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A CONSERVATIVE LEVEL SET METHOD FOR SHARP INTERFACE MULTIPHASE FLOW SIMULATION

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Abstract. *We present a finite difference method for the computation of the interface location in two two phase flows. The method is especially suited for flow situations where the surface tension plays an important role. Examples for such flows are falling droplets, liquid jets or applications in micro fluidics..*

The level set method is often used to describe the interface position. It's major drawback is that it does not conserve the mass of the fluids. To address this problem we use a finite difference implementation of the conservative level set method. The signed distance function is replaced by a hyperbolic tangent function. This allows to write the advection and the reinitialisation as conservation laws. High order methods are employed for the advection of the level set function, to ensure an accurate representation of the interface location and to keep the shape of the level set function close to to its hyperbolic tangent shape, which minimises the effort for the reinitialisation.

As a result we get an explicit method which is relatively easy to implement and has favorable properties for two phase flows. As it emploies the same discretisation schemes which are used for the advection of an ordinary level set method it is relatively easy to implement in an existing two phase solver. In addition the extension to three dimensions is straightforward. We present results computed with our method and compare them with the results from the original methods. Especially the improvements in mass conservation will be discussed.

1 Introduction

Drop impacts on dry surfaces can be found in many industrial and natural processes. Applications where the behavior of the impacting drops plays an important role include ink-jet printing, spray cooling, pesticide spraying, erosion processes due to rain and thermal spray coating. Drop impacts also play an important role in gas-liquid separation in the process industry and the gas and oil industry. In these processes the surface tension plays often an important role. The spreading of the drop on the target surface is driven by inertia forces, whereas the surface tension acts against the spreading. In certain cases the surface tension is strong enough such that the drop can bounce back from the target. In order to simulate such flows it is important to have an accurate description of the surface tension force.

The surface tension in multiphase flows introduces a jump in the normal stress across the interface. A widely used method to deal with such flows is the continuous surface force (CSF) model. The surface tension force and the change of the fluid properties e.g. density and viscosity are smeared out over several grid points. The result of those diffuse interface methods are numerically smooth solutions, which in turn make it possible to apply standard finite difference methods. The ghost-fluid method (GFM) [1], which uses a fixed Cartesian grid, was extended to incompressible two-phase flows [2]. The GFM allows to retain the jumps across the interface and therefore it is possible to eliminate the error which stems from the artificial smearing of the fluid properties. To use the GFM it is necessary to know the location of the interface, as well as its curvature, a level set approach [3] is working well to retrieve this geometrical information about the interface. Another advantage of the level set is its ability to handle topological changes of the interface. However, the level set method has an important disadvantage, it does not conserve the mass of the two fluids [4]. Different approaches were developed to satisfy the mass conservation of the level set method. Examples include the conservative level set method [5] [6], the particle level set method (PLS) [7] or the coupled level set/volume-of-fluid (CLSVOF) [8]. The added complexity for both PLS and CLSVOF are significant. On the other hand the conservative level set methods improves the mass conservation and keeps the simplicity of the original method.

The main idea of the conservative level set method is to replace the signed distance function from the traditional level set method with a hyperbolic tangent profile. As a result the conservative level set method can be advected and reinitialized by conservative numerical methods.

1.1 Conservative level set method

In level set methods the interface is defined as the iso contour of a smooth function. For ordinary level set methods this function is the signed distance form the interface, and the interface location is where the distance function is zero. The conservative level set function replaces the distance function by a hyperbolic tangent function ϕ with values between zero and one. The position of the interface is located at the $\phi = 0.5$ contour line. Since we have smooth functions which are defined in the entire computational domain in both cases, we can easily extract additional geometrical informations about the interface. For example the interface normals $\mathbf{n}$ and the curvature κ are defined as

$$\mathbf{n} = \frac{\nabla\phi}{|\nabla\phi|} \tag{1}$$

and

$$\kappa = \nabla \cdot \mathbf{n}. \tag{2}$$

The interface is transported simply by advecting the level set function $\phi_t = -\mathbf{u} \cdot (\nabla\phi)$. If we have a divergence free velocity field, as it is the case for incompressible flow, the interface transport can be written as a conservation law.

$$\frac{\partial\phi}{\partial t} + \nabla \cdot (\mathbf{u}\phi) = 0 \tag{3}$$

Since all numerical methods will introduce an error as ϕ is advected, it will loose its hyperbolic tangent shape. The diffusion of the advection schemes will increase the distance in which ϕ rises from zero to one. Ollson and Kreiss [6] propose the following reinitialisation equation to force ϕ back to its hyperbolic tangent shape:

$$\frac{\partial\phi}{\partial\tau} + \nabla \cdot (\phi(1-\phi)\hat{\mathbf{n}} - \epsilon\left((\nabla\phi \cdot \hat{\mathbf{n}})\hat{\mathbf{n}}\right)) = 0, \tag{4}$$

where $\hat{\mathbf{n}}$ are the normals at the beginning of the reinitialisation, and ϵ determines the width of the hyperbolic tangent. It is important to note that also the reinitialisation equation is a conservation law. The first flux term causes a compression of the profile, whereas the second term is a diffusive flux. By multiplications with the normals $\hat{\mathbf{n}}$ there are only fluxes in the direction of the normals. This forced flux direction for both the compression and the diffusion term are essential to improve the mass conservation of the method. To illustrate the nature of Equation (4), we use a 1 dimensional example. Suppose that the interface is located at $x = 0$, then the normals reduce to $n = -1$ or $n = 1$, in the example we use the latter. In this case a steady state solution to Equation (4) is:

$$\phi = \frac{1}{2}\left(1 + \tanh\left(\frac{x}{2\epsilon}\right)\right) \tag{5}$$

The solution is shown Figure 1, together with the compression and the diffusion term. It is clearly visible that at steady state the compression and the diffusion are balanced. If the ϕ would be too diffusive the compression term would outweigh the diffusive term and ϕ would be forced back to the steady state solution.

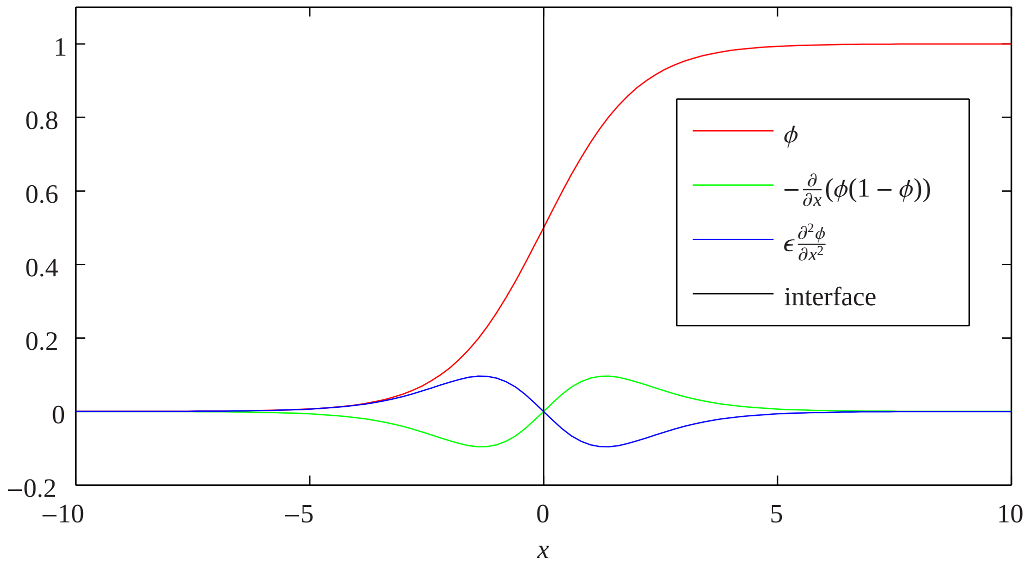

Figure 1: Illustration of the reinitialisation equation

2 Numerical Method

2.1 Advection

Since the conservative level set method will be a part of a multiphase solver, which uses the GFM to describe the jumps at the interface in a sharp way, it is a natural choice to use finite differences for its discretization. The spacial discretization for the advection Equation (3) is done with a standard 5th order finite difference WENO method as described in [9]. The advantage of the WENO scheme is that they do not produce artifical oscillations and therefore keep ϕ between zero and one. At the boundaries zero flux is imposed.

2.2 Normals

Before the reinitialisation Equation (4) can be solved the normals need to be computed. Far away from the interface the gradient of ϕ will be very small. As a result of the small gradients the direction of the normals will be extremely sensitive to small spurious errors in ϕ. If Equation (1) would be discretised directly using central differences with one sided stencils at the boundary, the resulting normals would point in arbitrary directions. Especially near the boundaries of the computation domain this problem will be amplified since the one sided stencils are less accurate. Such arbitrary normals pointing towards each other will lead to the accumulation of ϕ at wrong places during the reinitialisation.

Desjardins et. al. [10] propose to compute a singed distance function from ϕ using the fast marching method (FMM)[11]. The FMM is an efficient method to reinitialize the signed distance function ϕ_d for ordinary level set methods. The signed distance function has a gradient with unity length everywhere in the computation domain. Therfore the computation of the normals using (1) where ϕ is replaced by ϕ_d will be much more robust with regard to small errors in ϕ_d. We use a the FMM from the LSMLIB [12] which is second order in the L_2-norm to compute ϕ_d from ϕ. The normals $\hat{\mathbf{n}}$ are then computed from ϕ_d using a 4th order summation by parts (SBP) operator [13], with one sided stencils at the boundary.

2.3 Reinitialisation

Using twice a central difference approximation for the first derivative will not damp oscillations with a wavelength of $2\Delta x$. But the diffusive term in Equation (4) can not be computed using a central stencil for the second derivative because of the multiplications with the normals. Therefore $\nabla\phi$ is computed with a 4th order SBP operator and then the divergence total flux $\phi(1-\phi)\hat{\mathbf{n}} - \epsilon\left((\nabla\phi\cdot\hat{\mathbf{n}})\hat{\mathbf{n}}\right)$ is approximated by the same 5th order WENO scheme which is used for the advection. Again a zero flux boundary condition is enforced.

3 Examples

To calculate the area inside the level set contour an unbiased level set contouring is used as it is described in [14]. This method is only second order accurate. The error of the interface location is measured with

$$\frac{1}{L}\int \left|\mathrm{H}(\phi_{expected}) - \mathrm{H}(\phi_{computed})\right| \mathrm{d}A. \tag{6}$$

Where L is the length of the interface and $\mathrm{H}(\phi) = 0$ for $\phi \leq 0.5$ or $\mathrm{H}(\phi) = 1$ otherwise. The numerical calculation of the integral is done as described in [3].

In all examples the forward Euler scheme is used for the time discretisation. Every 1000 time steps we perform 20 reinitialisation steps.

3.1 Vortex test

A stream function of

$$\psi(x, y, t) = \frac{1}{\pi}\sin^2(\pi x)\cos^2(\pi y)\cos(\pi t/T) \tag{7}$$

is given in a square unit domain. Initially a circle with a diameter of 0.3 is placed at $(0.5, 0.75)$. The circle will be transported in the vortex and reach its maximum deformation at $t = T/2$. From then on the velocity components will change their sign and the vortex should reach its initial position at $t = T$. The time step Δt is set to $5\cdot 10^{-5}$ and the width of the hyperbolic tangent is $\epsilon = 0.8\Delta x$. In the literature two common values for T can be found, $T = 2$ will not lead to very thin filaments and is therefore often used for to show the method's ability at low numbers of grid points. On the other hand $T = 8$

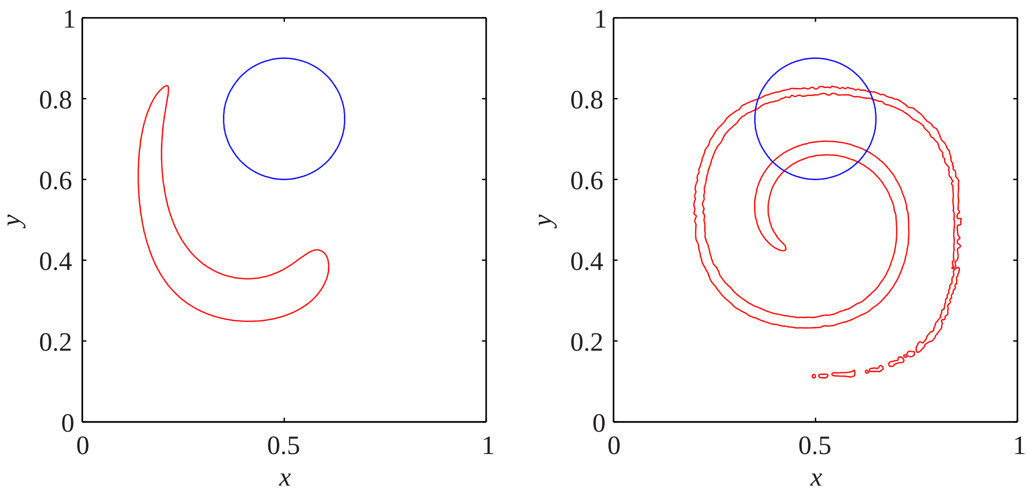

Figure 2: Circle undergoing deformation in a vortex at $t = 0$ blue, and $t = T/2$ red, for $T = 2$ on the left and $T = 8$ on the right

will lead to significant deformation of the circle. The the contour line where $\phi = 0.5$ at the maximum deformation is shown in Figure 2 for both values of T.

In Table 1 the results on three different grids are presented for $T = 2$. The accuracy is comparable to the results from Sun and Beckermann [15] who used a the phase-field equation to track the interface, which is similar to our method. The main difference is that using the phase-field equation the reinitialisation and the advection are combined in one equation. Since the conservative level set method separates those two tasks it is possible to use fixed normals for the reinitialisation which leads to the better area conservation compared to the method from [15].

Grid cells	Error	Order	% Area change
32	9.86E-3		1.48
64	2.26E-3	2.1	0.75
128	7.52E-4	1.58	0.71

Table 1: Error and mass loss for vortex test with $T = 2$

If the circle is advected longer in the vortex its develops very small structures and a corresponding resolution is required. As soon as the method is not able to resolve small structures in the interface, it develops small droplets which separate from the main structure as can be seen in Figure 2. This is caused by the fact that the method is conserving the quantity ϕ whereas in an ordinary level set method the unresolved parts simply vanish and therefore cause a mass loss. As the velocity is inverted and the the circle should be recovered at $t = T$ it becomes clear that the small, separated droplets will cause a big distortion of the interface (Figure 3). With a finer mesh the number of droplets which separate decreases and the error at $t = T$ is decreasing. Table 2 summarises the error and the area change for two different grid sizes. The error of the presented method is similar to the error of an ordinary level set method [7] but the area conservation is improved considerably. On the other hand we achieve a lower accuracy and area conservation than the PLS [7].

Grid cells	Error	Order	% Area change
128	1.75E-2		1.47
256	2.19E-3	2.9	0.77

Table 2: Error and mass loss for vortex test with $T = 8$

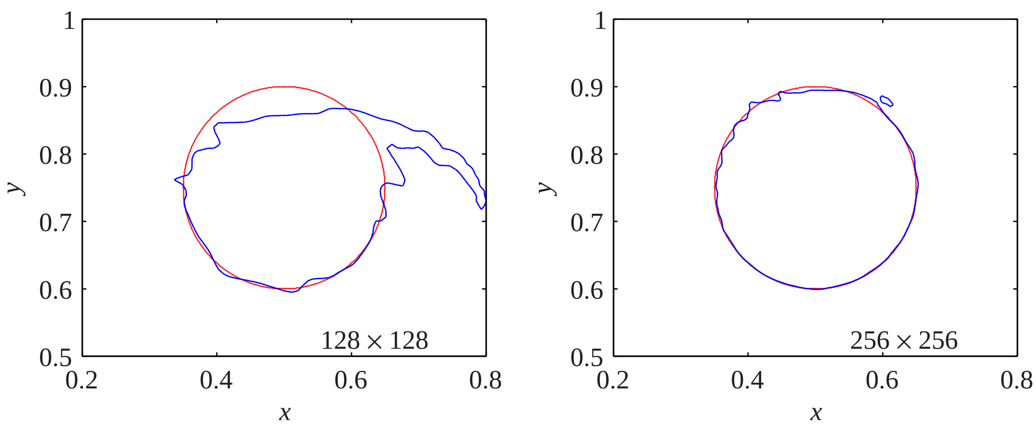

Figure 3: Interface at $t = T = 8$ on a 128×128 and 256×256 grid

3.2 Rigid Body Rotation of Zalesak's Disk

A stream function of

$$\psi(x, y) = -\frac{\pi}{628}\left(x^2 + y^2 - x - y\right) \tag{8}$$

is given in a square unit domain. Initially a slotted circle is placed at $(0.5, 0.75)$. The radius of the circle is 0.15, the width and the length of the slot are 0.05 and 0.25 respectively. In $t = 628$ the slotted disk completes a Rigid Body Rotation around the center of the domain. The time step is set to $\Delta t = 5 \cdot 10^{-3}$ and the width of the hyperbolic tangent is $\epsilon = 0.7\Delta x$.

Figure 4 shows the interface location of interface after one revolution. The errors and area changes are shown in Table 3. Also in this thest the accuracy is slightly better than for phase-field method [15]. The area change is the same for the coarse grid but decreases much faster in our method (0.04% versus 0.8% on the finest grid). If our results

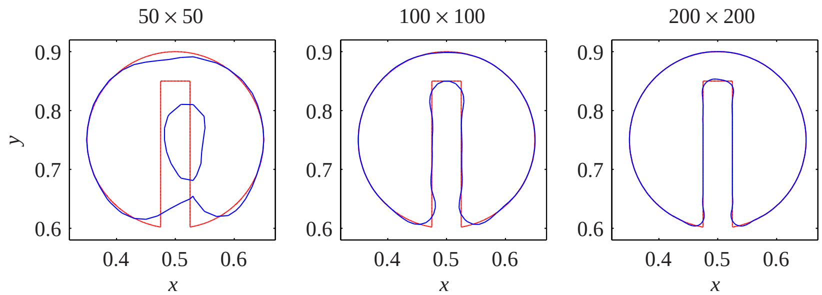

Figure 4: Zalesak's Disk after one revolution on different grids

are compared to an ordinary level set method and a hybrid particle level set method the improvement in mass conservation is evident. Enright et. al. [7] report that on the coarse grid the disk vanishes completely using a level-set method whereas the PLS suffers form a area loss of 15.9%. On the other hand the area loss of the accurate conservative level set method [10] is an order of magnitude smaller than in our method. Note that our errors can not be compared directly with the errors reported in [7] since a different domain size is used and the error measurement in Equation (6) is not dimensionless.

Grid cells	Error	Order	% Area change
50	8.67E-3		3.03
100	1.20E-3	2.85	0.28
200	3.49E-4	1.79	0.04

Table 3: Error and mass loss for one revolution of Zalesak's Disk

4 Conclusion

A finite difference implementation of the conservative level set method has been proposed. The employed discretisation schemes are well documented and widely used, therefore it is relatively easy to implement the conservative level set method into existing flow solvers especially to those which already contain an ordinary level set method. Mass conservation is considerably improved compared to an ordinary level set method and some related methods. Form the results in the test cases it can be seen that our method does not handle very thin interface structures as well as other methods. But this shortcoming can probably be improved by optimising the parameters for the reinitialisation, e.g. the number and frequency of the reinitialisation steps and the width of the hyperbolic tangent.

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