A non-monotone Fast Marching scheme for a Hamilton-Jacobi equation modeling dislocation dynamics *

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Summary. In this paper we introduce an extension of the Fast Marching Method introduced by Sethian [6] for the eikonal equation modeling front evolutions in normal direction. The new scheme can deal with a *time-dependent* velocity without *any restriction on its sign.* This scheme is then used for solving dislocation dynamics problems in which the velocity of the front depends on the position of the front itself and his sign is not restricted to be positive or negative.

1 Introduction

In this paper, we propose a new Fast Marching Method for the following eikonal equation

$$\begin{cases} u_t(x,y,t) = c(x,y,t)|\nabla u(x,y,t)| & Q \subset \mathbb{R}^2 \times (0,T) \\ u(x,y,0) = u^0(x,y) & Q \subset \mathbb{R}^2. \end{cases} \tag{1}$$

This equation describes the propagation of a front $\Gamma_t = \partial\Omega_t$, where $\Omega_t = \{(x,y) \in Q \; s.t. \; u(x,y,t) \geq 0\}$, with a normal speed $\mathbf{c} = c(x,y,t)\mathbf{n}$.
We consider here the case where the velocity $c(x,y,t)$ depends on time *without any restrictions on his sign.*
The main objective is to extend the Fast Marching Method to the following non-local Hamilton-Jacobi equation

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$$\begin{cases} u_t(x,y,t) = c^0(x,y) \star [u](x,y,t)|\nabla u(x,y,t)| & Q \subset \mathbb{R}^2 \times (0,T) \\ u(x,y,0) = u^0(x,y) & Q \subset \mathbb{R}^2. \end{cases} \tag{2}$$

The 0-level set of the solution of (2) represents a dislocation line in a 2D plane, here the kernel c^0 depends only on the space and $\star$ denotes the convolution in space (see [4] for a physical presentation of the model for dislocation dynamics).
To approach this problem, we first attack equation (1) generalizing the Fast Marching Method (FMM) introduced by Sethian [6] to fronts propagating with local unsigned speed $c(x,y,t)$. We will come back to equation (2) in the numerical section and in a future work.
It is well known that FMM is based on the following equation

$$c(x,y)|\nabla T(x,y)| = 1 \tag{3}$$

which is the stationary version of the equation (1) in the case that $c = c(x,y) > 0$ or $c = c(x,y) < 0$ (see [7]). The front can be recovered as the level sets of the function $T(x,y)$.
In classical FMM the computation of the solution proceeds in a crescent ordering accepting at each iteration the smallest value of the nodes in the current *narrow band* (see [6] and [5]). The minimal value of the *narrow band* can be considered *exact* (within the discretization error) in the sense that it can not be improved in the following iterations. This result allows us to deal easily with a *time-dependent* speed function using the current minimal value of the *narrow band* as time t and then to evaluate the speed function $c(x,y,t)$ during computation. Using this basic idea, Vladimirsky [8] extended FMM to a *signed* explicit time-depending function $c = c(x,y,t)$ and proved that in this case the evolution of front can be recovered as the level sets of the time-independent function $T(x,y)$ which is the unique viscosity solution of the equation

$$c(x,y,T(x,y))|\nabla T(x,y)| = 1. \tag{4}$$

In order to treat the *non-monotone* case in which speed is allowed to have different signs in different regions and/or to change sign in time, we introduce some important modifications to the classical scheme.
1) We perform a slightly modification of the function c. If there are two or more regions with different sign for c at the same time, we force the speed to be exactly zero on the boundaries of these regions so that the evolution of the front in each region can be considered completely separate. The modified function will refer to as *numerical speed* and it will be indicated with $\hat{c}$.
2) Our new *narrow band* is the set of nodes which are going to be reached by the front *and* the nodes just reached by the front. This allows to deal with changes of sign of the velocity in time.

2 The FMM algorithm for unsigned velocity

In this section we give details for our FMM algorithm for unsigned velocity. We describe the evolution of the front Γ_t using an auxiliary function:

$$\theta(x,y,t) = \begin{cases} 1 & \text{if } u(x,y,t) \geq 0 \\ -1 & \text{otherwise.} \end{cases}$$

Notations and preliminary definitions

We consider a lattice $Q_\Delta = \{(i,j) \in \mathbb{Z}^2 : (x_i, y_j) = (i\Delta, j\Delta) \in Q\}$ with space step Δ, we indicate with $0 < t_1 < ... < t_n < ... < t_N \leq T$ a non uniform lattice on $[0,T]$, where t_n is the physical evolution time computed in each iteration of the FMM. We note that partition of the time interval is not known *a priori.* We introduce some definitions which will be useful in the following.

Definition 1. *We define* **neighborhood of the node** (i,j) *the set* $V(i,j) \equiv \{(l,m) \in Q_\Delta \text{ such that } |(l,m)-(i,j)| = 1\}$.

Definition 2. *Given the speed* $c^n_{i,j} \equiv c(x_i, y_j, t_n)$ *we define* **numerical speed** *the function*

$$\hat{c}^n_{i,j} \equiv \begin{cases} 0 & if\ there\ exists\ (l,m) \in V(i,j)\ such\ that \\ & (c^n_{i,j} c^n_{l,m} < 0\ and\ |c^n_{i,j}| \leq |c^n_{l,m}|), \\ c^n_{i,j} & otherwise. \end{cases}$$

Definition 3. *Given* $\theta^n_{ij} = \theta(x_i, y_j, t_n)$ *we define the* **fronts** F^n_+ *and* F^n_- *by*

$$F^n_\pm \equiv V(E) \backslash E, \quad where \quad E = \{(i,j) \in Q_\Delta : \theta^n_{i,j} = \pm 1\}.$$

Description of the algorithm

We describe now the FMM algorithm for unsigned velocity.
We need a discrete function T_I to indicate the approximated physical time for the front propagation on the nodes $I = (i,j)$ of the fronts.

Initialization

1. $n = 1$

2. *Initialization of the matrix* θ^0
$$\theta^0_I = \begin{cases} 1 & \text{if } (x_i, y_j) \in \Omega_0 \\ -1 & \text{if } (x_i, y_j) \in Q \setminus \Omega_0 \end{cases}$$

3. *Initialization of the time on the fronts*
$T^0_I = 0$ for all $I \in F^0_+ \cup F^0_-$

Main cycle

4. *Computation of* $\tilde{T}_I^{n-1}$, $\forall I \in F_+^{n-1} \cup F_-^{n-1}$. Let $I \in F_\mp^{n-1}$, then
   a) if $\pm \hat{c}_I^{n-1} \le 0$, $\tilde{T}_I^{n-1} = \infty$,
   b) if $\pm \hat{c}_I^{n-1} > 0$, then we compute $\tilde{T}_I^{n-1}$ as the greater solution of the following second order equation:

$$\sum_{k=1}^{2}\left(\max_{\pm}\left(0, \tilde{T}_I^{n-1} - \hat{T}_{+,I^{k,\pm}}^{n-1}\right)\right)^2 = \frac{(\Delta x)^2}{|\hat{c}_I^{n-1}|} \text{ if } I \in F_-^{n-1}$$

$$\sum_{k=1}^{2}\left(\max_{\pm}\left(0, \tilde{T}_I^{n-1} - \hat{T}_{-,I^{k,\pm}}^{n-1}\right)\right)^2 = \frac{(\Delta x)^2}{|\hat{c}_I^{n-1}|} \text{ if } I \in F_+^{n-1}$$

   where

$$I^{k,\pm} = \begin{cases} (i \pm 1, j) \text{ if } k = 1 \\ (i, j \pm 1) \text{ if } k = 2. \end{cases}$$

   and

$$\hat{T}_{\pm,J}^{n-1} = \begin{cases} T_J^{n-1} & \text{if } J \in F_\pm^{n-1} \\ \infty & \text{else} \end{cases}$$

5. $\hat{t}_n = \min\left\{\tilde{T}_I^{n-1},\ I \in F_+^{n-1} \cup F_-^{n-1}\right\}$.

6. $\tilde{t}_n = \begin{cases} \hat{t}_n & \text{if } \hat{t}_n < \infty \\ t_{n-1} + dt & \text{if } \hat{t}_n = \infty \end{cases}$
   where dt is a small constant, see following Remark 1.

7. *Initialization of new accepted points*
   $NA_\pm^n = \{I \in F_\pm^{n-1},\ \tilde{T}_I^{n-1} = \tilde{t}_n\}$

8. $t_n = \max(t_{n-1}, \tilde{t}_n)$

9. *Reinitialization of* θ^n

$$\theta_I^n = \begin{cases} 1 & \text{if} \quad I \in NA_+^n \\ -1 & \text{if} \quad I \in NA_-^n \\ \theta_I^{n-1} & \text{else} \end{cases}$$

10. *Reinitialization of* T^n

    a) If $I \in NA_\pm^n$ then $T_I^n = t_n$.
    b) If $I \in (F_+^{n-1} \cup F_-^{n-1}) \cap (V(NA_+^n) \cup V(NA_-^n)) \backslash (NA_+^n \cup NA_-^n)$, then $T_I^n = T_I^{n-1}$.
    c) If $I \in (V(NA_+^n) \cup V(NA_-^n)) \backslash (F_+^{n-1} \cup F_-^{n-1})$ then $T_I^n = t_n$

11. $n = n + 1$

12. Go to 4.

Remark 1. The *step 6* allows to advance in time in any case. For example, if at time step n, we have $\hat{c}_I^{n-1} = 0 \ \forall I \in F_{\pm}^{n-1}$, then there will not be new accepted point and the time will not change. As consequence the algorithm will be blocked. The term dt have to be small enough (like $\frac{\Delta}{|\hat{c}^{n-1}|}$). More details will be given in a paper in preparation focused on the convergence of the scheme.

Remark 2. In *step 10* we change T_I^n only if a point of the neighborhood of I has been accepted.

Boundary conditions on ∂Q_Δ

The management of the boundary conditions is quite simple, as in the classical FMM (see for example [5]). We can assign to the nodes of the boundary the value $+\infty$ despite which is the value computed by the algorithm and at the end of computation these nodes are cut off.

3 Numerical tests

3.1 Given velocity

We present some simulations which show that this new scheme seems reasonable. We propose a first test regarding the rotation of a line. We consider the square $[-1,1]^2$ and we approximate the evolution of a line crossing the $\{x = 0\}$ axis with the velocity $c(x,y,t) = -x$. We set $\theta^0 = -1$ above the line and $\theta^0 = 1$ below. Formally, one expects that a straight line remains a

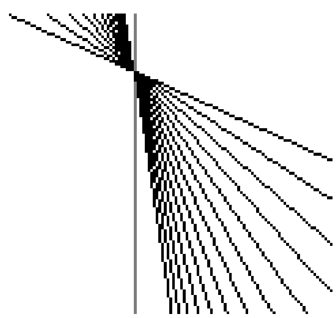

Fig. 1. Rotation of a line

straight line for all $t > 0$ and that it rotates around the axis $\{x = 0\}$ (where the velocity is zero). Indeed, let us consider a generic straight line

$$r = \{(x,y) : y = ax + b\}$$

and a point $(x_0, y_0) \in r$. We denote by (x_1, y_1) the image of (x_0, y_0) after the time δt. A first order expansion gives

$$\begin{aligned}(x_1, y_1) =& (x_0, y_0) - \delta t x_0 (b, -a) = \\ =& (x_0(1 - b\delta t), a x_0 (1 + \delta t) + b).\end{aligned}$$

Then

$$y_1 = a \left(\frac{1 + \delta t}{1 - b\delta t} \right) x_1 + b,$$

and we deduce that a straight line always remains a straight line. Fig. 1 shows that our algorithm computes what one expects.

Moreover, one can observe that the velocity of rotation of the line decreases when it approaches the axis $\{x = 0\}$. This is due to the fact that the velocity decreases near this axis.

We propose a second test regarding the evolution of a circle centered in the origin, with a speed $c(x, y, t) = 0.1t - x$. As shown in Fig. 2, the circle translates on the left and propagates in a self similar way. This test is run with $\Delta x = 2\pi/100$. The front is plotted every 0.5 physical time iterations with final time $T = 5$ and the solution is compared with that approximated by the classical finite difference scheme for equation (1).

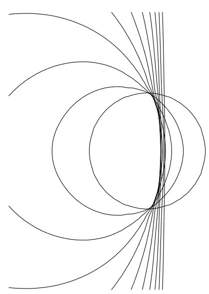

Fig. 2. Evolution of a circle with FD

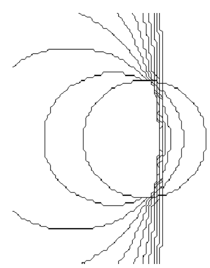

Fig. 3. Evolution of a circle with the FMM

Finally we propose a third test regarding the evolution of two circles. We set $\theta^0 = 1$ inside the circles and $\theta^0 = -1$ outside. We choose a velocity which changes sign in time, $c(x, y, t) = 1 - t$. This test is run with $\Delta x = 2\pi/100$. The front is plotted every 0.2 physical time with final time $T = 2.6$.
In Fig. 4 and 5 we show the result and we compare it with the approximation computed by the classical finite difference scheme for (1).

Fig. 4. Increasing (left) and decreasing (right) evolution of two circles with FMM

Fig. 5. Increasing (left) and decreasing (right) evolution of two circles by classical FD scheme

3.2 Dislocation Dynamics

As we said in the introduction, our method can be extended to dislocations dynamic problems. In this case, we introduce a time step Δt and we consider a uniform lattice over the time interval $[0,T]$, $\Delta t = \frac{T}{N}$ with $t_m = m\Delta t, m = 0, ..., N$.
We consider the function c as *time-independent* in each interval $\Delta t_m = [m\Delta t, (m+1)\Delta t]$. Once the algorithm completed the computation for the front's evolution in every interval Δt_m, it updates the speed function. We need to fix the velocity on each time interval Δt_m, since it depends on the front itself. This avoid spurious oscillations which arise when the velocity is updated before all the nodes of the front are evolved for a physical time Δt.
We propose one test regarding the relaxation of a dislocation line with sinusoidal shape. The problem (2) is approximated in $[-1,1]^2$ with

$$u(x,y,0) = \begin{cases} -1 & \text{if } y + 0.3\sin(x\pi) \leq 0 \\ 1 & \text{otherwise.} \end{cases}$$

We refer to [3] for the computation of the discrete convolution and for the description of the physical kernel. We remark that in this case the front has speed with different sign. In fact the upper part of the sinusoidal line moves

on the left and the other part moves on the right. The three points where the line changes convexity do not move since they have speed equal to 0.
This test has been run with $\Delta x = 0.01$, $\Delta t = 0.1$ for a final time T=4. Fig. 6 represents the 0-level set of the discrete function θ plotted every 10 time iterations.

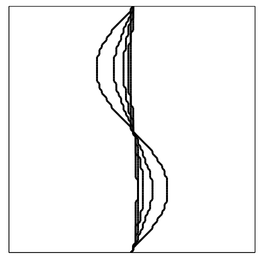

Fig. 6. Relaxation of a sinusoidal dislocation line

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