Modified Level Set Equation for Gas-Liquid Interface and Its Numerical Solution

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Abstract

This paper is devoted to further modification of the Level Set approach, which is well-known for simulation of gas-liquid flows with the interface. In our development, we addressed to the case of a strong velocity gradient at the free interface. This is a typical situation, for example, when this interface interacts with the turbulent flow. In this case, the gradients of the level set scalar, in the vicinity of the interface, increase with time very rapidly. In order to maintain the accuracy of the numerical solution, the Level Set methods are combined usually with the Eikonal equation for a signed distance function from the zero level set. In the standard procedure (Sussman et al., J. Comput. Phys. 114, 1994), in order to be consistent with evolutional type of the Level Set equation, the non-evolutional Eikonal equation is replaced by quasi-evolutional one, with the artificial time providing iterations at each time step. Our idea is to modify the Level Set equation, in such a way that the Eikonal equation is satisfied directly by the form of the modified equation. This was done in the proposed paper. The efficiency of the proposed method is demonstrated by using various tests problems with interface.

Introduction

There are numerous physical phenomena in which discontinuities in physical properties are described by evolution of an interface. Examples include premixed flames, gas-liquid systems with a free interface, solidification and melting processes (e.g. [1]-[3]). In simulation of these phenomena, the moving interface is simulated often by level set methods. The details of this theory can be found in classical books [4]-[6]. Namely, the interface is associated with the zero level set (front) $G_0 = \{\mathbf{x} : G(\mathbf{x},t) = 0\}$ of the continuous level set function G, which is governed by the following field-equation:

$$\frac{\partial G}{\partial t} + \mathbf{u} \cdot \nabla G = u_F \left|\nabla G\right|, \qquad G(\mathbf{x}, t=0) = f(\mathbf{x}) \qquad (1)$$

Here $\mathbf{u}(\mathbf{x},t)$ is the flow velocity field, $\mathbf{n}(\mathbf{x},t) = -\nabla G(\mathbf{x},t) / \left|\nabla G(\mathbf{x},t)\right|$ is the local outward pointing unit normal, u_F is the propagation velocity of the front relative to the flow in the normal direction (as in the premixed flames, for example). In the application of level set methods, the statement of usual problem is this: if the flow velocity in (1) is not constant (a simple example is the interface subjected to the non-rotational uniform strain), the gradient of the level set scalar may grow or decay rapidly (exponentially) with time. In the vicinity of the zero level set, this leads to a strong distortion of the level set function, with loss of accuracy in numerical integration of (1). In level set methods, this problem is remedied by re-initialization procedure (e.g. [7]- [9]), i.e. by the reconstruction of the level set function with the aid of the Eikonal equation (e.g. [10]):

$$\left|\nabla G\right| = 1 \qquad (2)$$

The solution of (2) is the signed distance function with respect to the zero level set. However, strictly from a mathematical viewpoint, equations (1) and (2) are not compatible (e.g. [11]): equation (2) is not the evolution equation, while equation (1) is evolutional. As a consequence, even if the initial G-function is defined to be the

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signed distance function, the solution of (1), in the general case, does not retain this property. In order to circumvent this problem, the prevalent practice is to replace the non-evolutional Eikonal equation (2) by the evolutional one, with iterative time (e.g. [9], [12]):

$$\frac{\partial G^{\nu}}{\partial \tau} + S(\tilde{G})\left(\left|\nabla G^{\nu}\right| - 1\right) = 0, \tag{3}$$

Here $\tilde{G}$ is the solution of (1), which does not satisfy (2), and $S(\tilde{G})$ is the smoothed sign function presumed in the following form:

$$S(\tilde{G}) = \frac{\tilde{G}}{\sqrt{\tilde{G}^2 + \varepsilon^2}}, \qquad \varepsilon^2 << 1 \tag{4}$$

Analytically, it is stated that in the limit $\tau \to \infty$, the solution of (3) tends to the unique viscosity solution of (2) without pertubation of the zero level set. However, it has been noted by several authors [13, 14], that discretization and numerical solution of (3) may shift significantly the zero level set. Thereby the substantial errors may be incurred by the reinitialization procedure. In a number of approaches [13,14], the ways of alleviation this problem were proposed.

The following question does however remain: along with satisfaction of property (2), is it possible to reformulate the level set problem directly in terms of evolution equation of the level set function. In answer, let us first note that distances between different level sets are governed by the velocity gradient. Thus, one of the possibilities to avoid breaking of property (2) is to control the velocity field outside of the zero level set, requiring that velocity at the zero level set is unchanged. This idea was introduced in [15] by the velocity extension method. Let us note that application of the velocity extension method to the gas liquid systems ($u_F = 0$) has the following consequence: the level sets move relative material surfaces, as it does in the case of premixed combustion ($u_F \neq 0$).

In the present study, our objective is to modify equation (1) in such a way that the velocity field is not perturbed in the whole domain, and simultaneously, the Eikonal equation (2) is satisfied. This is accomplished by the specific source term in G-equation, which is equal to zero at the zero level set. In fact, our modification of (1) is equivalent, in principle, to the velocity extension method [15], but it offers a significant simplification in realization. First, the following lemma is introduced:

Lemma: the sign of solution of the G-equation, with a source term proportional to G,

$$\frac{\partial G}{\partial t} + \mathbf{u} \cdot \nabla G = u_F \left|\nabla G\right| + A(\mathbf{x}, t) G, \tag{5}$$

is conserved ($A(\mathbf{x}, t)$ is an arbitrary function), and consequently, (5) gives the same evolution of the zero level set $G(\mathbf{x}_f(t), t) = 0$, where $\mathbf{x}_f(t)$ is the local coordinate of points on the zero level set isosurface. The function $A(\mathbf{x}, t)$ will be determined by use of the constraint (2).

Derivation

Based on the above lemma, let us consider the following initial value problem

$$\frac{d\varphi}{dt} = \frac{\partial \varphi}{\partial t} + \mathbf{u} \cdot \nabla \varphi = A(\mathbf{x}, t)\varphi + u_F, \tag{6}$$

$$\varphi(\mathbf{x}, t = 0) = \varphi_0(\mathbf{x}) \tag{7}$$

$$\left|\nabla \varphi(\mathbf{x}, t = 0)\right| = \left|\nabla \varphi_0(\mathbf{x})\right| = 1, \tag{8}$$

where $\varphi(\mathbf{x},t)$ is a new scalar field with $\varphi(\mathbf{x}_f(t),t)=0$, representing the flame isosurface, i. e. $\varphi(\mathbf{x},t)\propto G(\mathbf{x},t)$. The Eikonal equation (2) is:

$$\left|\nabla\varphi(\mathbf{x},t)\right|=1, \qquad t>0 \tag{9}$$

By virtue of initial condition (8), we have the same also for initial time : $t=0$, $\left|\nabla\varphi(\mathbf{x},t=0)\right|=1$.
We now determine the function $A(\mathbf{x},t)$ by requiring $\left|\nabla\varphi(\mathbf{x},t>0)\right|=1$. Let us differentiate (6) with respect to x_i, and then multiply it by $2\nabla_i\varphi$, where $\nabla_i\varphi=\frac{\partial\varphi}{\partial x_i}=-n_i$. Summing over the suffix i, one yields:

$$n_i\varphi\frac{\partial A}{\partial x_i}-A(\mathbf{x},t)=-n_i\frac{\partial u_k}{\partial x_i}n_k \tag{10}$$

Introducing the coordinate n along the normal vector $\mathbf{n}$ to the isorsurface $\varphi(\mathbf{x},t)=0$, we obtain the following expression:

$$A(\mathbf{x},t)\Big|_{n=0}=n_i\,n_k\left.\frac{\partial u_k}{\partial x_i}\right|_{n=0}=n_k\left.\frac{\partial u_k}{\partial n}\right|_{n=0}=\left.\frac{\partial(\mathbf{u}\cdot\mathbf{n})}{\partial n}\right|_{n=0} \tag{11}$$

The following properties were used in (11). The first one is the definition of the derivative along the normal vector $\mathbf{n}(\mathbf{x},t)$: $n_i\frac{\partial}{\partial x_i}=\frac{\partial}{\partial n}$. Recognizing that this derivative is along the characteristic of the Eikonal equation, and since the characteristics of the the Eikonal equation are the straight lines at each time [10], it is clear that the normal vector $\mathbf{n}(\mathbf{x},t)$ does not change along the characteristics. Thus we have: $\frac{\partial n_k}{\partial n}=0$. We note also that the condition $(\;)\big|_{n=0}$ denotes $(\;)\big|_{\varphi(\mathbf{x},t)=0}$, i.e. $(\mathbf{u}\cdot\mathbf{n})\big|_{n=0}=\mathbf{u}(\mathbf{x}_f(t),t)\cdot\mathbf{n}(\mathbf{x}_f(t),t)$.
The next step is to recast (10) by taking into accound that by virtue of $\left|\nabla\varphi(\mathbf{x},t)\right|=1$ and $\mathbf{n}(\mathbf{x},t)=-\nabla\varphi(\mathbf{x},t)$, the following relation is valid

$$\varphi=-n. \tag{12}$$

Then the equation equation (10) can be recasted as:

$$\frac{\partial\left(An-\mathbf{u}\cdot\mathbf{n}\right)}{\partial n}=0 \tag{13}$$

The solution of (13) is straightforward

$$A(\mathbf{x},t)n=\mathbf{u}\cdot\mathbf{n}-(\mathbf{u}\cdot\mathbf{n})\big|_{n=0}, \qquad A(\mathbf{x},t)=\frac{\left(\mathbf{u}\cdot\mathbf{n}-(\mathbf{u}\cdot\mathbf{n})\big|_{n=0}\right)}{n} \tag{14}$$

It is seen that at $n\to 0$ (14) gives (11).
The final set of equations for $\varphi(\mathbf{x},t)$ and its normal $\mathbf{n}(\mathbf{x},t)=-\nabla\varphi(\mathbf{x},t)$ can be written in the following form

$$\frac{d\varphi}{dt}=\frac{\partial\varphi}{\partial t}+\mathbf{u}\cdot\nabla\varphi=A(\mathbf{x},t)\varphi+u_F \tag{15}$$

$$\frac{dn_i}{dt} = \frac{\partial n_i}{\partial t} + \mathbf{u} \cdot \nabla n_i = -\frac{\partial u_k}{\partial x_i} n_k - \frac{\partial A \varphi}{\partial x_l} \quad (16)$$

where the product $A\varphi$ satisfies equation (13) with initial condition (11). Note that equation for the normal was already considered in [16]- [18].

Computation

In this study, our computations are based on equation (15) only, without application of equation for the outwards normal (16). Two forms of the source term were considered. One is (10):

$$A(\mathbf{x},t) - \varphi \nabla_i \varphi \nabla_i A = \nabla_i \varphi \nabla_i u_k \nabla_k \varphi \quad (17)$$

without re-initialization. Another one is given by simplifed expression, as $\varphi \to 0$:

$$A(\mathbf{x},t) = \nabla_i \varphi \nabla_i u_k \nabla_k \varphi \quad (18)$$

In this case, the re-initialization procedure is applied. The solutions with two forms (17) and (18) were assessed by comparison with the standard approach. In simulation, the governing equations are discretized in time using the 3-stage third-order TVD Runge-Kutta scheme. For spatial discretization, the fifth-order upwind finite difference WENO scheme is used with the Roe flux splitting. The mean curvature is calculated by:

$$\kappa = -\frac{\varphi_x^2 \varphi_{yy} - 2\varphi_x \varphi_y \varphi_{xy} + \varphi_y^2 \varphi_{xx}}{\left(\varphi_x^2 + \varphi_y^2\right)^{3/2}} \quad (19)$$

The both forms (17) and (18) are taken locally in the narrow band, which is moving with the interface. The criteria of convergency for the re-initializaton procedure is proposed in [7]. This criteria is applied in the narrow band, and it is expressed as:

$$\frac{1}{N} \sum_{i,j:\left|\varphi_{i,j}\right| < \varepsilon} \left| \varphi_{i,j}^{\upsilon+1} - \varphi_{i,j}^{\upsilon} \right| < \Delta\tau \Delta x^2 \quad (20)$$

where N is the number of nodes in the narrow band (blues points in Fig.1), ε is the thickness of the inner zone, $\varphi_{i,j}^{\upsilon+1}$ and $\varphi_{i,j}^{\upsilon}$ are the computed values of the level set function at a given point for two successive itterations. The error in computation of level set function gradient is estimated by the following expression:

$$E_{\nabla\varphi} = \frac{1}{N} \sum_{i,j:\left|\varphi_{i,j}\right| < \varepsilon} \left| \left| \nabla \varphi_{i,j} \right| - 1 \right| \quad (21)$$

Here the 4th-order central difference is used for computation of spatial derivative. The various tests problems were used. These tests included the advection of a circle of fluid in the vortex flow; the advection of Zalesak's rotating disk; the oscillating circle test, the flame propagation across the presumed flow structure. The interface location error, the mean deviation from the signed distance property, and the errors of the interface curvature were analyzed. Three tests are illustrated hereafter.

a. Oscillating circle [19]. In this test, the initial circular interface of radius 3, being centered on (0,0), is considered in the computational domain $\vec{x} \in [-5,5] \times [-5,5]$. This interface is subjected to the presumed velocity field, in which only the normal component is non-zero. The modulus of this component is dependent on azimuth periodically, and it is harmonic in time:

$$\vec{u} = s\vec{n},\ s = \cos(8\theta)\sin(\omega t);\quad \theta = \mathrm{arctg}\left|\frac{y}{x}\right|,\ \omega = \frac{2\pi}{T} \tag{22}$$

Here we used the simplified expression (18) with (15). The results of computation and comparison with the standard approach are illustrated in Fig. 1-3. In Fig.1, the evolution of interface in such a velocity field illustrates the extensions (outwards and inwards, until t = T/2) and the subsequent contractions back to the original shape (attained at t = T). The time-step $\Delta t = \Delta x / 4$ corresponds to CFL number equal to 0.25. The quantitative analysis of the accuracy is given in Fig.2, for the curvature of interface; in Fig. 3, for the error in computation of the level set function gradient on the interface, and also in Table 1, where the interface location error is reported. The advantage of the modified level set equation is seen from these figures: return to the circled shape is better presented, with more accurate curvature. Also, Fig.3 shows that the error in signed distance property is significantly reduced. Additionally, it is seen in Fig. 4 that the number of iterations is reduced three times at least.

Table 1 : Front location error at t = T.

	Grid			
Method	642	1282	2562	5122
Standard	1.89e-2	6.01e-2	2.41e-3	8.23e-4
New	7.30e-2	2.85e-4	5.62e-5	1.88e-5

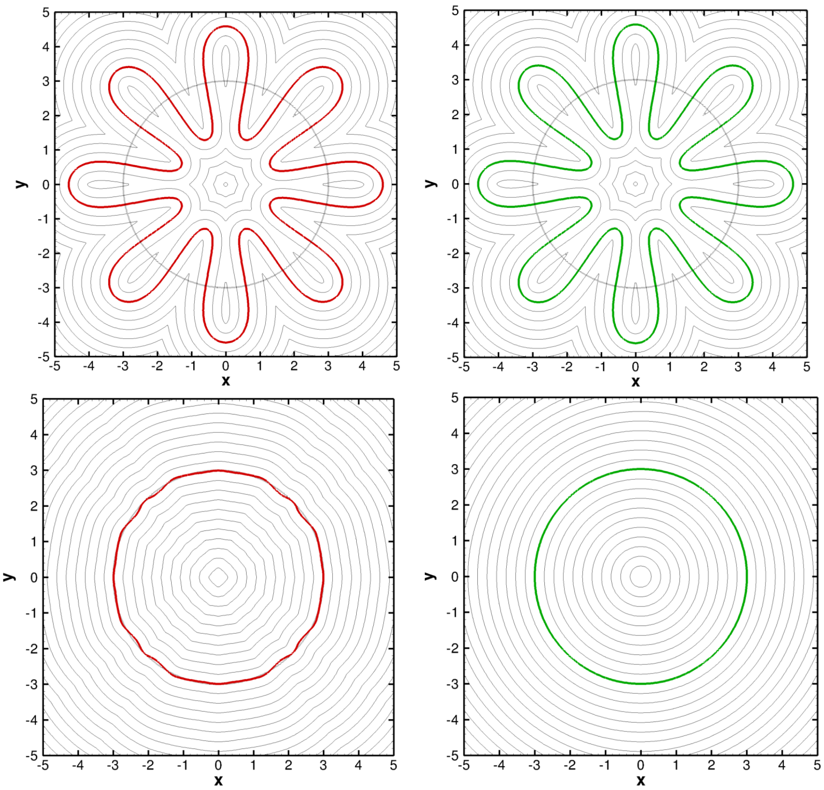

Figure 1: Oscillating circle test. Snapshots of isolines of G-scalar at two different times: t = T/2; T. On the left-hand side: standard method; on the right-hand side: new method.

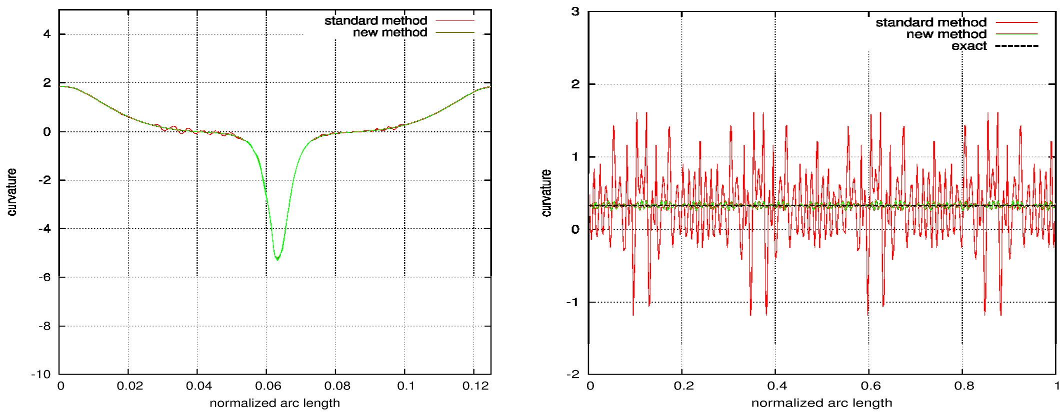

Figure 2 : Oscillating circle test. Interface curvature at t = T/2 and t = T.

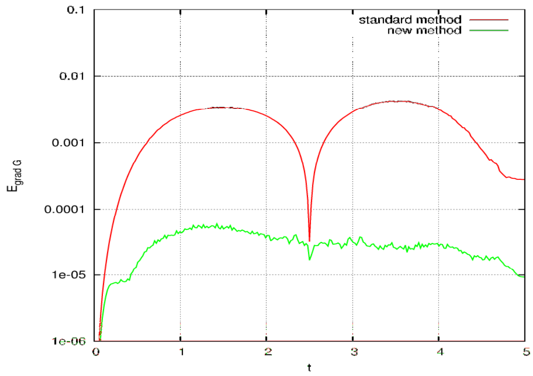

Figure 3 : Oscillating circle test. Gradient error Interface curvature

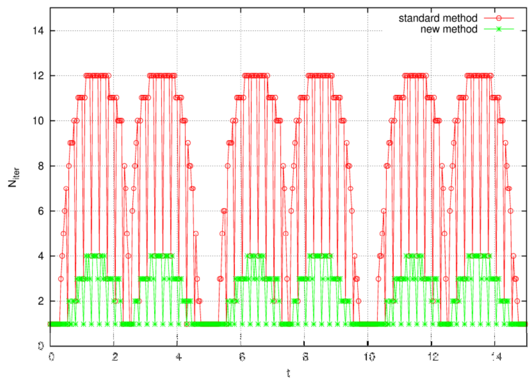

Figure 4 : Oscillating circle test.

b. Interface stretching in a 2D single-vortex [20].

The conditions for this test problem are taken from the paper of Rider and Kothe [20]. Here the initial interface represents circle with radius 0.15, centered at x = 0.5, y = 0.75 in unit square computational domain given in Fig.5. The velocity field is defined by following stream function:

$$\psi(x, y) = \frac{1}{\pi}\sin^2(\pi x)\sin^2(\pi y) \tag{23}$$

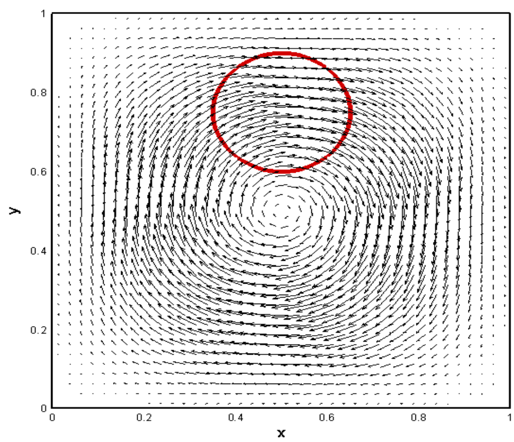

Figure 5: Representation of the vortical flow field defined in Eq. (23) on the domain

$$(0 \le x \le 1, 0 \le y \le 1)$$

The initial circle is stretched by this flow field forming filaments. In computations, the CFL number (based on the maximum velocity) is set to 0.5; The grid contains 1282 grid points. The reference solution is obtained by standard level set approach on 5122 computational grid. In Fig.6, we compared the stretched resolved filaments for both methods; in the new method the exact form (17) was used without re-initialization. It is seen that the modified level set equation leads to better resolution of stretched filaments, compared to the case of standard approach. In Fig.7, the number of iterations is indicated in order to satisfy the convergence criteria in standard approach. Fig. 8 shows that results are almost not sensible when the different thickness of the narrow band is used. This is also confirmed by Table 2.

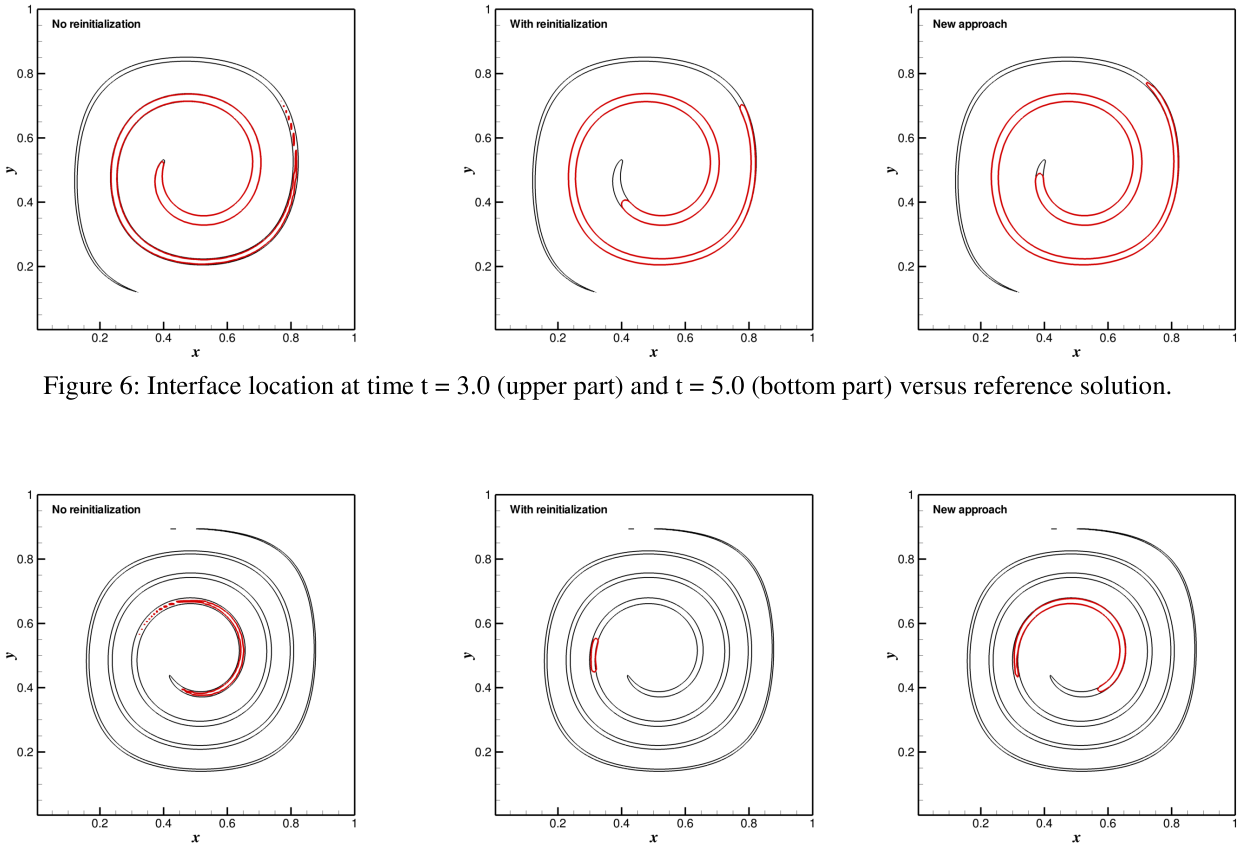

Figure 6: Interface location at time t = 3.0 (upper part) and t = 5.0 (bottom part) versus reference solution.

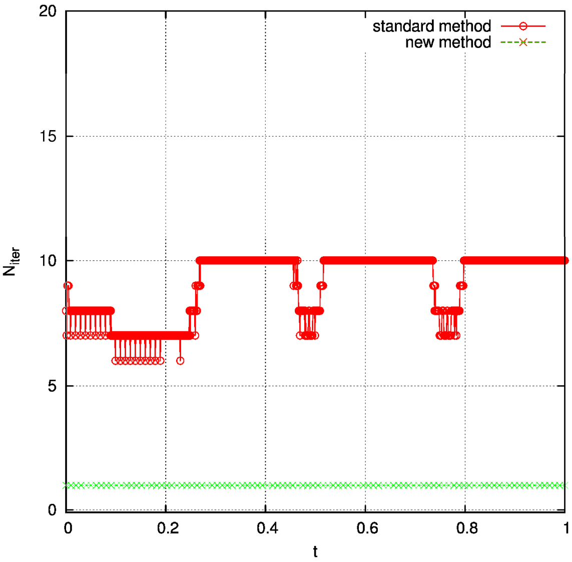

Figure 7: Number of iterations needed to satisfy the convergence criteria

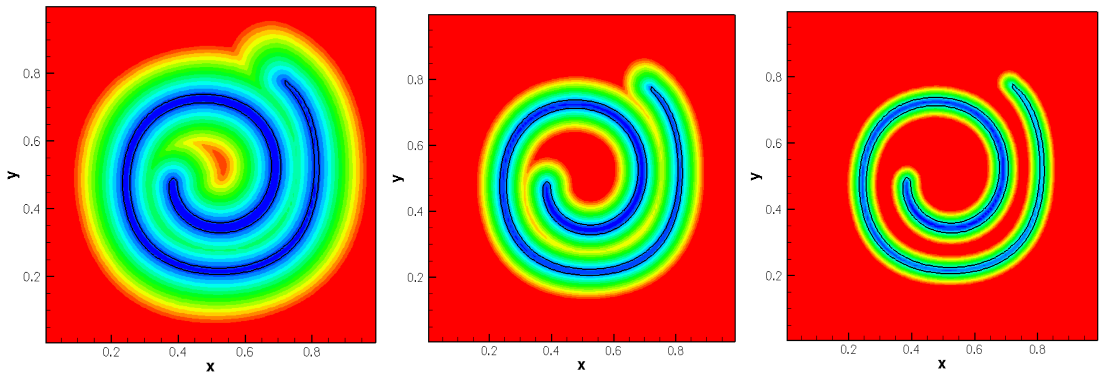

Figure 8. Interface location at time t = 3.0 obtained with the new method on 1282 computational grid. 3 cases are presented : $\varepsilon = 20\Delta x$, $\varepsilon = 10\Delta x$, $\varepsilon = 5\Delta x$.

Table 2. Influence of the size of the narrow band on the approximation errors

Grid size	Half-width	Gradient error
128	5	8.3491e-5
	10	7.9788e-5
	20	7.0738e-5
256	5	1.1549e-5
	10	1.0613e-5
	20	1.2449e-5

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