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DIRECT APPROACH TO MEAN-CURVATURE FLOW WITH TOPOLOGICAL CHANGES

PETR PAUŠ AND MICHAL BENEŠ

This contribution deals with the numerical simulation of dislocation dynamics. Dislocations are described by means of the evolution of a family of closed or open smooth curves $\Gamma(t) : S \rightarrow \mathbb{R}^2$, $t \geq 0$. The curves are driven by the normal velocity v which is the function of curvature κ and the position. The evolution law reads as: $v = -\kappa + F$. The motion law is treated using direct approach numerically solved by two schemes, i. e., backward Euler semi-implicit and semi-discrete method of lines. Numerical stability is improved by tangential redistribution of curve points which allows long time computations and better accuracy. The results of dislocation dynamics simulation are presented (e. g., dislocations in channel or Frank–Read source). We also introduce an algorithm for treatment of topological changes in the evolving curve.

Keywords: mean curvature flow, dislocation dynamics, parametric approach

AMS Subject Classification: 35L65, 76M12, 80A20

1. INTRODUCTION

In the field of material science, the dislocations are defined as irregularities or errors in crystal structure of the material. The presence of dislocations strongly influences many of material properties. This justifies the importance of developing suitable physical [8, 14] and mathematical models [13]. From the mathematical point of view, the dislocations are defined as smooth closed or open plane curves which evolve in time. They are located in a plain called slip plane. Their motion therefore is two-dimensional.

The evolving curves can be mathematically described in several ways. One possibility is to use the *level-set method* [5, 7, 15, 16, 20], where the curve is defined by the zero level of some surface function. One can also use the *phase-field method* [3]. Finally, it is possible to use the *direct (parametric) method* [6, 10] where the curve is parametrized in the usual way. This article discusses the direct approach.

2. PARAMETRIC DESCRIPTION

When using the parametric approach, the planar curve $\Gamma(t)$ is described by a smooth time-dependent vector function

$$X : S \times I \rightarrow \mathbb{R}^2,$$

where $S = \langle 0, 1 \rangle$ is a fixed interval for the curve parameter and $I = \langle 0, T \rangle$ is the time interval. The curve $\Gamma(t)$ is then given as the set

$$\Gamma(t) = \{X(u, t) = (X^1(u, t), X^2(u, t)), u \in S\}.$$

The family of curves satisfies the equation of motion

$$v = -\kappa + F, \tag{1}$$

where v is the normal velocity of the curve evolution, κ is the curvature, and F is the forcing term which can depend on position vector x and time t .

The evolution law (1) is transformed into the parametric form. The unit tangential vector \vec{T} is defined as $\vec{T} = \partial_u X / |\partial_u X|$. The unit normal vector \vec{N} is perpendicular to the tangential vector and $\vec{N} \cdot \vec{T} = 0$ holds. In case of closed curve, \vec{N} is the outer vector to the interior of the curve. In case of open curve, \vec{N} has a selected, pre-defined direction (e.g., upwards). The orientation of the curve is clockwise. The curvature κ is expressed as

$$-\kappa = \frac{\partial_u X^\perp}{|\partial_u X|} \cdot \frac{\partial_{uu} X}{|\partial_u X|^2} = \vec{N} \cdot \frac{\partial_{uu} X}{|\partial_u X|^2},$$

where X^\perp is a vector perpendicular to X . The normal velocity v is defined as the time derivative of X projected into the normal direction,

$$v = \partial_t X \cdot \frac{\partial_u X^\perp}{|\partial_u X|}.$$

The equation (1) can now be written as

$$\partial_t X \cdot \frac{\partial_u X^\perp}{|\partial_u X|} = \frac{\partial_{uu} X}{|\partial_u X|^2} \cdot \frac{\partial_u X^\perp}{|\partial_u X|} + F(X, t),$$

which holds provided

$$\partial_t X = \frac{\partial_{uu} X}{|\partial_u X|^2} + F(X, t) \frac{\partial_u X^\perp}{|\partial_u X|}. \tag{2}$$

This equation is accompanied by the periodic boundary conditions for closed curves, or by fixed-end boundary condition for open curves, and by the initial condition. These conditions are considered similarly as in [6]. The solution of (2) exhibits a natural redistribution property which is useful for short-time curve evolution [9, 17]. The redistribution of curve discretization points is operated by tangential forces discussed below.

The term $\partial_{uu}X/|\partial_u X|^2$ in (2) contains a tangential component which makes the curve points to move along the curve. To modify or cancel this tangential force, a term α in the tangential direction can be considered as follows

$$\partial_t X = \frac{\partial_{uu}X}{|\partial_u X|^2} - \alpha \frac{\partial_u X}{|\partial_u X|} + F(X, t) \frac{\partial_u X^\perp}{|\partial_u X|}. \tag{3}$$

Consequently, one can derive an equation without a tangential force. Consider the expression

$$\frac{1}{|\partial_u X|} \partial_u \left(\frac{\partial_u X}{|\partial_u X|} \right).$$

Here

$$\partial_u \left(\frac{\partial_u X}{|\partial_u X|} \right) = \frac{\partial_{uu}X(|\partial_u X|) - \partial_u X \partial_u |\partial_u X|}{|\partial_u X|^2},$$

with

$$\partial_u (|\partial_u X|) = \partial_u \sqrt{\partial_u X \cdot \partial_u X} = \frac{\partial_u X \cdot \partial_{uu}X}{|\partial_u X|}.$$

Then

$$\partial_u \left(\frac{\partial_u X}{|\partial_u X|} \right) = \frac{(\partial_u X)^2 \partial_{uu}X - (\partial_u X \cdot \partial_{uu}X) \partial_u X}{|\partial_u X|^3}.$$

Therefore, we have

$$\begin{aligned} \frac{1}{|\partial_u X|} \partial_u \left(\frac{\partial_u X}{|\partial_u X|} \right) &= \frac{|\partial_u X|^2 \partial_{uu}X - (\partial_u X \cdot \partial_{uu}X) \partial_u X}{|\partial_u X|^4} \\ &= \frac{\partial_{uu}X}{|\partial_u X|^2} - \frac{\partial_u X \cdot \partial_{uu}X}{|\partial_u X|^4} \partial_u X. \end{aligned}$$

Hence the tangential term contained in equation (3) has the form

$$\alpha = \frac{\partial_{uu}X \cdot \partial_u X}{|\partial_u X|^3}. \tag{4}$$

Then the equation without a tangential force has the following form:

$$\partial_t X = \frac{\partial_{uu}X}{|\partial_u X|^2} - \frac{\partial_{uu}X \cdot \partial_u X}{|\partial_u X|^4} \partial_u X + F(X, t) \frac{\partial_u X^\perp}{|\partial_u X|}. \tag{5}$$

This equation is not suitable for numerical simulations because the curve points do not move along the curve and can accumulate in some parts or move from each other in other parts of the curve. This can cause a slow-down in computation. The equation (2) is better for numerical simulations but still for long time simulations similar accumulation of points can happen. Additional algorithm for tangential redistribution of points has to be considered.

For long time computations with time and space variable external force $F(X, t)$, the algorithm for curvature adjusted tangential velocity is used. This algorithm moves points along the curve according to the curvature, i. e., areas with higher curvature contain more points than areas with lower curvature. This improves numerical stability and also accuracy of computation. Unlike the case with no tangential force (Eq. 5), the term α is not given by a simple formula but it is based on the relative local length between points. Details are described in [21]. Another approach based on finite-element discretization of equations for curve parametrization is in [2], where existing multiple junctions are treated as well.

3. NUMERICAL SCHEME

For numerical approximation we consider a regularized form of (3) which reads as

$$\partial_t X = \frac{\partial_{uu} X}{Q(\partial_u X)^2} - \alpha \frac{\partial_u X}{Q(\partial_u X)} + F(X, t) \frac{\partial_u X^\perp}{Q(\partial_u X)}, \tag{6}$$

where $Q(x_1, x_2) = \sqrt{x_1^2 + x_2^2 + \varepsilon^2}$ with ε being a small parameter. Two numerical schemes are used for numerical solution of the differential equation (3), i. e., backward Euler semi-implicit and semi-discrete method of lines. With two numerical schemes it is possible to compare the solution and error of computation.

In the semi-discrete scheme of method of lines, spatial derivatives are approximated by fourth-order central differences. The first derivative is approximated as

$$\partial_u X|_{u=jh} \approx \left[\frac{X_{j-2}^1 - 8X_{j-1}^1 + 8X_{j+1}^1 - X_{j+2}^1}{12h}, \frac{X_{j-2}^2 - 8X_{j-1}^2 + 8X_{j+1}^2 - X_{j+2}^2}{12h} \right],$$

and the second one as

$$\partial_{uu} X|_{u=jh} \approx \left[\frac{-X_{j-2}^1 + 16X_{j-1}^1 - 30X_j^1 + 16X_{j+1}^1 - X_{j+2}^1}{12h^2}, \frac{-X_{j-2}^2 + 16X_{j-1}^2 - 30X_j^2 + 16X_{j+1}^2 - X_{j+2}^2}{12h^2} \right],$$

where X_j^i denotes an approximation of $X^i(jh, \cdot)$, $i \in \{1, 2\}$, $h = 1/m$. Here m is a number of intervals dividing S . The difference expressions above are denoted as X_u for the first difference and X_{uu} for the second difference.

The equation (6) in the semi-discrete scheme of method of lines has the following form:

$$\frac{dX_j}{dt} = \frac{X_{uu,j}}{Q^2(X_{u,j})} - \alpha_j \frac{X_{u,j}}{Q(X_{u,j})} + F(X_j, t) \frac{X_{u,j}^\perp}{Q(X_{u,j})}, \tag{7}$$

$j = 1, \dots, m - 1, t \in (0, T)$

where again $Q(x_1, x_2) = \sqrt{x_1^2 + x_2^2 + \varepsilon^2}$, $X_{u,j}^\perp$ is a vector perpendicular to $X_{u,j}$, and α_j is the redistribution coefficient. The term with ε serves as a regularization to

avoid singularities when the curvature tends to infinity. This scheme is solved by the fourth order Runge–Kutta method [4, 15].

The second approach uses the backward Euler semi-implicit scheme. In this case lower order differences are used. The first derivative is discretized by the backward difference as follows

$$\partial_u X|_{u=jh} \approx \left[\frac{X_j^1 - X_{j-1}^1}{h}, \frac{X_j^2 - X_{j-1}^2}{h} \right],$$

and the second derivative as

$$\partial_{uu} X|_{u=jh} \approx \left[\frac{X_{j+1}^1 - 2X_j^1 + X_{j-1}^1}{h^2}, \frac{X_{j+1}^2 - 2X_j^2 + X_{j-1}^2}{h^2} \right].$$

The approximation of the first derivative is denoted as $X_{\bar{u},j}$ and of the second derivative as $X_{\bar{u}\bar{u},j}$.

The semi-implicit scheme for equation (3) has the following form

$$X_j^{k+1} - \tau \frac{X_{\bar{u}\bar{u},j}^{k+1}}{Q^2(X_{\bar{u},j}^k)} + \tau \alpha_j \frac{X_{\bar{u},j}^{k+1}}{Q(X_{\bar{u},j}^k)} = X_j^k + \tau F(X_j^k, k\tau) \frac{X_{\bar{u},j}^{\perp k}}{Q(X_{\bar{u},j}^k)},$$

$$j = 1, \dots, m - 1, k = 0, \dots, N_T - 1, \quad (8)$$

where $Q(x_1, x_2)$, $X_{\bar{u},j}^\perp$, m , and α_j have the same meaning as for semi-discrete scheme. $X_j^k \approx X(jh, k\tau)$, τ is a time step and N_T is the number of time steps. The matrix of the system (8) for each component of X^{k+1} has the following tridiagonal structure:

$$\begin{pmatrix} 1 + \frac{2\tau}{h^2 Q^2} - \frac{\tau \alpha}{h Q} & \frac{-\tau}{h^2 Q^2} & 0 & \dots \\ \frac{-\tau}{h^2 Q^2} + \frac{\tau \alpha}{h Q} & \ddots & \ddots & \ddots \\ 0 & \ddots & \ddots & \ddots \\ \vdots & \ddots & \ddots & \ddots \end{pmatrix}.$$

The scheme (8) is solved for each k by means of matrix factorization. Since there are two components of X , two linear systems are solved in each timestep.

4. TOPOLOGICAL CHANGES

In curve dynamics in general, and in dislocation dynamics in particular, topological changes may occur (e.g., connecting or splitting, closing of open curves, etc.). The parametric approach does not handle them intrinsically, and we therefore need an additional algorithm allowing for such changes of discretized curves.

The algorithm we present is not supposed to be universal for every situation and possibility. Main purpose is to simulate topological changes that can happen during dislocation dynamics (see [18]), i.e., topological changes such as merging or splitting of curves, closing of open curves, etc. As the initial condition, we consider only curves

which do not intersect itself and do not touch each other. The orientation of curves is clockwise. The algorithm is designed for topological changes of curves which touch only at one point. More complex changes can be treated by multiple application of the algorithm in one timestep. The evolution after merging or splitting behaves as expected. Normal vectors and evolution speed correspond to the situation captured by the level-set method. The results of the algorithm were compared with the level-set method in [19].

Let us consider two closed or open curve parametrizations discretized as $X = \{x_1, x_2, \dots, x_n\}$ and $Y = \{y_1, y_2, \dots, y_m\}$ in \mathbb{R}^2 . Curves evolve independently according to the equation (3). The algorithm for merging two curves is as follows:

1. Compute the distance between X and Y and find one point from each curve where the minimum is reached. Let us denote the distance as d , the point from X as x_{\max} and from Y as y_{\max} .
2. Check if the distance d between curves is smaller than a given tolerance δ . If not, compute new timestep and go to 1.
3. Create new empty curve Z . We must take into account the type of merged curves. Merging two closed curves will produce one closed curve. Merging one open and one closed curve will produce one open curve and merging two open curves will produce two open curves.
4. Copy points from X from the beginning (i. e., from x_1) up to x_{\max} to Z .
5. Copy points from Y from y_{\max} up to the end (i. e., up to y_m) to Z .
6. Copy points from Y from the beginning (i. e., from y_1) up to y_{\max} to Z .
7. Copy points from X from x_{\max} up to the end (i. e., up to x_n) to Z .
8. Delete X and Y .
9. Compute a new timestep for Z and go to 1.

We also consider that one curve can intersect itself and thus split itself into 2 parts. Let us consider a closed or open curve discretized as $X = \{x_1, x_2, \dots, x_n\}$. The curve evolves independently according to the equation (3). The algorithm for splitting into two curves is as follows:

1. Compute the distance between points in X and find two points where the minimum was reached. Let us denote the distance as d , and the points as $x_{\max 1}$ and $x_{\max 2}$. We do not consider several points in the neighbourhood of each point when measuring the distance to avoid finding minimal distance for two neighbor points. The number has to be computed according to the value of a given tolerance δ (see the next step). We recommend to omit all points with the distance smaller than at least 4δ .
2. Check if the distance d between points is smaller than a given tolerance δ . If not, compute new timestep and go to 1.

3. Create two new empty curves X_{new1} and X_{new2} . If X is an open curve, X_{new1} will be open and X_{new2} closed curve. If X is a closed curve then X_{new1} and X_{new2} will be closed curves.
4. Copy points from X from the beginning (i. e., from x_1) up to x_{max1} to X_{new1} .
5. Copy points from X from x_{max1} up to x_{max2} to X_{new2} .
6. Copy points from X from x_{max2} up to the end (i. e., up to x_n) to X_{new1} .
7. Delete X .
8. Compute new timestep for X_{new1} and X_{new2} and go to 1.

The numerical simulation is shown in Figure 8.

5. RESULTS OF NUMERICAL SIMULATION

In this section, the results of numerical simulation are presented. Schemes were tested on open or closed curves with or without tangential redistribution of points. At first, we simulated evolution of a circle and compared with analytical solution. Experimental order of convergence and absolute error were measured. For more details see [17].

Figure 1 (a) illustrates the evolution of a closed curve with external force variable in space. Values are as follows: $F = 10$ for $|X| < 0.35$, $F = -5$ for $|X| > 0.35$. The initial curve is a four-leaf clover curve. The positive force moves the curve to the center but the negative force move the rest of the curve from the center. In a short time, high curvature appears and overcomes the positive external force $F = 10$. This causes the whole curve to expand.

Figure 1 (b) shows the evolution of the curve which intersects itself. Intersections can evolve into singularities and it is not possible to continue evolution because curvature goes to infinity. However, the regularization term $Q(x_1, x_2) = \sqrt{x_1^2 + x_2^2 + \varepsilon^2}$ allows the curve to be evolved beyond singularities. One can see that the curve asymptotically adopts the circular shape. In this case, the algorithm for splitting and merging curves is not used since we needed to check how the curve evolution with regularization term behaves in singularities. Singularities are studied in detail in [1].

Figure 2 shows the evolution of a star shaped curve using the scheme (8) with $\alpha = 0$ (Figure 2(a)) and α computed by (4) (Figure 2(b)). The equation (2) contains some tangential force which helps to move points along curve and improve the stability of the computation. In Figure 2(a), one can see that the points are almost uniformly distributed at the end of the simulation. On the other hand, when the tangential force is removed by computing α according to (4), the curve points remain accumulated. This configuration requires smaller timestep and therefore larger CPU time. Numerical error also increases.

In practical applications such as dislocation dynamics, long time computations with variable external force are considered. In this case, accumulation of points occurs even for the evolution by (2). A redistribution algorithm then has to be

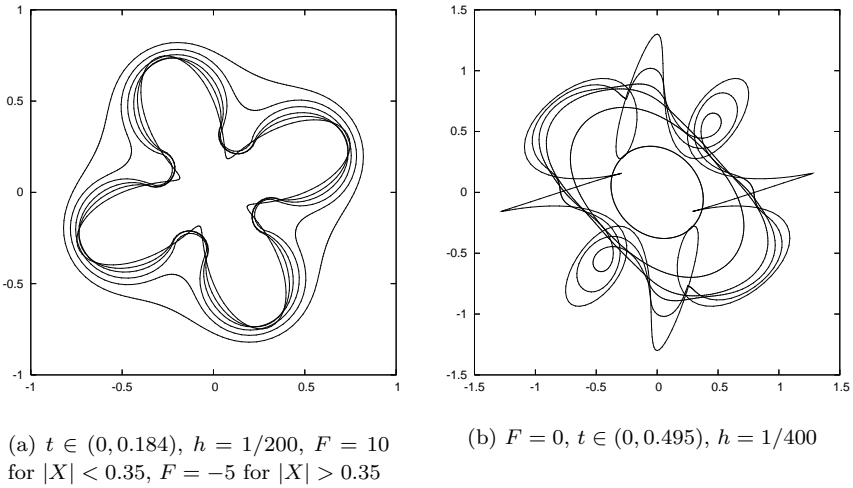


Fig. 1. Time evolution of closed curves, scheme (7).

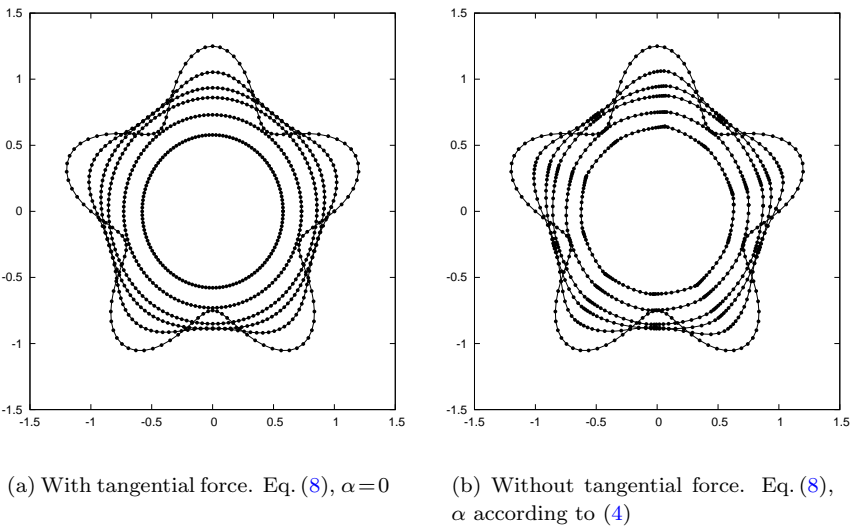


Fig. 2. Comparison of evolution with and without tangential force.

considered (see the remarks in Section 3 and [21]). Figures 3 (b) and 3 (a) present the position of an open curve at $t = 1.38$. There is an external force $F = 3$ which

changes the sign (i. e., $F = 3$ or $F = -3$) with the period of 0.3. This force causes the curve to move up and down. Figure 3 (a) shows the evolution by equation (2). One can see that in the central part of the curve the points accumulate. If tangential redistribution (mentioned in Section 2 and described in [21] is used (Figure 3 (b)), the points tend to be uniformly distributed along the curve.

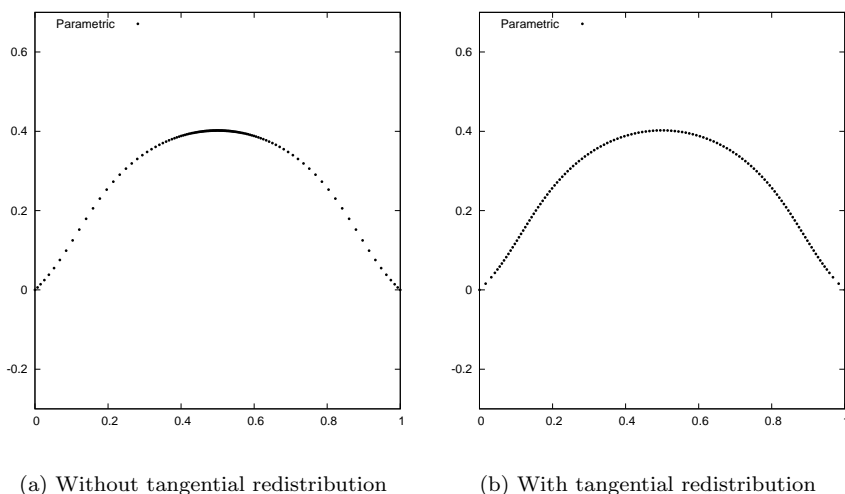


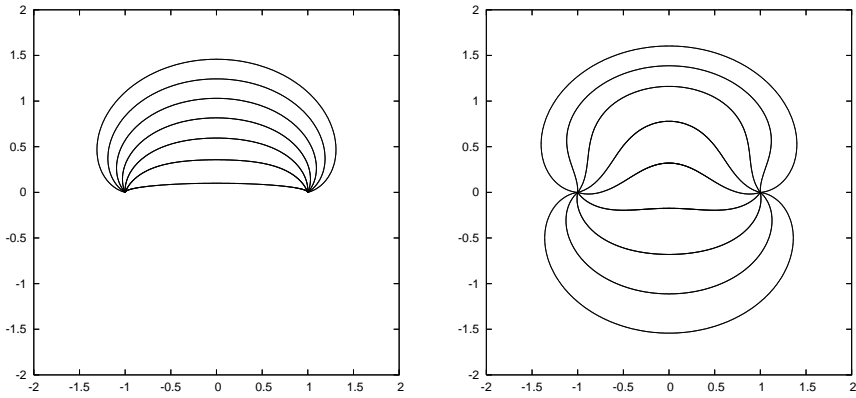
Fig. 3. Comparison of evolution with and without tangential redistribution at time $t = 1.38$.

6. APPLICATION IN DISLOCATION DYNAMICS

Dislocation curves as defects in material evolve in time. The dislocation evolution history contains shape changes of open curves, closing of open dislocation curves up to collision of dipolar loops (see [14]). Interaction of dislocation curves and dipolar loops has been studied, e. g., in [11, 12, 13].

Figure 4 illustrates the evolution of a dislocation curve in time. The external force $F = -3$ is applied to the curve which causes the expansion in the upward direction. At time $t = 0.54$, the sign of the force is changed. The curve then moves downwards. In a real material, one can observe similar behavior.

Dislocations can interact with other defects through the stress field. In this case, dislocation curve can be blocked by a potential barrier. Figure 5 shows this case with a weak barrier. Dislocation curve expands by means of $F = -3$ until it reaches the barrier made by the spatially variable force $F = 9$ at $x_2 = 1.7$. This barrier is not strong enough to lock the curve. At the ends of the barrier there is a very high curvature. High curvature results into a strong force resisting the barrier. The curve can leave the barrier and continue to expand. The simulation in Figure 6 was computed for $t \in (0, 2.1)$.



(a) Dislocation curve expands ($F = -3$) for $t \in (0, 0.54)$.

(b) Curve goes back and expands to the other side ($F = 3$) for $t > 0.54$.

Fig. 4. The evolution of the dislocation curves with variable external force F .

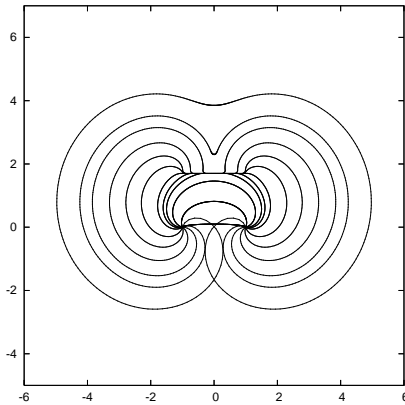
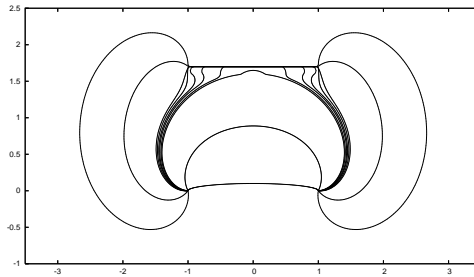
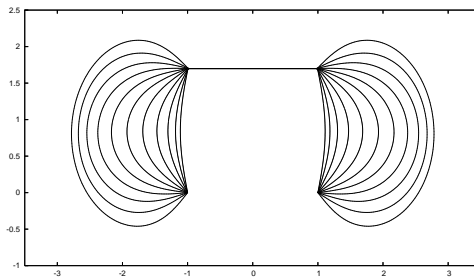


Fig. 5. The dislocation curve expands over a barrier created by spatially variable external force.

In the case of a strong barrier, the curve is locked in it and cannot continue in the evolution. The curve can expand to sides only. The barrier is at $x_2 = 1.7$ and the value of a barrier force is $|F| = 35$. Figure 6 (a) illustrates the curve expansion by $F = -3$ and the case when it is locked at the barrier ($t \in (0, 1.5)$). Figure 6 (b) shows the curve shrinking by $F = 3$ for $t \in (1.5, 3)$. The curve is locked at the barrier and cannot go back to a straight line. This example should represent a real



(a) Curve expansion



(b) Curve moves back

Fig. 6. Spatially variable external force F with high value, $t \in (0, 1.5)$.

dislocation curve expansion when the curve is locked in a *channel*.

The evolution of the curve at the infinite channel is shown in Figure 7. The infinite channel is created by a spatially variable external force. The curve cannot cross the barrier (at $x_2 = 1.2$ and $x_2 = 0$).

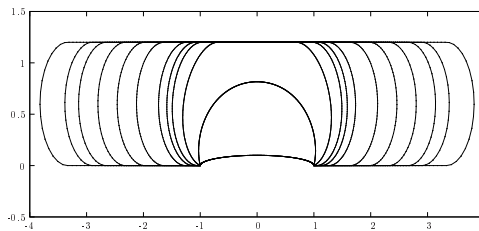


Fig. 7. Curve evolution at the channel.

The last example shows the simulation of the Frank–Read mechanism (see [14]) which describes how new dislocation loops are created. A force is applied to the dislocation line (similar to Figure 4). The curve keeps expanding until it touches itself. At this moment, the curve splits into two parts – dipolar loop and dislocation line. The loop continues in expansion. The dislocation line will again undergo the same process.

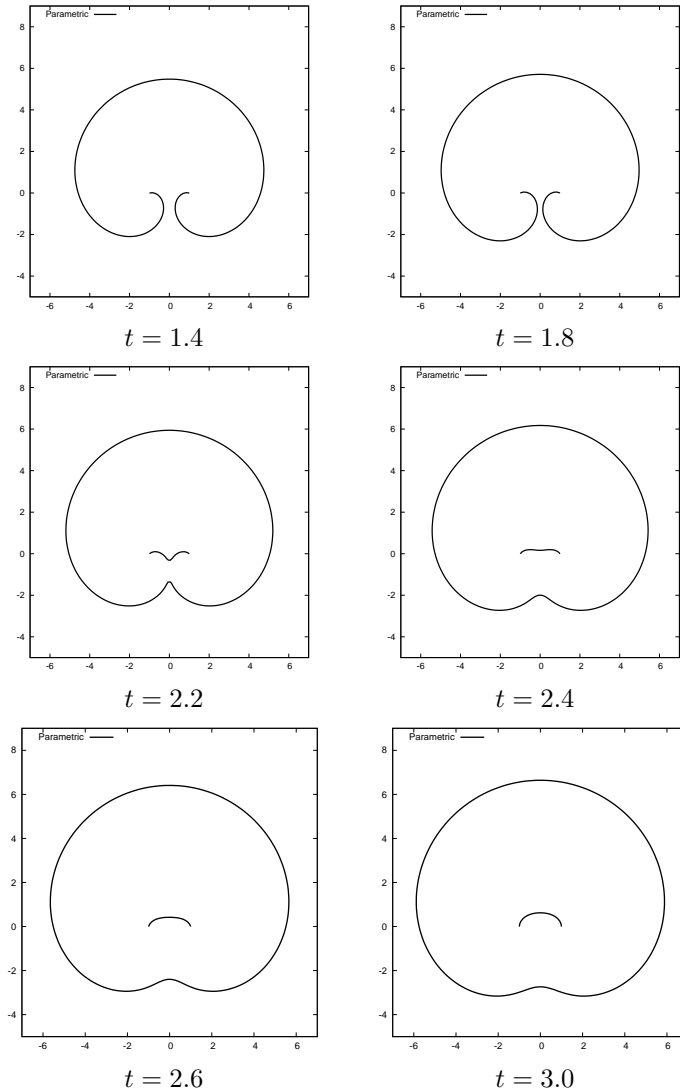


Fig. 8. The Frank–Read mechanism.

7. CONCLUSION

The simulation of dislocation dynamics is important in practice as dislocations affect many material properties. Dislocation dynamics can be mathematically simulated by the mean curvature flow. We presented a method based on a parametric approach and two numerical schemes. We applied the model to situations similar to the real context including a mechanism of creating new dislocations (i. e., Frank–Read source). The scheme had to be improved by an algorithm for tangential redistribution of points and by an algorithm for topological changes for parametric model.

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