num}(A, p)$ for monotone kernel $c^0 = -\delta_0 + J$



Figure 7 Level sets of the effective Hamiltonian $\overline{H}^{num}(A, p)$



In Figure 5, we present the effective Hamiltonian $\overline{H}^{num}(A, p)$ as a function of A for several densities of dislocations p. Again we check numerically the qualitative properties of the effective Hamiltonian.

In Figure 6, we represent the graph of the effective Hamiltonian \overline{H}^{num} . The X-axis (respectively Y-axis and Z-axis) corresponds to the density of dislocations p (respectively the parameter A and the effective Hamiltonian \overline{H}^{num}). The projection of this graph on the plane (A, p) gives Figure 7 which represents the level sets of \overline{H}^{num} .

In Figure 7, the central region is the set where there is a pinning of the dislocations on the defects represented by the field c^1 , i.e., where the effective Hamiltonian vanishes. Moreover the monotonicity of \overline{H}^{num} in p reveals that in this model, the ability of the dislocations to pass the obstacles is increased when we increase the density of dislocations. This is typically a collective behaviour.

5 Computation of the effective Hamiltonian for other equations

In this section we study numerically the effective Hamiltonian for models where in equation (1) the non-local velocity $c^{int}[u]$ is replaced by

$$c^{\rm int}[u] = c^0 \star \lfloor u \rfloor \tag{35}$$

where $\lfloor \cdot \rfloor$ is the floor function.

Figure 8 Linear trajectories



Here the positions of dislocations are given by the jumps of $\lfloor u \rfloor$ (see Ghorbel and Monneau, 2006). Let us mention that even for monotone kernel c^0 , the theoretical existence of an effective Hamiltonian is not known, we numerically check that this effective Hamiltonian exists in two cases: the monotone kernel (Subsection 5.1) and the Peierls-Nabarro kernel (Subsection 5.2).

5.1 The monotone kernel with one type of dislocations

In this subsection we set $c^0 = -\delta_0 + J$ with $J^* = \frac{1}{Q}$ with the notation of Section 4. This case is strongly related to the homogenisation of a Slepčev formulation (see Forcadel et al., xxxx).





Figure 10 The motion of the dislocations becomes periodic in time



First, we represent in Figure 8 the trajectories of three dislocations (initially located at x = -1/3, x = 0, x = 1/3) in the case where there are no obstacles (i.e., $c^1 = 0$).

In this case the trajectories of dislocations are straight lines. A different situation happens (see Figure 9), when we add sufficient obstacles in order to obtain the pinning of dislocations (with $B \ge A$). This case corresponds to the situation where \overline{H}^{num} is equal to zero.



Figure 11 Effective Hamiltonian $\overline{H}^{num}(A, p)$ as a function of A for $c^0 \star \lfloor u \rfloor$, $c^0 = -\delta_0 + J$

Figure 12 Graph of $\overline{H}^{num}(A, p)$ for Peierls-Nabarro model with one type of edge dislocations



Now, if we increase the parameter A, without changing the obstacles, i.e., with the same c^1 , we observe a persistent motion of dislocations (see Figure 10). Numerically, this

motion becomes periodic in time. Moreover, we also present in Figure 11 the effective Hamiltonian whose behaviour is similar to the case of Section 4.

5.2 The Peierls-Nabarro kernel with one type of edge dislocations

In this subsection, we consider the Peierls-Nabarro kernel (see Hirth and Lothe, 1992; Alvarez et al., 2006) given by:

$$c^{0}(x) = \frac{-\mu |\vec{b}|^{2}}{2\pi(1-\nu)} \frac{x^{2}-\zeta^{2}}{(x^{2}+\zeta^{2})^{2}}.$$
(36)

where $\nu = \frac{\lambda}{2(\lambda+\mu)}$ is the Poisson ratio and λ and $\mu > 0$ are the Lamé coefficients for isotropic elasticity and \vec{b} is the Burgers vector. We choose $\frac{\mu |\vec{b}|^2}{2\pi(1-\nu)} = 1$ and $\zeta = 0.01$ for our simulations.

Again we compute the effective Hamiltonian in Figure 12 which turns out to provide a behaviour similar to the one of Section 4.

6 Computation of the effective Hamiltonian for systems of equations

In this section, we consider systems of equations describing the motion of dislocations of opposite Burgers vector $(+\vec{b})$ and $(-\vec{b})$. More precisely we study numerically the following system:

$$\begin{cases} \frac{\partial u^{+}}{\partial t}(x,t) = -c[u^{+},u^{-}](x,t) \left| \frac{\partial u^{+}}{\partial x}(x,t) \right| & \text{in } \mathbb{R} \times (0,+\infty) \\ \frac{\partial u^{-}}{\partial t}(x,t) = c[u^{+},u^{-}](x,t) \left| \frac{\partial u^{-}}{\partial x}(x,t) \right| & \text{in } \mathbb{R} \times (0,+\infty) \\ u^{+}(x,0) = p^{+}x & \text{on } \mathbb{R} \\ u^{-}(x,0) = p^{-}x & \text{on } \mathbb{R} \end{cases}$$
(37)

where

$$c[u^{+}, u^{-}](x, t) = A + c^{0} \star (\lfloor u^{+}(\cdot, t) \rfloor - \lfloor u^{-}(\cdot, t) \rfloor).$$
(38)

Figure 13 Opposite motion of dislocations + and -

motion of dislocation + ++++++ + ----- xmotion of dislocation -



Figure 14 Graph of $\overline{H}^{num}(A, p)$ as a function of A for $p = p^+ = p^-$ with the monotone kernel

Figure 15 Effective velocity $\frac{\overline{H}^{num}(A,p)}{p}$ as a function of A for $p = p^+ = p^-$ in the case of Peierls-Nabarro kernel



Here the positions of dislocations of Burgers vector $(+\vec{b})$ (respectively $(-\vec{b})$) are represented by the jumps of $\lfloor u^+(\cdot,t) \rfloor$ (respectively $\lfloor u^-(\cdot,t) \rfloor$). The motion is schematically represented on Figure 13.

In the following three subsections we will compute the numerical effective Hamiltonian for the two types of dislocations $\overline{H}^{num}(A,p)$ with the same densities $p = p + p = p - (\text{or the velocity } \frac{\overline{H}^{num}(A,p)}{p})$ using a numerical method similar to the one used in Sections 4 and 5. We present successively our result in the case of monotone kernel, Peierls-Nabarro kernel for edge dislocations, and the kernel describing the motion of walls of dislocations.

Figure 16 Walls of dislocations + and walls of dislocations -



6.1 Monotone kernel

Here we take $c^0 = -\delta_0 + J$ with $J^* = \frac{1}{Q}$ with the notation of Section 4. We present in Figure 14 the effective Hamiltonian $\overline{H}^{num}(A, p)$. We observe a threshold phenomenon, similar to the one of Section 4. Here the dislocations of type – can be seen as obstacles to the motion of the dislocations of type + and vice-versa.

6.2 Peierls-Nabarro kernel for edge dislocations

In this case we take the kernel c^0 given in equation (36) and the numerical values of Subsection 5.2. We observe in Figure 15 the mean velocity and a threshold effect which increases (apparently linearly) where we increase the density $p = p^+ = p^-$ of dislocations, as physically expected.

6.3 Kernel for walls of dislocations

Here we take

$$c^{0}(x) = \frac{\partial \bar{\sigma}}{\partial x}(x) \quad \text{with } \bar{\sigma}(x) = \frac{\mu |\vec{b}|^{2} \pi}{1 - \nu} \frac{\frac{x}{\varepsilon}}{\left(\cosh(2\pi \frac{x}{\varepsilon}) - 1\right)}$$
(39)

with μ is a Lamé coefficient, ν is the Poisson ratio, \vec{b} is the Burgers vector and ε is the distance between dislocations along the y direction (see Figure 16 and Appendix B).

Here we take $\frac{\mu b^2 \pi}{1-\nu} = 1$ and $\varepsilon = 1$. We present the effective velocity $\frac{\overline{H}^{\text{num}}(A,p)}{p}$ in Figure 17, and get similar result as in Subsection 6.2 and in Ghorbel et al. (2006).



Figure 17 Effective velocity $\frac{\overline{H}^{num}(A,p)}{p}$ as a function of A for $p = p^+ = p^-$ with the kernel for walls of dislocations

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Appendix

A Proof of Lemma 2.1

With the notation of Lemma 2.1, we set $c = \frac{Y+y}{2}$ and $\delta = \frac{Y-y}{2} \in \left] -\frac{1}{2}, \frac{1}{2}\right[$. Then we compute

$$(c^{0} \star u)(Y) - (c^{0} \star u)(Y) = \int dz \ J(z)(u(Y+z) - u(Y))$$

$$- \int dz \ J(z)(u(y+z) - u(y))$$

$$= \int d\bar{z} \ J(\bar{z} - \delta)(u(c+\bar{z}) - u(Y))$$

$$- \int d\tilde{z} \ J(\tilde{z} + \delta)(u(c+\tilde{z}) - u(y))$$

$$\leq - \int dz \ \inf(J(z-\delta), J(z+\delta))$$

$$\times (u(Y) - u(c+z) + u(c+z) - u(y))$$

$$\leq -(u(Y) - u(y))c_{2}$$

where we have used the change of variables $\bar{z} = z + \delta$, $\tilde{z} = z - \delta$ in the second line and used the fact that $u(c + \bar{z}) - u(Y) \leq 0$ and $u(c + \tilde{z}) - u(y) \geq 0$ to get the third line.

B Computation of the kernel for walls of dislocations

We recall (see Hirth and Lothe, 1992) that the stress created by one dislocation at the origin is given by:

$$\sigma_{xy}^0(x,y) = \frac{\mu b}{2\pi(1-\nu)} \frac{x(x^2-y^2)}{(x^2+y^2)^2}.$$
(40)

Now the stress created by a wall of dislocations at the positions $x = 0, y = k\varepsilon$ for $k \in \mathbb{Z}$ is given by:

$$\sigma_{xy}(x,y) = \sum_{k \in \mathbb{Z}} \sigma_{xy}^0(x,y-k\varepsilon)$$
$$= \frac{\mu b\pi}{1-\nu} \frac{\frac{x}{\varepsilon} \left(\cosh\left(2\pi\frac{x}{\varepsilon}\right)\cos\left(2\pi\frac{y}{\varepsilon}\right)-1\right)}{\left(\cosh\left(2\pi\frac{x}{\varepsilon}\right)-\cos\left(2\pi\frac{y}{\varepsilon}\right)\right)^2}.$$
(41)

(see Hirth and Lothe, 1992, p.733, formula (19-73)). Then

$$c^{0}(x) = b \frac{\partial \sigma_{xy}}{\partial x}(x,0) = \frac{\partial \bar{\sigma}}{\partial x}(x)$$
(42)

with $\bar{\sigma}(x) = b\sigma_{xy}(x,0)$.