Numerical approximation of dislocation dynamics

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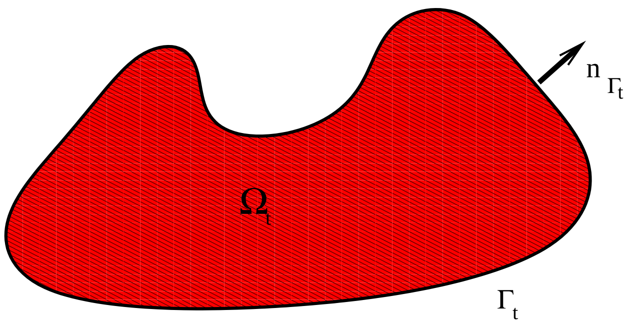
Outline

- The model problem for dislocation dynamics
- Finite Difference scheme
- Generalised Fast Marching Method (GFMM)
- Numerical tests for GFMM applied to dislocation dynamics

Idealisation of dislocations

We assume that the dislocation line is represented by the boundary Γ_t of a smooth bounded domain $\Omega_t \subset \mathbb{R}^2$. We define

$$u(x,t) = \begin{cases} > 0 & \text{if} \quad x \in \Omega_t, \\ < 0 & \text{if} \quad x \notin \Omega_t \\ = 0 & \text{if} \quad x \in \partial\Omega_t. \end{cases}$$



$$\begin{cases} u_t = c(1_{u>0}, x, t)|Du| & \text{in} \quad \mathbb{R}^2 \times (0, +\infty), \\ u(x,0) = u_0(x) & \text{on} \quad \mathbb{R}^2. \end{cases} \tag{1}$$

Dislocations dynamics, Peierls-Nabarro model

The resolved Peach-Koehler force acting on the dislocation is

$$c(x,t) = \ c_0 * 1_{u>0}(x,t)$$

The Fourier transform of c_0 is given by:

$$\widehat{c_\delta^0}(\xi_{x_1},\xi_{x_2}) = -\frac{1}{2}\left(\frac{\xi_{x_1}^2 + (\frac{1}{1-\nu})\xi_{x_2}^2}{\sqrt{\xi_{x_1}^2 + \xi_{x_2}^2}}\right) e^{-\delta\sqrt{\xi_{x_1}^2+\xi_{x_2}^2}}, \qquad (2)$$

$\delta \simeq$ size of the core of the dislocation

ν influences the anisotropy of the evolution

Short time existence and uniqueness

Theorem (Alvarez, C., Monneau, Rouy)
Let $c^0 \in L^\infty(\mathbb{R}^2) \cap BV(\mathbb{R}^2)$*. If* u^0 *satisfies*

$$|\nabla u^0(x,y)| < B \quad in\ \mathbb{R}^2$$

and

$$\frac{\partial u^0}{\partial y}(x,y) > b > 0 \quad in\ \mathbb{R}^2,$$

then there exists T^* *such that a unique viscosity solution of the problem in* $\mathbb{R}^2 \times [0, T^*)$ *exists .*

A finite difference scheme for the continuous model

A finite difference scheme for the continuous model

$$\begin{cases} v_{i,j}^{n+1} = S(c_{i,j}(1_{\{v^n>0\}}), v^n) & n = 0, ..., N \\ v_{i,j}^{n} = u^0(x_i, y_j) \end{cases}$$

$$S(c_{i,j}(1_{\{v^n>0\}}), v^n) = v_{i,j}^n + \Delta t H_d(c_{i,j}(1_{\{v^n>0\}}), D_x^{\pm} v_{i,j}^n, D_y^{\pm} v_{i,j}^n)$$

where the discrete numerical Hamiltonian reads

$$H_d = \begin{cases} c_{i,j}(1_{\{v^n>0\}}) H^+ & c_{i,j} 1_{\{v^n>0\}} \geq 0 \\ c_{i,j}(1_{\{v^n>0\}}) H^- & c_{i,j} 1_{\{v^n>0\}} < 0. \end{cases}$$

H^+, H^- are the standard numerical Hamiltonian:

$$H^+ = \left\{ \max(D_x^+ v_{i,j}^n, D_y^+ v_{i,j}^n, 0)^2 + \min(D_x^- v_{i,j}^n, D_y^- v_{i,j}^n, 0)^2 \right\}^{\frac{1}{2}}$$

A finite difference scheme for the continuous model

The FD scheme is

- consistent
- NOT monotone
- convergent under the CFL condition

$$0 < \frac{\Delta t}{\Delta x} \leq \frac{1}{2\sqrt{2}|c_\delta^0(\cdot,\cdot)|_1}$$

for small time

Convergence result

Theorem (Alvarez, C., Monneau, Rouy)

If u^0 satisfies

$$|\nabla u^0(x,y)| < B \quad in\ \mathbb{R}^2$$

and

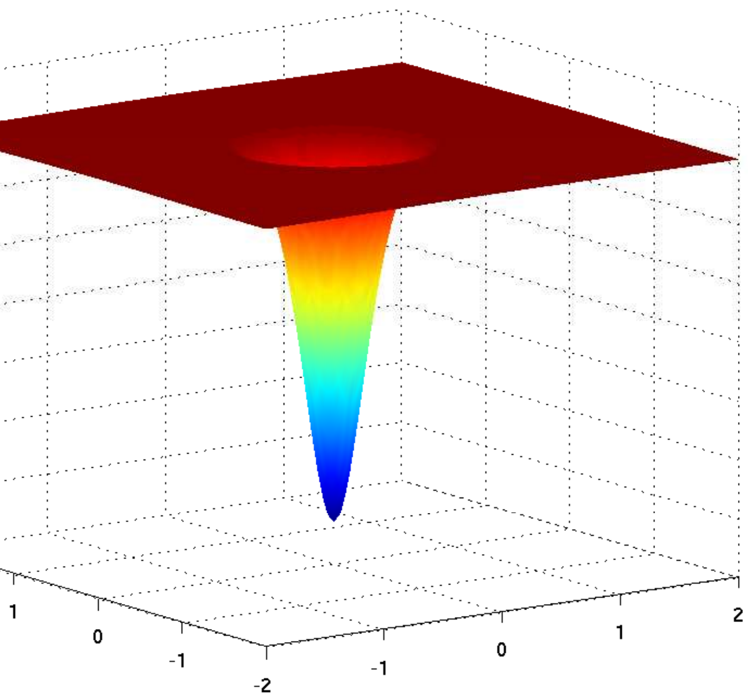
$$\frac{\partial u^0}{\partial y}(x,y) > b > 0 \quad in\ \mathbb{R}^2,$$

then there exists a positive constant C such that

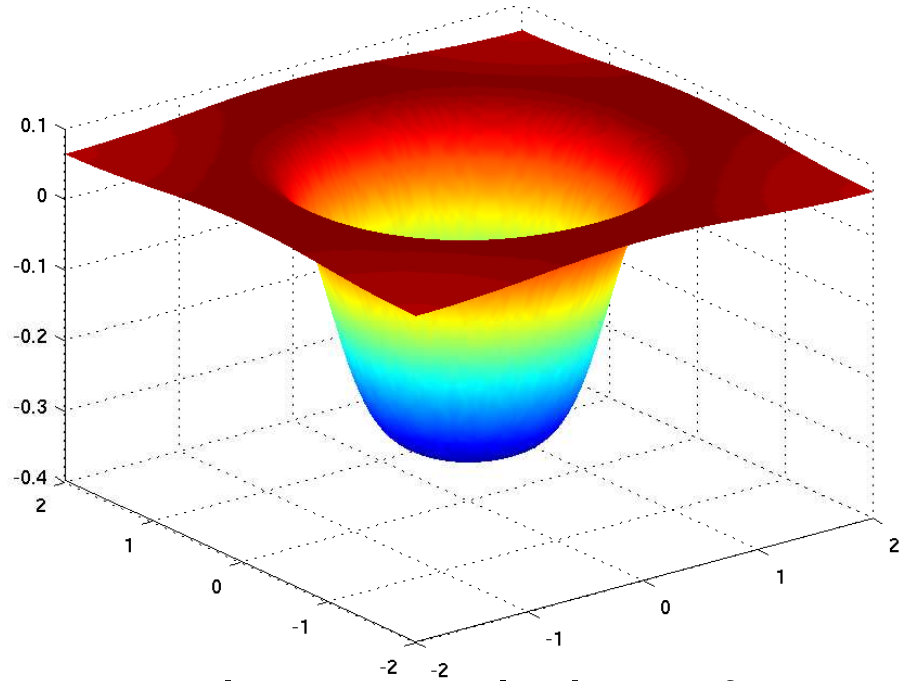
$$\sup_{i,j\in\mathbb{Z}} |u(x_i, y_j, n\Delta t) - v_{i,j}^n| \leq C\sqrt{\Delta t} \quad n = 1, ..., N_{T^*}$$

with $\Delta t \simeq \Delta x$.

Dislocations dynamics, Peierls-Nabarro model

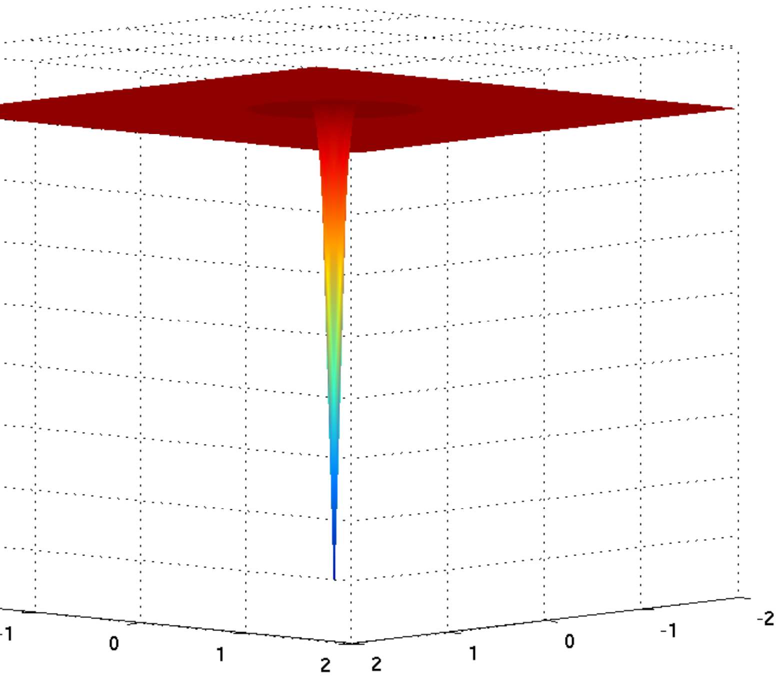


Kernel c_0 ($\nu = 0$,$\delta = 0.5$)

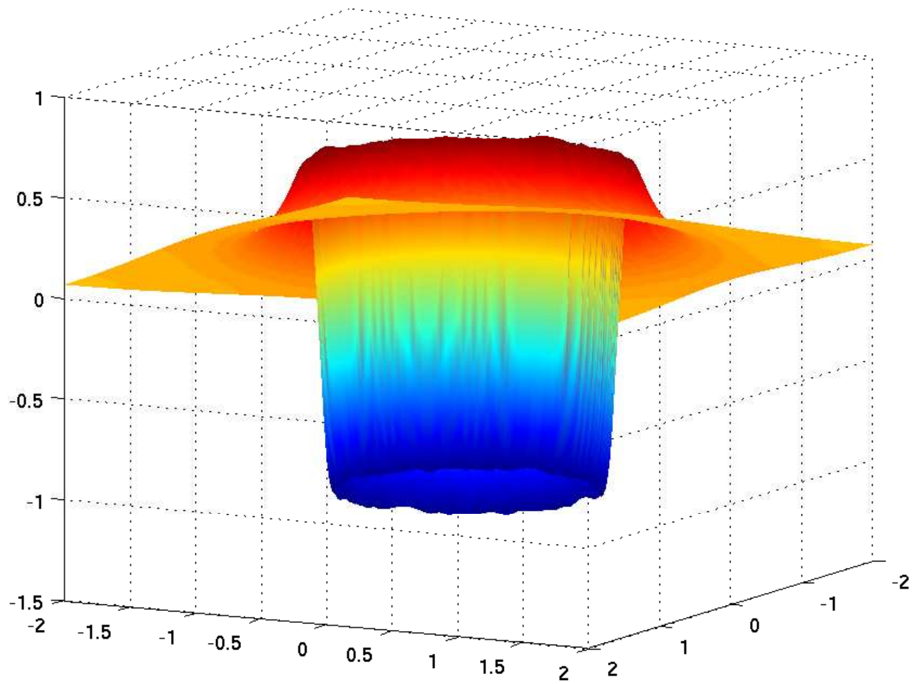


The convolution of c_0
by the characteristic function
of a circle

Dislocations dynamics, Peierls-Nabarro model

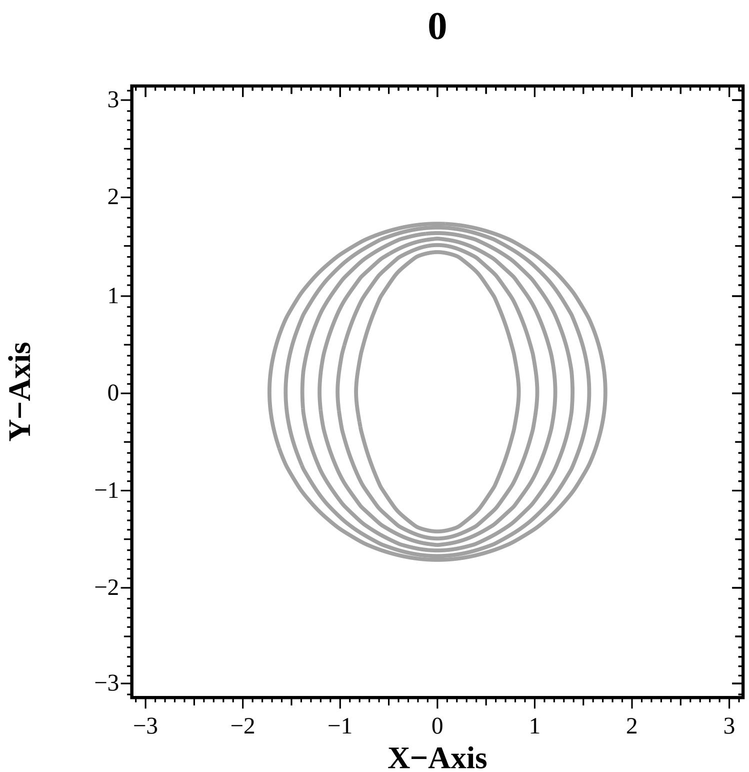


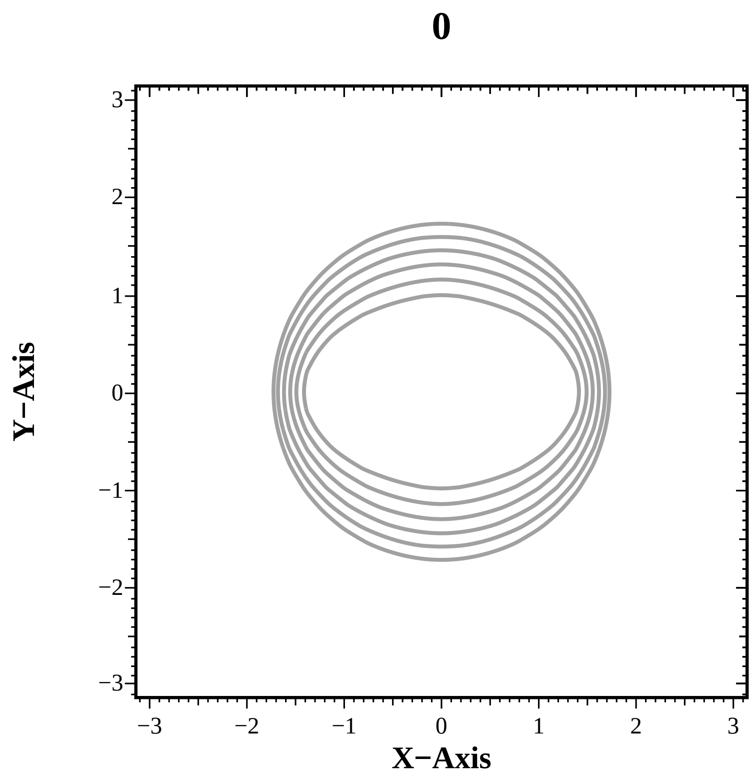
Kernel c_0 ($\nu = 0$,$\delta = 0.1$)



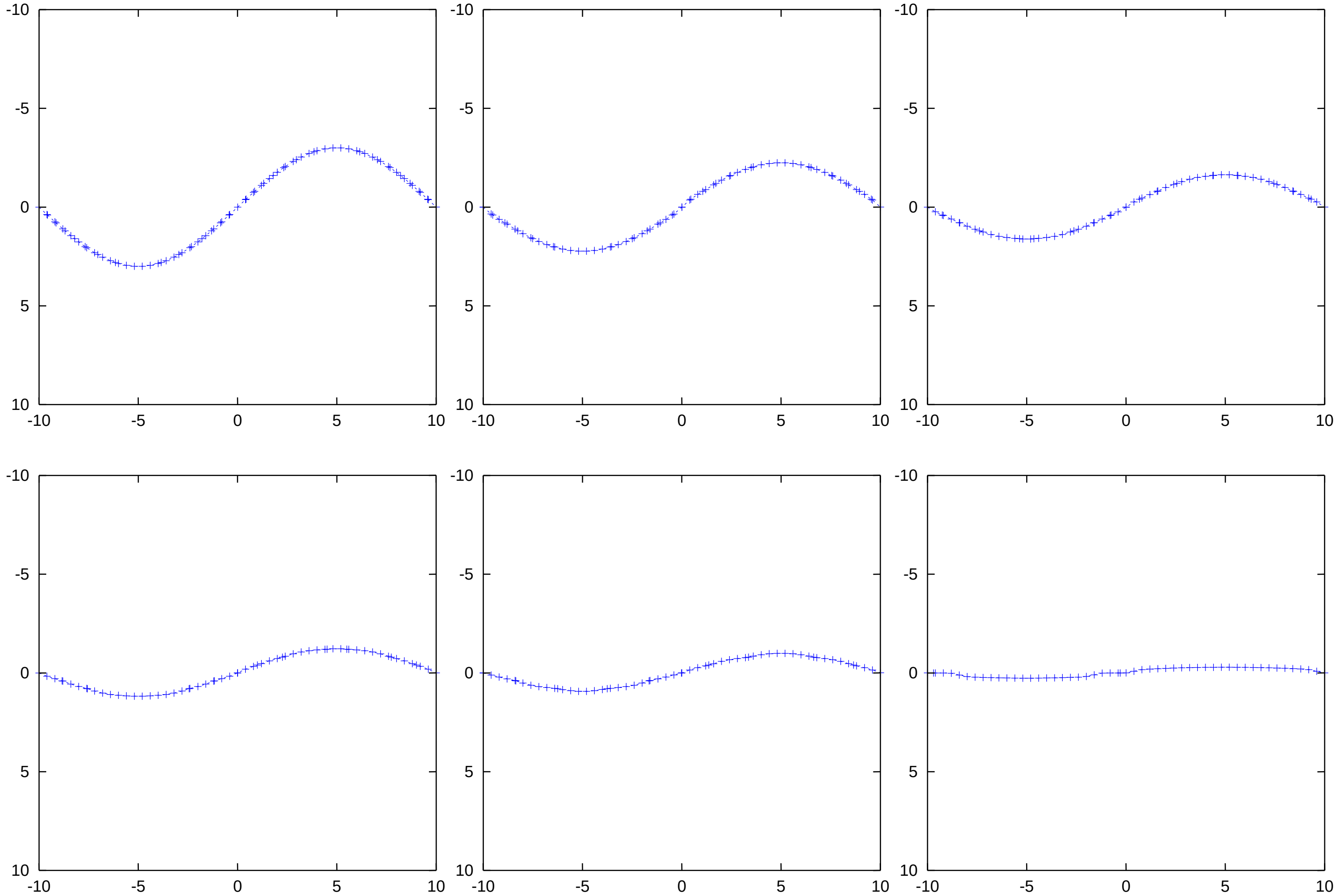
The convolution of c_0
by the characteristic function
of a circle

Numerical tests: Anisotropic Shrinking of a circle



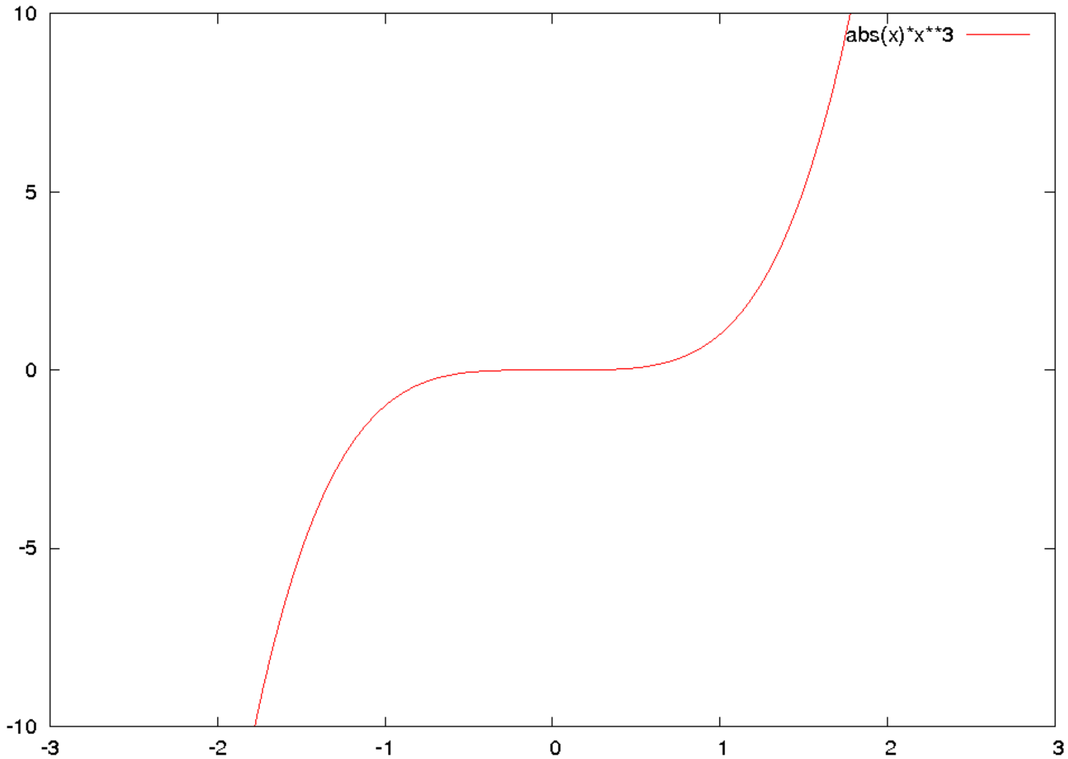


Numerical tests: Relaxation of a sinusoidal dislocation line



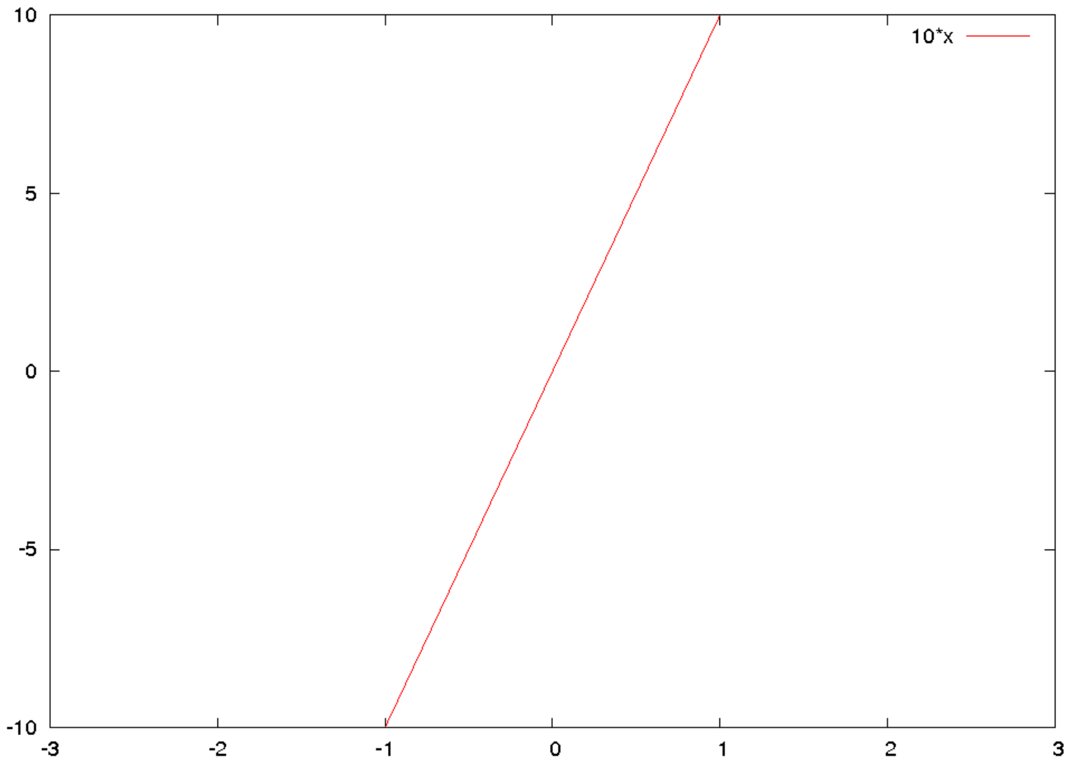
A numerical difficulty in the finite difference scheme

if we choose the size of the dislocation core δ such that $\delta \simeq \Delta x$, the gradient can get too small



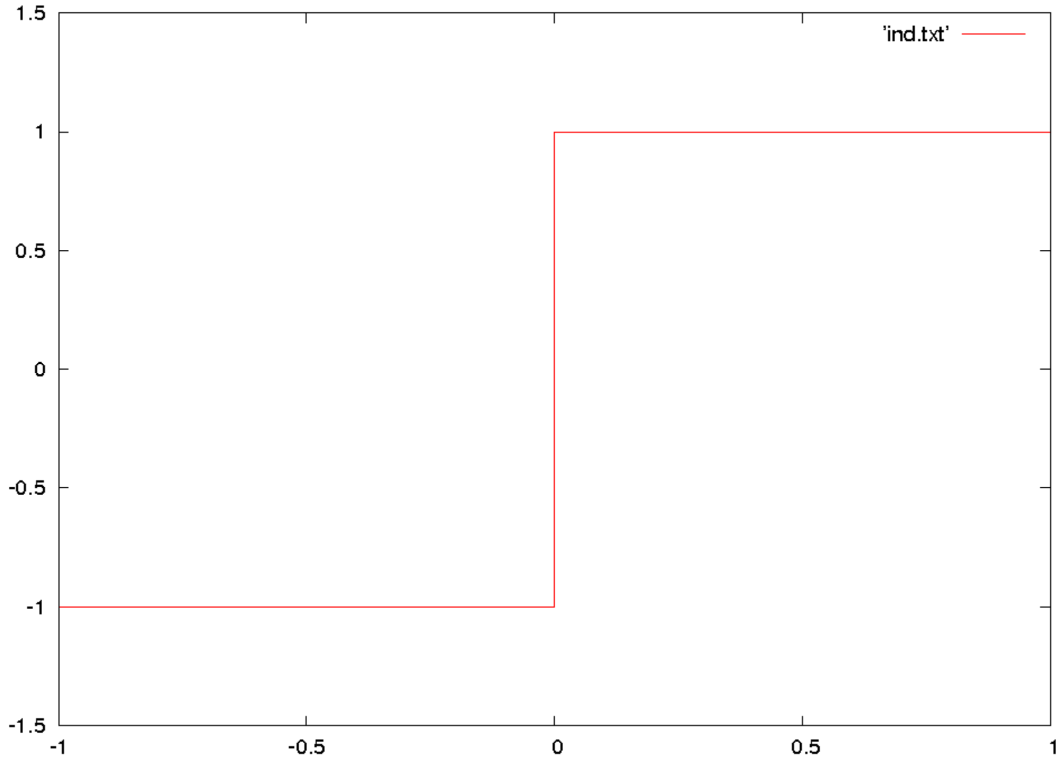
A numerical difficulty in the finite difference scheme

You need to reinitialize your representing function



A numerical difficulty in the finite difference scheme

We decide to use a different type of representation of the front



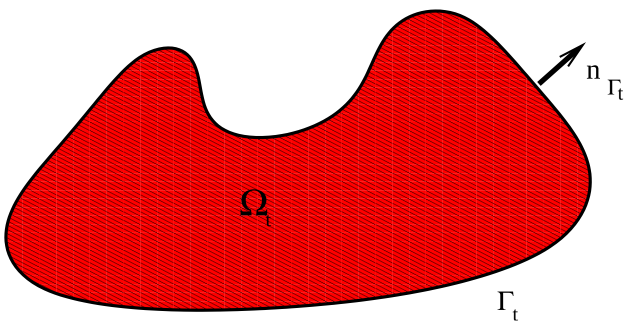
and apply different type of scheme:

the Fast Marching Method

Discontinuous solution

We assume that the dislocation line is represented by the boundary Γ_t of a smooth bounded domain $\Omega_t \subset \mathbb{R}^2$. We define

$$\theta(x,t) = \begin{cases} 1 & \text{if} \quad x \in \Omega_t, \\ -1 & \text{if} \quad x \notin \Omega_t. \end{cases}$$



$$\begin{cases} \theta_t = c(\theta, x, t)|D\theta| & \text{in} \quad \mathbb{R}^2 \times (0, +\infty), \\ \theta(x, 0) = \theta_0(x) & \text{on} \quad \mathbb{R}^2. \end{cases} \tag{2}$$

The present Fast Marching schemes

- $c(x, y) > 0$
  Fast Marching Method
  (Tsitsiklis ’95, Sethian ’96)
- $c(x, y) \geq 0$
  Semi-Lagrangian Fast Marching Methods
  (Falcone-Cristiani ’05)
- $c(x, y, t) > 0$

$$\begin{cases} c(x, y, T, \frac{\nabla T}{|\nabla T|})|\nabla T(x, y)| = 1 & \Omega \\ T(x, y) = q(x) & \partial\Omega \end{cases}$$

Ordered Upwind Method
(Sethian-Vladimirsky ’01)

GFMM for non monotone evolution

If the speed function is NOT always positive then the crossing time $T(x, y)$ is NOT single-valued function.
We introduce an auxiliary discrete function

$$\theta^n_{i,j} \simeq \theta(x_j, t_n)$$

and we approximate the evolutive front $\Gamma_t = \partial\Omega_t$ by the discontinuity of the field $\theta^n_{i,j}$

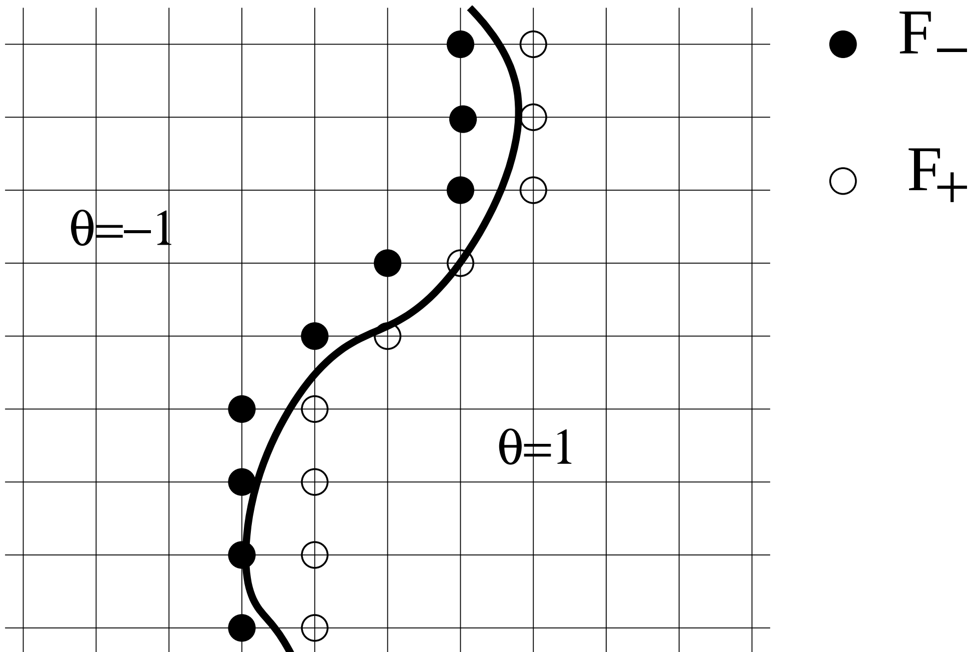
GFMM : non monotone evolution

Def. Given a field $\theta^n_{i,j}$ with values $+1$ and -1, we define the two phases

$$\Theta^n_\pm \equiv \{i,j\,:\,\theta^n_{i,j}=\pm 1\},$$

and the fronts

$$F^n_+ \equiv \partial\Theta^n_-, \qquad F^n_- \equiv \partial\Theta^n_+$$

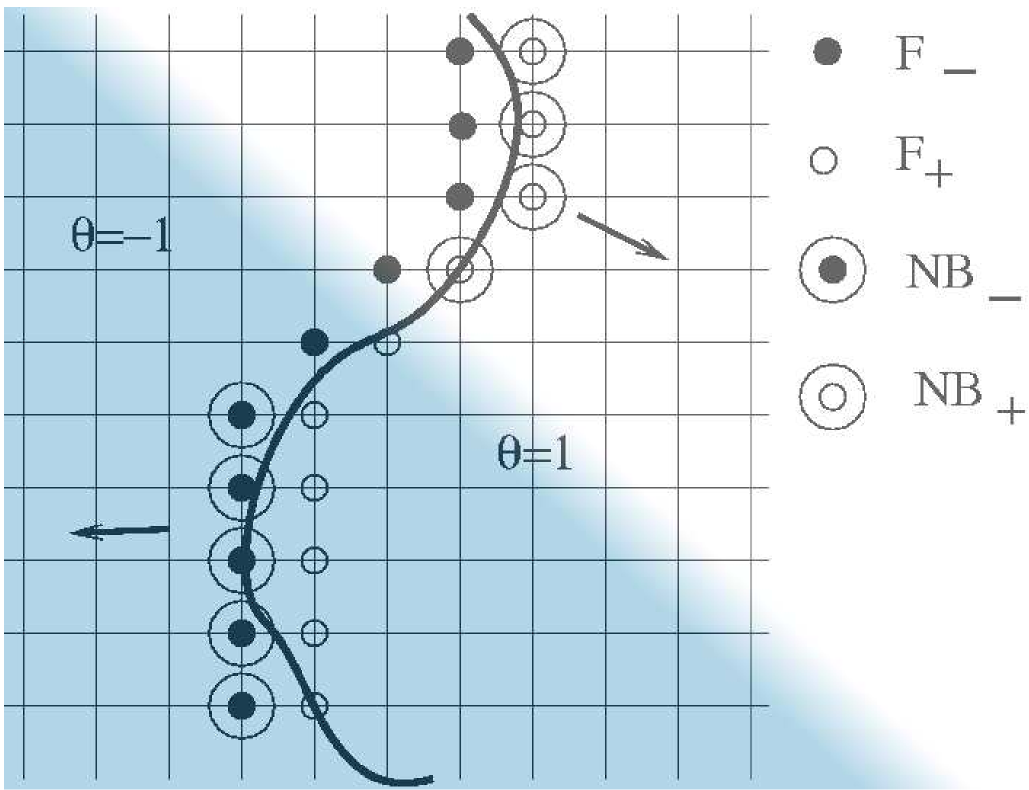


GFMM : non monotone evolution

We define two different **narrow bands**:

$$NB_+^n = F_+^n \cap \{(i,j), c_{i,j}^n < 0\}, \quad NB_-^n = F_-^n \cap \{(i,j), c_{i,j}^n > 0\}.$$

$$NB^n = NB_+^n \cap NB_-^n$$

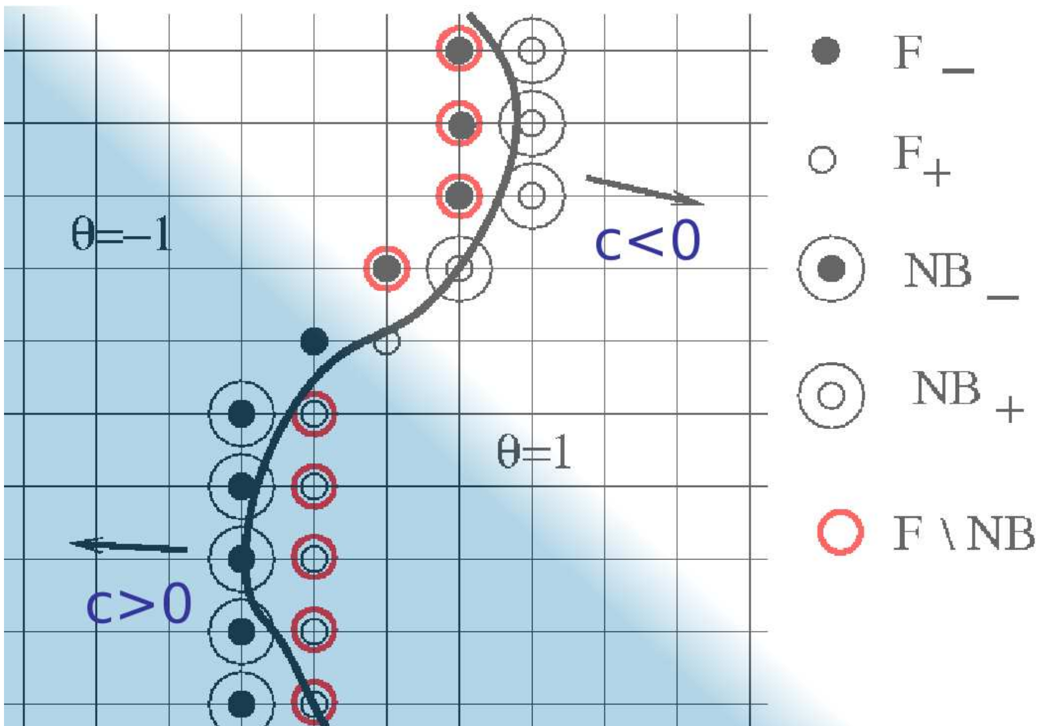


GFMM : non monotone evolution

If a node $(l,m) \in NB^n$ then we define the set of points useful for this node as

$$U^n(l,m) = \{(i,j) \text{s.t.} |(i,j)-(l,m)| = 1, \text{ and } \theta^n_{i,j} = -\theta^n_{l,m}\}$$

$$U^n = \bigcup_{(l,m)\in NB^n} U^n(l,m)$$



$\Rightarrow$ the nodes really used for the computation

GFMM : Initialisation

Initialisation

- *Initialisation of the matrix* θ^0

$$\theta^0_{i,j} = \begin{cases} 1 & (i,j) \in \Omega_0 \\ -1 & (i,j) \notin \Omega_0 \end{cases}$$

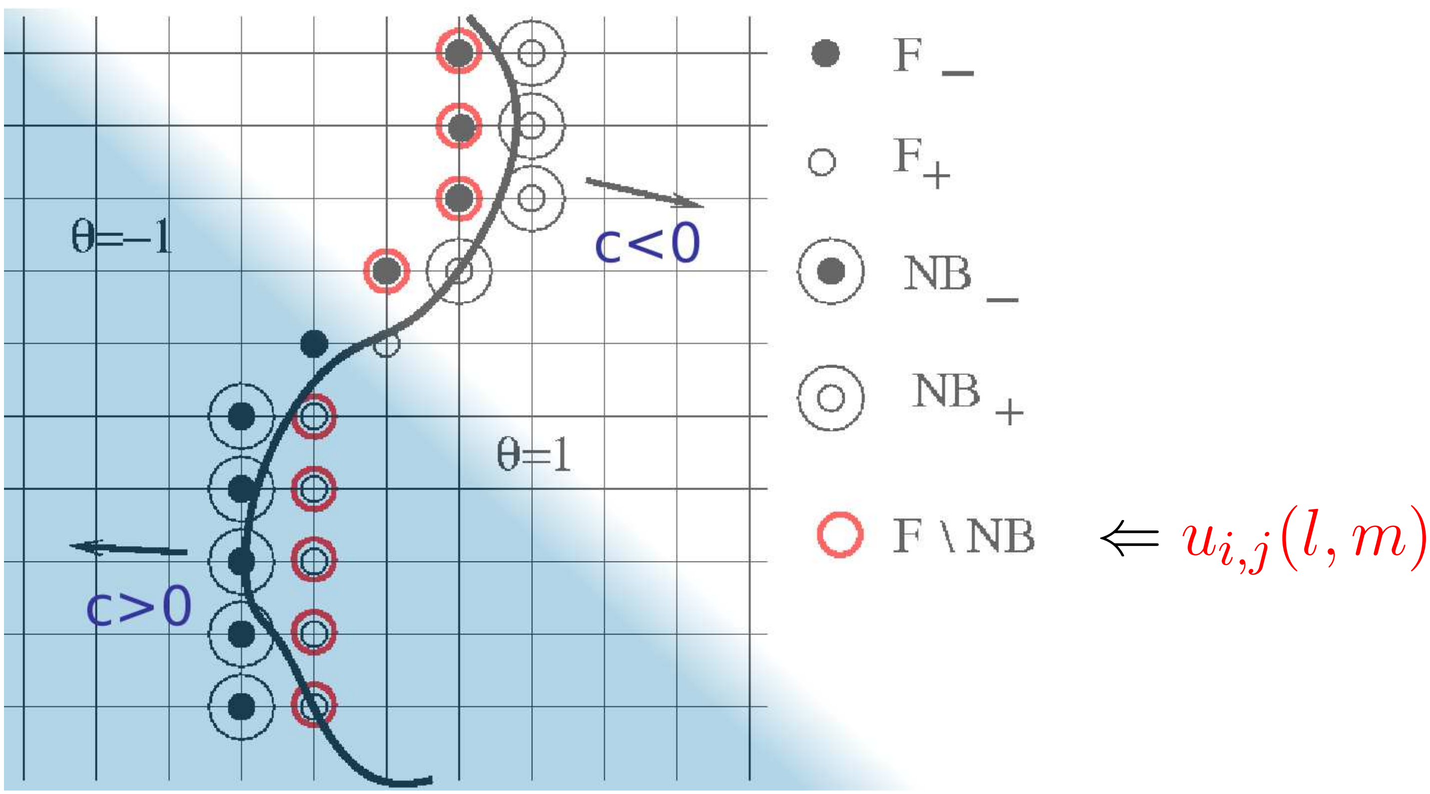
- *Initialisation of the time on the front*

$u^0_{i,j} = 0$ for all $(i,j) \in U^0$

GFMM : Main Cycle

- *Initialise of the useful time* U *everywhere on the grid*

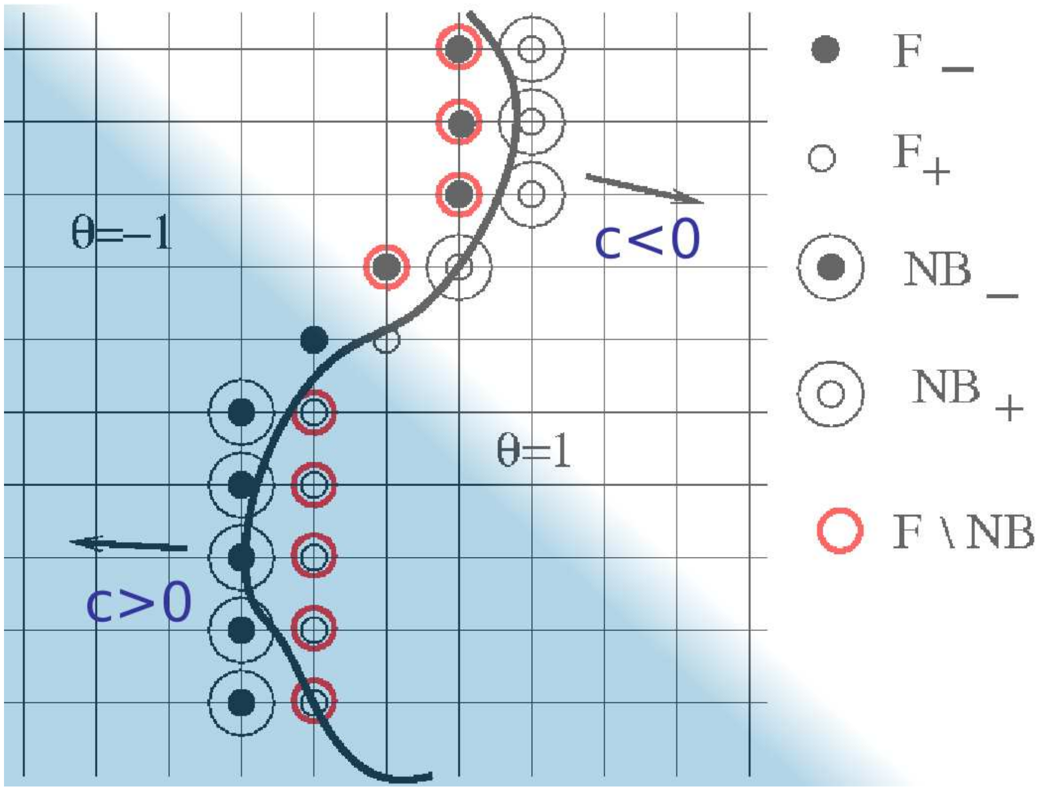
$$u_{i,j}(l,m) = \begin{cases} u_{i,j}^{n-1} & \text{for } (i,j) \in U^{n-1}(l,m) \\ \infty & \text{elsewhere.} \end{cases}$$



GFMM : Main Cycle

- *Compute* u^n *on* NB^{n-1}

$$\begin{array}{l}\max(0, u^n_{i,j} - u_{i-1,j}(i,j), u^n_{i,j} - u_{i+1,j}(i,j))^2 + \\ \max(0, u^n_{i,j} - u_{i,j+1}(i,j), u^n_{i,j} - u_{i,j-1}(i,j))^2\end{array} = \frac{(\Delta x)^2}{|c^{n-1}_{i,j}|^2}$$



NB _ $\Leftarrow u^n$

NB + $\Leftarrow u^n$

F \ NB $\Leftarrow u_{i,j}(l,m)$

GFMM : Main Cycle

- $t_n = \min \left\{ u^n_{i,j},\ (i,j) \in NB^{n-1} \right\}$.
- Initialisation of new accepted point
  $NA^n = \{(i,j) \in NB^{n-1},\ u^n_{i,j} = t_n\}$
- Re-initialisation of θ^n

$$\theta^n_{i,j} = \begin{cases} -1 & \text{if} \quad (i,j) \in NA^n \text{ and } \quad \theta^{n-1}_{i,j} = 1 \\ 1 & \text{if} \quad (i,j) \in NA^n \text{ and } \quad \theta^{n-1}_{i,j} = -1 \end{cases}$$

- Re-initialisation of u^n on U^n
  If $(i,j) \in U^{n-1}$ then $u^n_{i,j} = u^{n-1}_{i,j}$
  If $(i,j) \notin U^{n-1}$ then $u^n_{i,j} = t_n$

Non constant time step!

The time step $\Delta t_n = t_{n+1} - t_n$ is not constant and we can actually have:

1. $\Delta t_n >> 1$ too large time step
2. $\Delta t_n < 0$ not increasing time

To avoid case 1. we choose

$$\widehat{t_n} \equiv t_n + \Delta t$$

and to avoid case 2.

$$t_n = t_{n-1}.$$

Then one always gets

$$0 \leq \Delta t_n < \Delta t$$

If case 1) occurs: do not advance the front!

Some important modifications to the classical scheme

- We use a 'DOUBLE FRONT' (F_+) and (F_-), in order to be able to take into account the changes of sign of the velocity
- at each iterations the values of ALL the nodes in the NB are recomputed
- we introduce a time step Δt to avoid large jumps in time (it is not a CFL condition, small time steps are required for accuracy)
- we approximate the front by the discontinuity of a characteristic function
- when $c \geq 0$, our GFMM algorithm is the usual FMM algorithm

Convergence result

Theorem(C., Falcone, Forcadel, Monneau)

Let $c(x, y, t)$ be globally Lipschitz continuous in space and time, the initial set Ω_0 be with piece wise smooth boundary and $\theta^{\Delta}(x, y, t)$ be an appropriate extension of the discrete function $\theta^n_{i,j}$ over all the continuous space where $\Delta = (\Delta x, \Delta t)$,then

$$\overline{\theta}^0 = \limsup{}^* \theta^{\Delta}$$

(resp. $\underline{\theta}^0 = \liminf{}^* \theta^{\Delta}$) is a viscosity sub-solution (resp. super-solution) of the problem

$$\begin{cases} \theta_t = c(x, y, t)|\nabla\theta| & \mathbb{R}^2 \times (0, T) \\ \theta = 1_{\Omega_0} - 1_{\Omega_0^c} & \mathbb{R}^2. \end{cases}$$

Comparison Principle

Theorem (Forcadel)
For a slightly more complicated version of GFMM we have the following result:
Let two velocities c_u and c_v satisfy

$$\inf_{s\in[t,t+\Delta t]} c_v(x,s) \geq \sup_{s\in[t,t+\Delta t]} c_u(x,s).$$

Then

$$\theta_v^{\Delta}(x,0) \geq \theta_u^{\Delta}(x,0) \quad \Rightarrow \quad \theta_v^{\Delta}(x,t) \geq \theta_u^{\Delta}(x,t)$$

GFMM applied to dislocation dynamic

1. Initialisation

$$\theta^0_{i,j} = \begin{cases} 1 & \text{if} (i,j) \in \Omega \\ -1 & \text{if} \text{otherwise} \end{cases}$$

2. $\bar{t} = 0, \; n = 0$
   compute the speed $c^0_d \simeq c^0 \star \theta^0$
3. compute θ^n with the GFMM and speed c^n
4. if $t_n - \bar{t} > \Delta T$ compute $c^n_d \simeq c^0 \star \theta^n$
   otherwise return to 3

Convergence result for non-local dislocation dynamics

$$\begin{cases} \theta_t(x,t) = c[\theta](x,t)|D\theta(x,t)| \quad \text{on} \quad \mathbb{R}^N \times (0,T) \\ \theta(\cdot,0) = 1_{\Omega_0} - 1_{\Omega_0^c}. \end{cases} \quad (2)$$

$$c[\theta](x,t) = c_1(x,t) + (c_0 \star \theta(\cdot,t))(x).$$

Main assumptions:

(A1) Existence and uniqueness for problem (2)

(A2) Existence and uniqueness for the perturbed problem with $c^e(x,t) = c[\theta](x,t) + e$

(A3) Stability for the perturbed problem

$$|\theta^e - \theta|_{L^\infty((0,T);L^1(\mathbb{R}^N))} \leq CeT$$

Convergence result for non-local dislocation dynamics

Theorem (C., Forcadel, Monneau)
Under assumptions (A1)-(A2)-(A3).
Let $\theta^{\Delta}(x,t)$ be the solution of GFMM algorithm applied to problem (2) with discrete speed c^{Δ} defined by

$$c^{\Delta} = c[\theta^{\Delta}]$$

Then

$$\theta^{\Delta} \to \theta \quad L^{\infty}((0,T);L^{1}(\mathbb{R}^{N})).$$

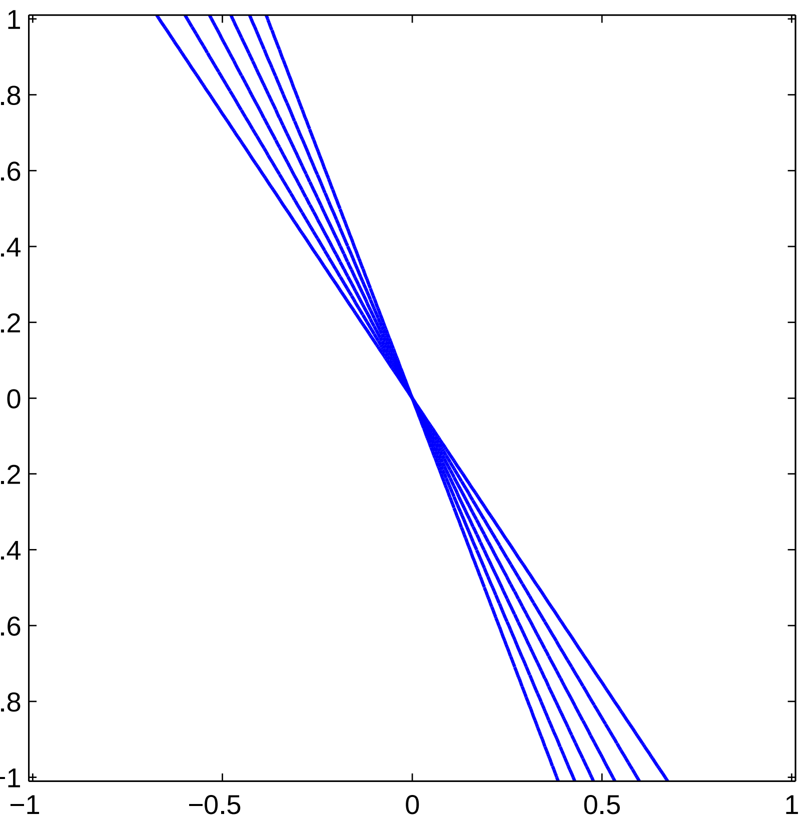
for T small enough.

Checking assumption

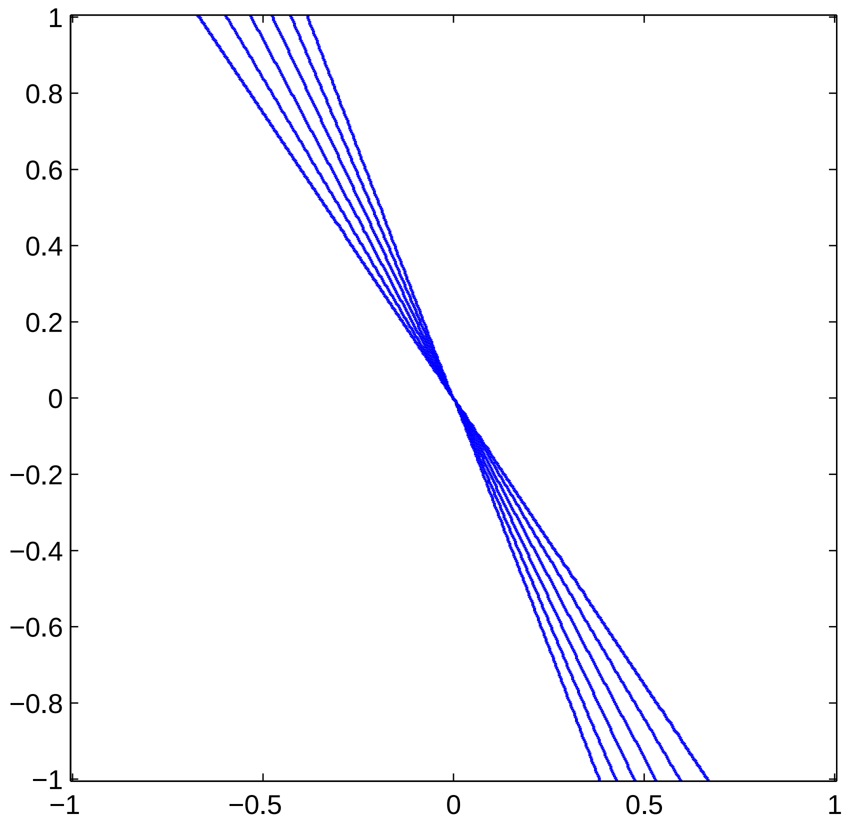
- If Ω_0 is C^3 and bounded and $\partial\Omega_0$ smooth enough and if $c_1 \in W^{1,\infty},\ c_0 \in W^{1,1} \cap L^\infty$ then (A1)-(A3) are verified for short time
(see Alvarez, Hoch, LeBouar, Monneau ’04).
- If dislocation dynamics has a non-negative velocity and the initial curve satisfies an *interior ball condition*, if $c_1 \in W^{2,\infty},\ c_0 \in W^{1,1} \cap L^1$ then (A1)-(A3) are verified for large time
(see Alvarez, Cardialiaguet, Monneau ’05).

Local dynamic: a rotating line

Speed: $c(x,t) = \sin(2\pi t)x_1$



FD



GFMM

Local dynamic a rotating line

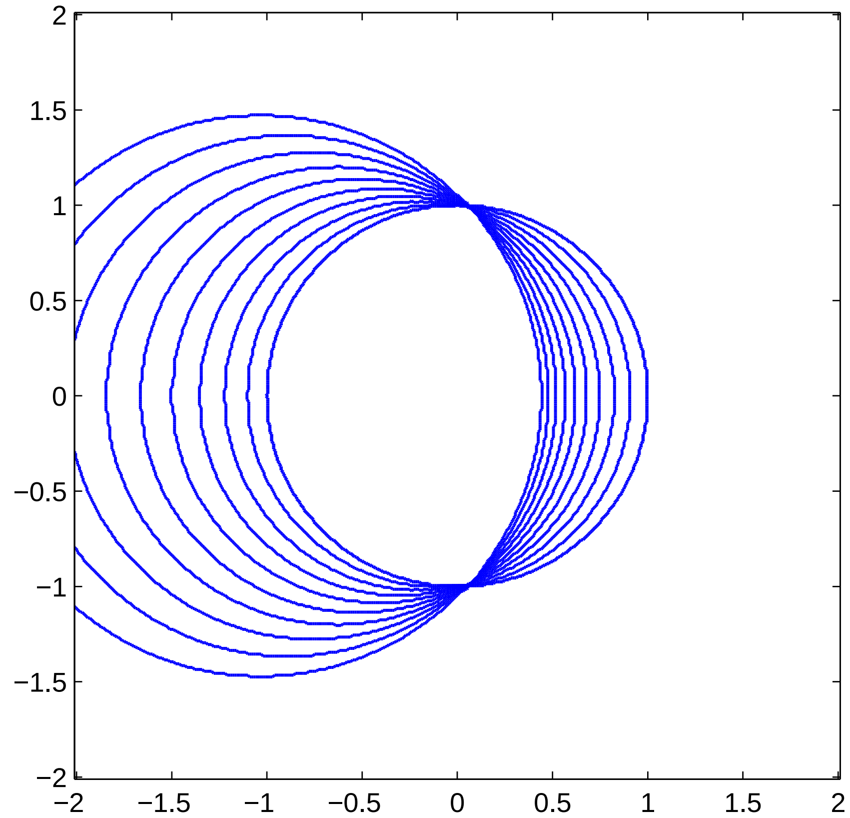
Speed: $c(x,t) = \sin(2\pi t)x_1$

	GFMM		**FD**	
Δx	$\mathcal{H}(\mathcal{C},\tilde{\mathcal{C}})$	CPU	$\mathcal{H}(\mathcal{C},\tilde{\mathcal{C}})$	CPU
0.04	$5.21 \cdot 10^{-2}$	$0.52s$	$4.82 \cdot 10^{-2}$	$1.82s$
0.02	$3.07 \cdot 10^{-2}$	$1.71s$	$2.46 \cdot 10^{-2}$	$13.3s$
0.01	$1.54 \cdot 10^{-2}$	$10.5s$	$1.35 \cdot 10^{-2}$	$102s$
0.005	$9.00 \cdot 10^{-3}$	$130s$	$7.00 \cdot 10^{-3}$	$842s$

Local dynamic a rotating line

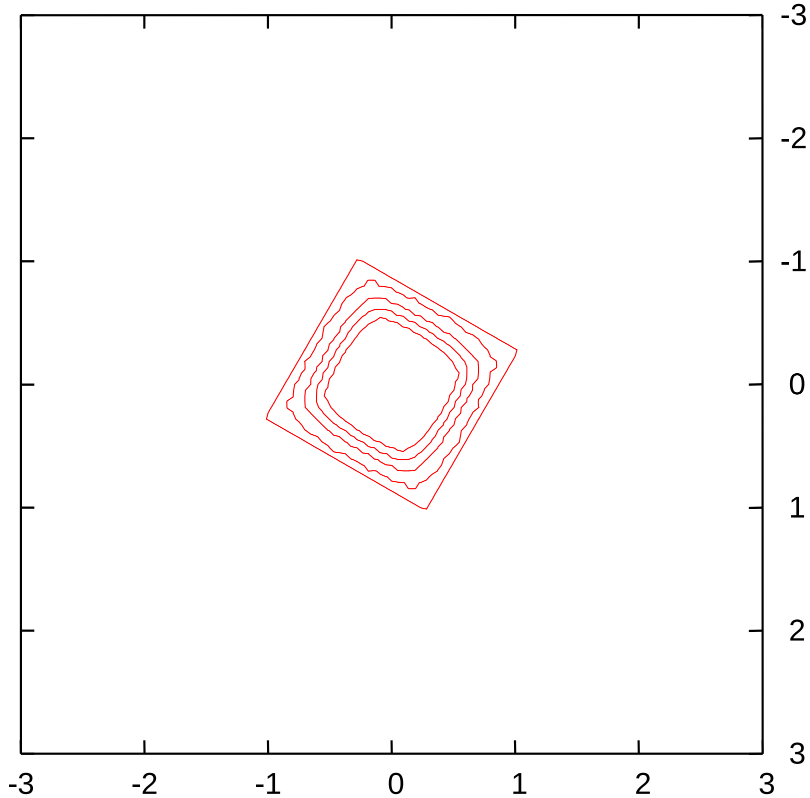
Speed: $c(x,t) = 0.1t - x_1$

Δx	$\mathcal{H}(\mathcal{C}, \tilde{\mathcal{C}})$
0.08	$8.52 \cdot 10^{-1}$
0.04	$4.42 \cdot 10^{-2}$
0.02	$2.41 \cdot 10^{-2}$
0.01	$1.24 \cdot 10^{-2}$

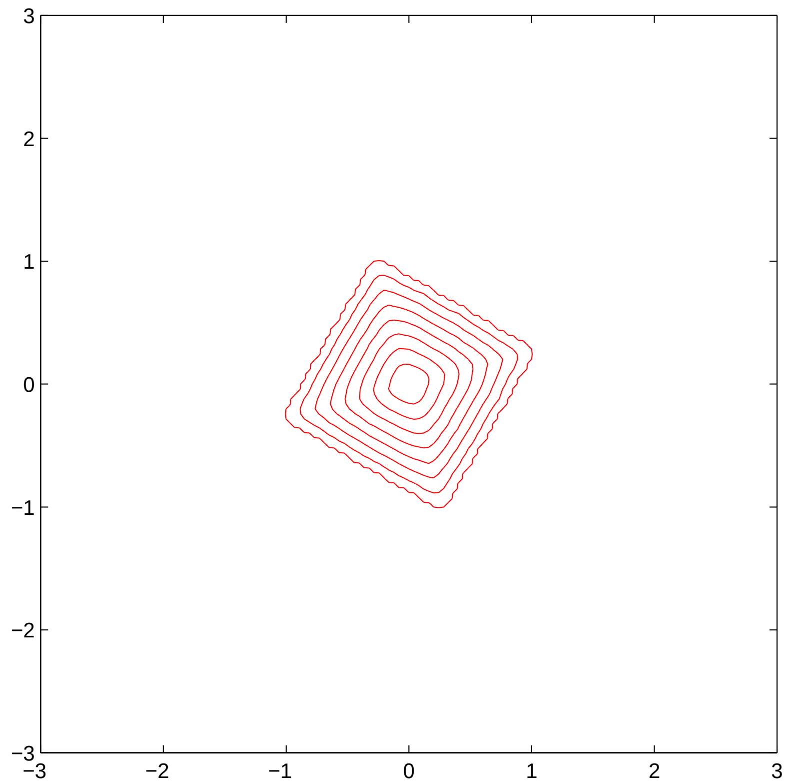


Non local Dynamics:Finite Difference versus GFMM

Non local Dynamics:Finite Difference versus GFMM



FD

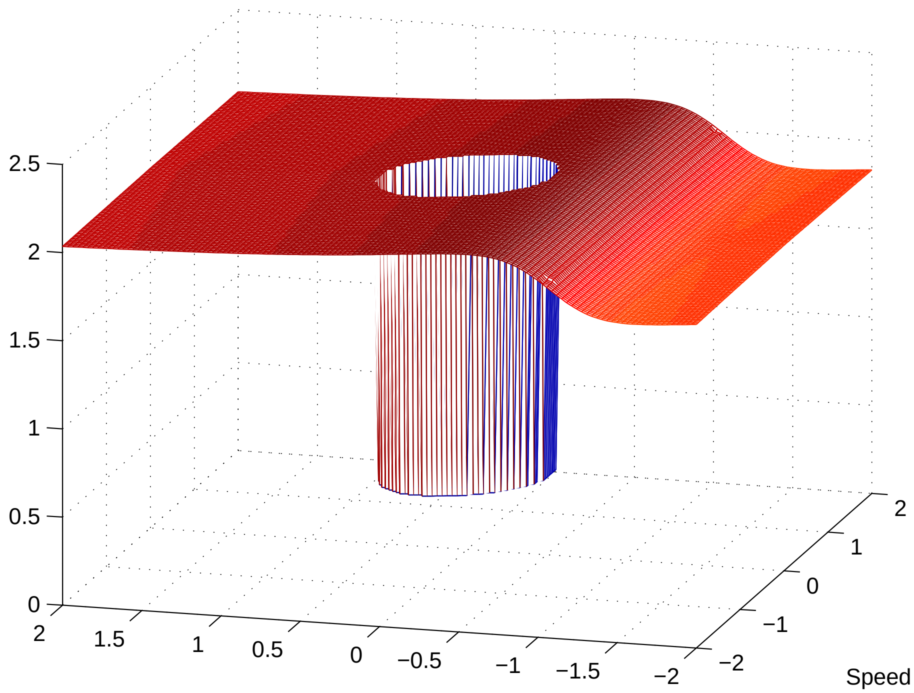


GFMM

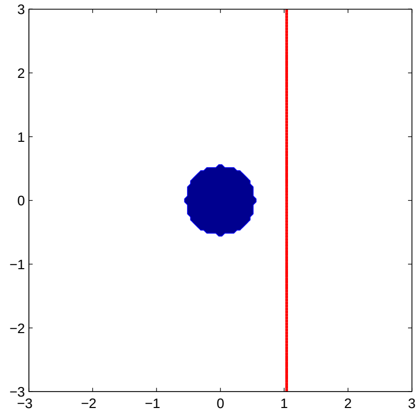
Non local dynamics: Propagation with external constraint

$$c(x,t) = (c^0_\delta \star \theta(\cdot,t))(x) + c^1(x,t)$$

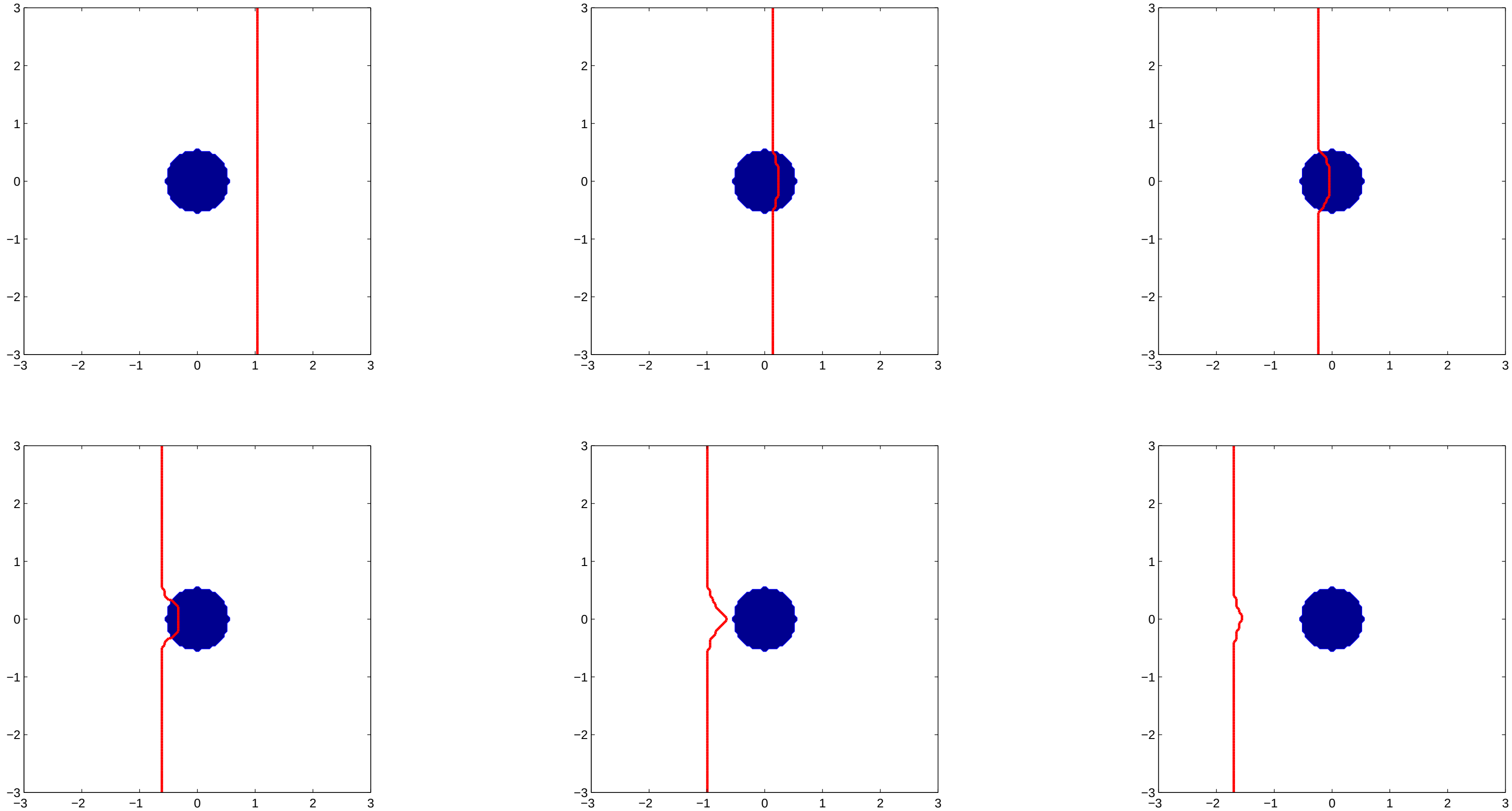
$$c^1(x,t) = \begin{cases} \alpha & \text{if } |x|^2 < 0.3 \\ 2 & \text{otherwise.} \end{cases}$$



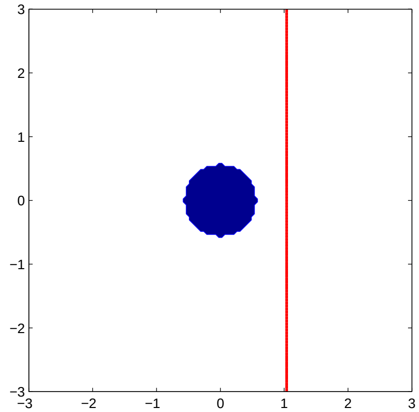
Propagation with external constraint, case $\alpha = 1.5$



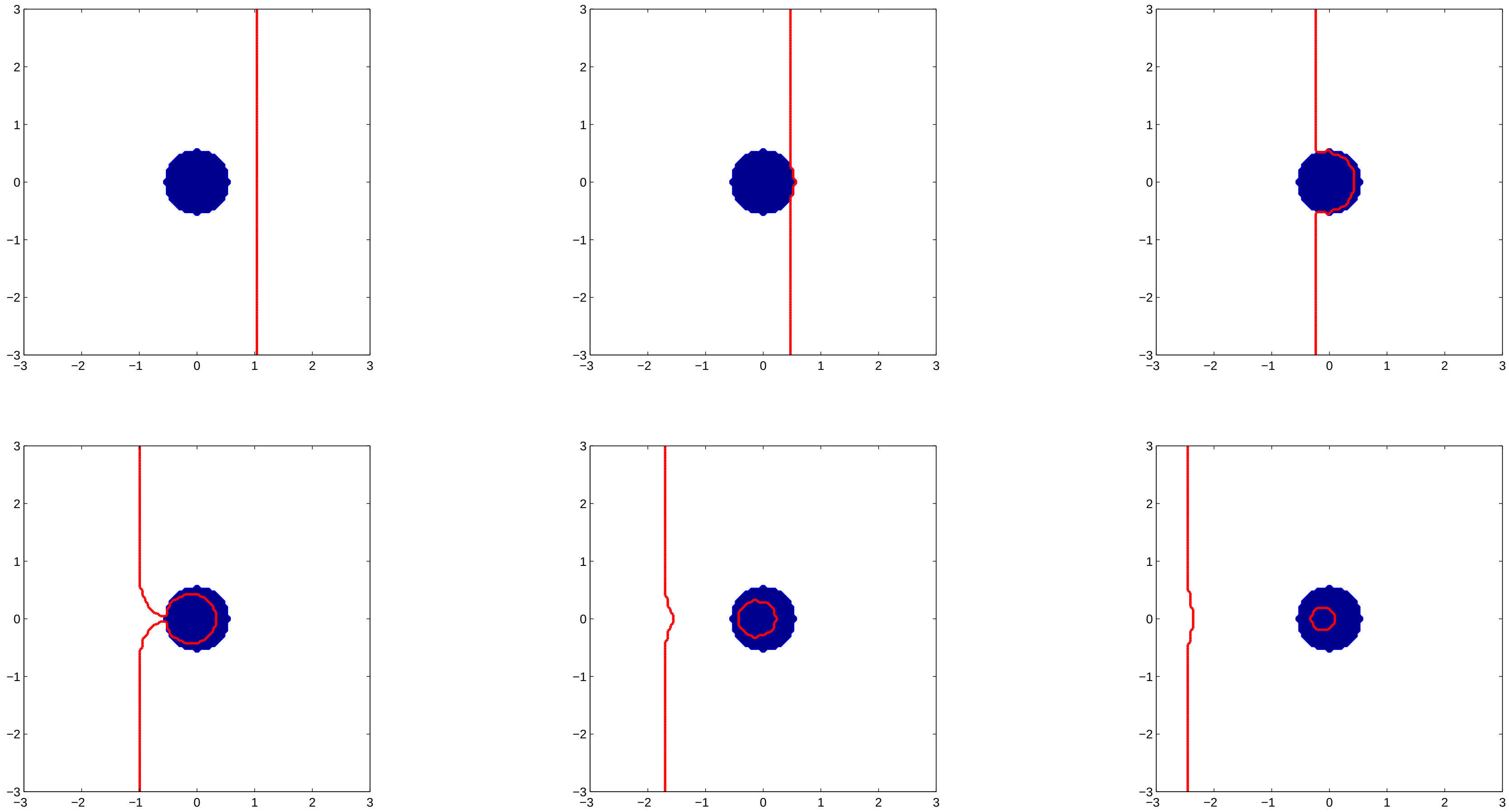
The line passes over the obstacle



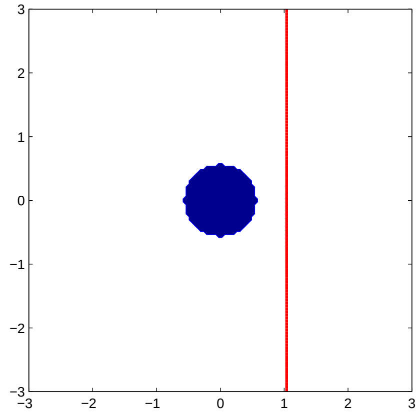
Propagation with external constraint, case $\alpha = 0.5$



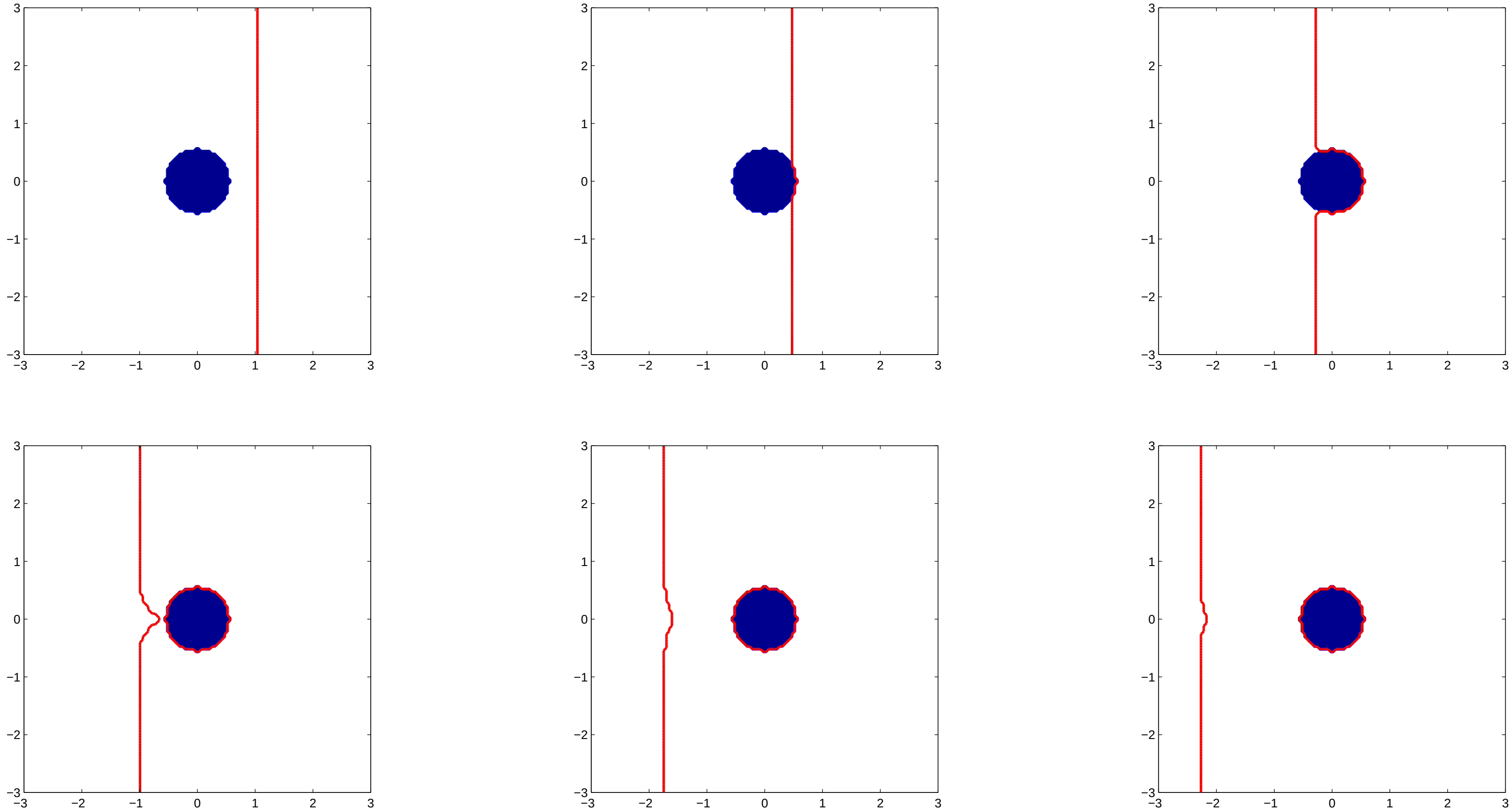
The obstacle breaks the line



Propagation with external constraint, case $\alpha = -0.5$



The obstacle capture the line



Future works

- Extensions to triangular meshes
- Different type of solver (Semi-Lagrangian, Weno,...)
- extend the numerical analysis to the model with the mean curvature term

Open problems

- extension to 3d dislocation curve's dynamic
- open curves
- more dislocations curves

References

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