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Wei Yang
China Agricultural University

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AN UNSPLIT LAGRANGIAN ADVECTION SCHEME FOR VOLUME OF FLUID METHOD*

YANG Wei, LIU Shu-hong, WU Yu-lin
Laboratory of Hydraulic Science and Engineering, Tsinghua University, Beijing 100084, China,
E-mail: yang-w03@mails.tsinghua.edu.cn

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Abstract: An Unsplit Lagrangian Advection (ULA) scheme for Volume Of Fluid (VOF) method is presented in this article. The ULA scheme is developed based on an algorithm of Piecewise Linear Interface Construction (PLIC). The volume fluxes between cells are calculated through solving the new equation of the linear interfaces in cells in the ULA scheme. The fluxes flowing out from one cell is the inflow fluxes for another cell. In this way the whole fluid volume is conserved strictly without using any redistribution algorithms. The ULA scheme is based on two-dimensional structured rectangular mesh and may be extended to three-dimensional structured mesh with more geometrical efforts. The results from three widely-used benchmark tests show that the ULA scheme can achieve the accuracy higher than Split Lagaragian Advection (SLA) scheme and the Flux-Corrected Transport (FCT) algorithm.

Key words: advection schemes, free surfaces, fluid interfaces, Volume Of Fluid (VOF) method

1. Introduction

The free surface flow exists widely in aerospace, marine and transport and other fields. The interface tracking method is particularly important in simulating numerically the free surface flow. The Volume Of Fluid (VOF) method is this kind of numerical methods, which was presented in the early 1970s. Debar used the VOF method to simulate two-dimensional compressible multiphase flow, which is one of the earliest application of VOF method. After that, the VOF method has got a rapid development and has been widely used in engineering problems[1-5].

For a certain material M in multiphase flow, in the VOF method the color function is defined as

$$f(x)=1 \quad \text{if there is material } M \text{ at } x \tag{1a}$$

$$f(x)=0 \quad \text{otherwise} \tag{1b}$$

and the volume of fraction of material M in cell (i, j) as

$$f_{ij}=\frac{\iint f(x,y)\mathrm{d}x\mathrm{d}y}{\Delta x\Delta y} \tag{2}$$

In literature, either the advective form of

$$\frac{\partial f}{\partial t}+\boldsymbol{u}\bullet\nabla f=0 \tag{3}$$

or the equivalent conservative form

$$\frac{\partial f}{\partial t}+\nabla\bullet(f\boldsymbol{u})=0 \tag{4}$$

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Biography: YANG Wei (1982-), Male, Ph. D.

in a divergence-free flow is often referred to as the governing equation of the VOF method. In Eqs.(3) and (4) $\boldsymbol{u}$ denotes the velocity vector.

During each time step, the interface is tracked by two sub-steps. In the first advection step, a new value of volume fraction, $f_{i,j}^{n+1}$, is calculated based on $f_{i,j}^{n}$ and the current interface locus, and in the second reconstruction step, the new interface locus is determined solely by $f_{i,j}^{n+1}$ in a neighborhood of cell $(i,\ j)$.

There are two normal interface reconstruction algorithms for the VOF method. One is based on Simple Line Interface Construction (SLIC) algorithm, and the other is based on Piecewise Linear Interface Construction (PLIC) algorithm. The SLIC algorithm is used in the early version of the VOF method, in which the interface is reconstructed with a piecewise constant function aligned to one of the coordinates. Since the constructed interface can only be either horizontal or vertical, these methods are crude in accuracy and generate spurious flotsam even in simulating simple flows. In the PLIC algorithm, the slope of the interface in cell is determined by the gradient of the volume of fraction distribution instead of a constant. Most modern versions of the VOF method are based on the PLIC algorithm to simulate the interfacial flows[6-11]. The calculation of the interface normal is an important part in the PLIC algorithm and it determines the accuracy of the PLIC algorithm. There are many algorithms to calculate the interface normal, such as the center of mass algorithm, the central difference algorithm[11], the Parker and Youngs method, the Least squares VOF Interface Reconstruction Algorithm (LVIRA) and the Efficient Least squares VOF Interface Reconstruction Algorithm (ELVIRA) and so on. Since the center of mass algorithm, the central difference algorithm and the Parker and Youngs method do not reconstruct all linear interface exactly, so at most the first-order accuracy can be achieved. In contrast, the LVIRA and ELVIRA can reconstruct a linear interface exactly and the second-order accuracy can be obtained. The ELVIRA method can save more computation time than the LVIRA method.

The advection schemes in the VOF method fall into two categories: the operator splitting method and the unsplit method. In most cases, the operator splitting method can reach the same accuracy as the unsplit methods. But in porous media problems, the unsplit method can give better results. Because of its simplicity, the operator splitting approach is dominant in the early development of the VOF method, such as the SLIC, Chorin, SOLA-VOF, FCT-VOF[12] and Youngs method. In recent years, the unsplit method[6,7,11] have become more popular. Rider and Kothe reported their advection schemes based on the PLIC algorithm. Their schemes need corner flux amendment. However double calculation fluxes are also inevitable. Therefore, the redistribution algorithms of the volume fraction are necessary as their method is used. An average transverse velocity is applied to avoid the corner fluxes amendment [8]. However the double fluxes also appear there. These problems are solved by using the Defined Donating Region (DDR) algorithm developed by Haivie and Fletcher[7]. But the DDR algorithm has a poor accuracy in flux calculation. They also established the stream scheme[6], in which no redistribution algorithm is needed while the integral error must be under control. A multidimensional advection scheme constructed by Lopez and Hernandez[9] supposed the same transverse velocity at the common nodes between neighbor cells and in this way they resolved the double fluxes problems. Most recently, a new advection method termed Polygonal Area Mapping (PAM) built by Zhang et al.[13] showed a better accuracy than existing advection schemes and the volume of the calculation did not significantly increase.

The unsplit methods is more efficient in calculating cell boundary fluxeses than the operator splitting schemes. Only one interface reconstruction per time step is required for the unsplit methods. The Unsplit Lagrangian Advection (ULA) scheme, as will be developed in this study, is a piecewise linear scheme with cell boundary fluxes integrated using an unsplit method. The ULA scheme owns the same advantages as the unsplit method, and hence it is different from the Split Lagrangian Advection (SLA) scheme[14,15].

In this article, the details of the new VOF advection scheme are described. Firstly, the new equation of the interface in cell is proposed, secondly, the fluxes between neighborhood cells are computed based on the new equation of the interface, finally, a comparison of the performance of the ULA scheme against the SLA scheme and FCT-VOF method is made by using three typical VOF advection tests.

2. Unsplit Lagrangian advection scheme

The present ULA scheme is based on structured rectangle mesh. There are two parts in the ULA scheme. One is to calculate the new positions of the interfaces in cells, the other is to compute the fluxes between cells based on the new calculated positions of the interfaces. A PLIC scheme is applied in the ULA scheme for interface tracking.

2.1 *Calculation of new position of interface*

In the PLIC scheme, the interface in cell is assumed to be a straight line with a normal calculated from the gradient of the volume fraction.

The general equation for a straight line in the (x, y) plane with the normal $\boldsymbol{n}$ is

$$n_1 x + n_2 y = \alpha \tag{5}$$

where n_1, n_2 are the components of the normal vector of interface, and α is a constant. Suppose the free surface in the i and jth grid cell at the moment t_n can be written as

$$n_1^n x^n + n_2^n y^n = \alpha^n \tag{6}$$

Then at the next moment $t_{n+1} = t_n + \tau$, where τ is time step, the free surface can be represented as

$$n_1^{n+1} x^{n+1} + n_2^{n+1} y^{n+1} = \alpha^{n+1} \tag{7}$$

The velocity components at any point on the free surface can be calculated through line interpolation of the velocity on cell faces, which can be expressed as

$$u(x) = U_0\left(1 - \frac{x}{c_1}\right) + U_h \frac{x}{c_1} \tag{8}$$

$$v(y) = V_0\left(1 - \frac{y}{c_2}\right) + V_h \frac{y}{c_2} \tag{9}$$

where U_0, U_h, V_0, V_h are normal velocities on cell faces respectively, and c_1, c_2 are the grid lengths in the x and y directions respectively. After time τ the new coordinates of any point on the free surface can be achieved according to the above velocities, which can be written as

$$x^{n+1} = x^n + u(x^n)\tau = \left[1 + \left(\frac{U_h - U_0}{c_1}\right)\tau\right] x^n + U_0\tau \tag{10}$$

$$y^{n+1} = y^n + v(y^n)\tau = \left[1 + \left(\frac{V_h - V_0}{c_2}\right)\tau\right] y^n + V_0\tau \tag{11}$$

From Eqs.(7)-(11) the following expressions can be derived:

$$x^n = \frac{x^{n+1} - U_0\tau}{1 + \left(\frac{U_h - U_0}{c_1}\right)\tau} \tag{12}$$

$$y^n = \frac{y^{n+1} - V_0\tau}{1 + \left(\frac{V_h - V_0}{c_2}\right)\tau} \tag{13}$$

Substituting Eqs.(12), (13) into Eq.(6) and rewriting Eq.(7) in the standard form lead to the following expressions:

$$n_1^{n+1} = \frac{n_1^n}{1 + \left(\frac{U_h - U_0}{c_1}\right)\tau} \tag{14a}$$

$$n_2^{n+1} = \frac{n_2^n}{1 + \left(\frac{V_h - V_0}{c_2}\right)\tau} \tag{14b}$$

$$\alpha^{n+1} = \alpha^n + \frac{n_1^n U_0\tau}{1 + \left(\frac{U_h - U_0}{c_1}\right)\tau} + \frac{n_2^n V_0\tau}{1 + \left(\frac{V_h - V_0}{c_2}\right)\tau} \tag{14c}$$

And the first step is finished here. The new interface Eq.(7) with the substitutions of expressions (14) is what we need.

If the new interface (i.e., the bold line in Fig.1) enters the neighboring cells, the fluxes between these cells need to be computed.

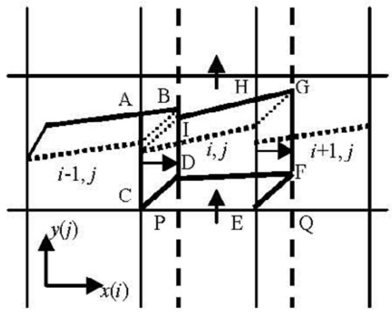

Fig.1 A 2-D sketch map of the ULA scheme. The dashed lines represent the initial interfaces in cells and the bold lines the new interface at next moment. The velocity on cell boundary is represented by arrow lines

2.2 *Fluxes computation*

The area of a region from a rectangle cut by a straight line can be given by a general formula

$$S = \frac{\alpha^2}{2n_1n_2}\left[1 - H(\alpha - n_1c_1)\left(\frac{\alpha - n_1c_1}{\alpha}\right) - \right.$$

$$\left. H(\alpha - n_2c_2)\left(\frac{\alpha - n_2c_2}{\alpha}\right)\right] \tag{15}$$

where $H(x)$ is the Heaviside step function defined as

$$H(x) = 0 \quad \text{for} \quad x < 0 \tag{16a}$$

$$H(x) = 1 \quad \text{for} \quad x > 0 \tag{16b}$$

Different from the SLA scheme fluxes computation, the ULA scheme is based on the new interface by cutting trapezoid instead of rectangle. Take Fig.1 for example, after a time step τ, the flux from cell (i, j) to cell ($i+1$, j) is the area of the trapezoid HGFE, S_{HGFE}, which can be calculated via

$$S_{\mathrm{HGFE}} = S_{\mathrm{HGQE}} - S_{\mathrm{EQF}} \tag{17}$$

where the area of the trapezoid HFQE, S_{HGQE}, can be calculated from Eq.(15) and the area of the triangle EQF, S_{EQF}, can be expressed as

$$S_{\mathrm{EQF}} = \frac{1}{2}U_hV_0\tau^2 \tag{18}$$

A coordinate transformation is needed to make use of Eq.(15) to calculate the area S_{HGQE}. Set

$$x^{n+1} = c_1 + x' \tag{19a}$$

$$y^{n+1} = c_2 + y' \tag{19b}$$

Substituting Eq.(19) into Eq.(7) yields

$$n_1^{n+1}x' + n_2^{n+1}y' = \alpha' \tag{20}$$

where

$$\alpha' = \alpha^{n+1} - n_1^{n+1}c_1 - n_2^{n+1}c_2 \tag{21}$$

Substituting the coefficients n_1^{n+1}, n_2^{n+1} and α' into Eq.(15) we can get calculate the area S_{HGQE}. Thereby the flux from cell (i, j) to cell ($i+1$, j) is obtained. All the fluxes through the boundary of cell (i, j) can be calculated in the same way as was described above. In the ULA scheme, the fluid volume changing in every cells are calculated directly, and then a new volume fraction f^{n+1} can be obtained:

$$f^{n+1} = f^n + \frac{\Delta\Phi}{A} = f^n + \frac{\Phi_+ + \Phi_-}{A} \tag{22}$$

where $\Delta\Phi$ is the volume change in cell, Φ_+ is the inflow volume for cell and it is positive, Φ_- is the outflow volume from cell and it is negative, $A = c_1c_2$ is the area of the cell. For the case of Fig.1 the outflow volume from cell (i, j), $\Phi_- = S_{\mathrm{HGFE}}$, and the inflow volume to cell (i, j), $\Phi_+ = S_{\mathrm{ABDC}} + S_{\mathrm{CDFE}}$. The area of the quadrilateral CDFE, S_{CDFE} can be calculated in the same way as S_{HGFE}. The flow chart of the ULA scheme is shown in Fig.2.

3. Tests

In this section three typical VOF advection tests are reported to make a comparison of the ULA scheme with the FCT-VOF scheme and the SLA scheme[15]. An analytical velocity field is given in Zalesak rotation test and shearing flow test. And the two fluids considered are inviscid and have constant density. Since the fluid velocity is specified during the above two advection scheme tests, it is easy to compare the advection methods without the effect of fluid behavior. While in the Rayleigh-Taylor instability test the viscosity of both the fluids is taken into consideration, resulting in a kind of real flow test.

In order to evaluate the accuracy of the advection schemes, two kinds of calculation errors are defined. One is the fractional error and defined as

$$E_1 = \frac{\sum_{i,j}\left|f_{i,j}^n - f_{i,j}^e\right|}{\sum_{i,j} f_{i,j}^0} \tag{23}$$

where f^n is the calculated solution after n time

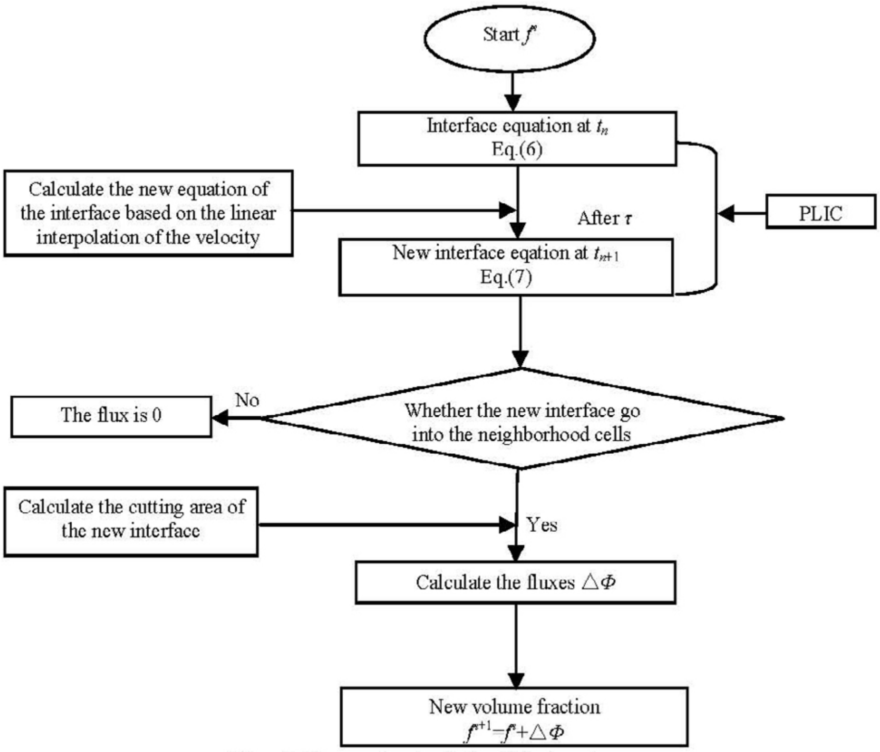

Fig.2 Flow chart of the ULA scheme

steps, f^e is the exact solution after n time steps and f^0 is the initial solution. The other is called percentage error and is estimated by

$$E_2 = 100\frac{\left|\sum_{i,j}^{N} f_{i,j}^{n} - \sum_{i,j}^{N} f_{i,j}^{0}\right|}{\sum_{i,j}^{N} f_{i,j}^{0}} \tag{24}$$

where N is the total number of cells in the domain, f^n is the volume fraction at the new time step and f^0 is the volume fraction at the initial time step. Equation (23) represents the local error of the advection scheme while Eq.(24) indicates the mass conservation ability of a given scheme.

3.1 *Zalesak rotation test*

Zalesak's solid-body rotation of a slotted circle is a widely-used test for the advection schemes. The computational domain is a square with dimensions 4 m×4 m with uniform mesh of size 200×200. The initial interface is shown in Fig.3(a). The diameter of the slotted circle is 50 mesh cells and the slot is 6 mesh cells in width and 25 mesh cells in depth. The center of the slotted circle is at (2.0, 2.75) and it rotates around the point (2.0, 2.0) with an angular velocity $\Omega = 0.5\text{rad/s}$. The velocity field is given by

$$U = -\Omega(y - y_0) \tag{25a}$$

$$V = \Omega(x - x_0) \tag{25b}$$

The time step is 0.005 s and one rotation corresponds to 2524 time steps. The calculation results of the ULA scheme, FCT-VOF method and the SLA scheme after one rotation are shown in Table 1 and Figs.3(b)-3(d).

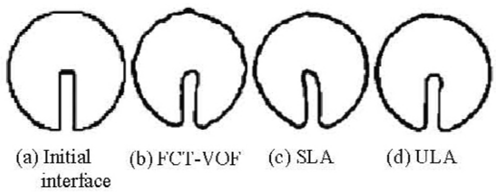

Fig.3 The slotted circle simulated after a rotation cycle

It is shown in Fig.3 that all the three advection schemes can achieve acceptable interface shapes, although the right angle corners at both ends of the slot are not reconstructed well. The ULA scheme gives a smoother circle. From Table 1, the fractional error of the ULA scheme is the smallest, which indicates that the ULA scheme can give a more accurate result than the other two schemes. It is noticed that only the ULA scheme gives a zero percentage error while the other two advection schemes give a limited value. It means that the ULA scheme can keep mass conservation exactly without any amendment.

Table 1 The fractional error and percentage error of the FCT-VOF method, SLA scheme and ULA scheme in Zalesak rotation test

Errors	FCT-VOF	SLA	ULA
E_1	0.0810	0.1761	0.0451
E_2	3.29×10^{-4}	6.37×10^{-5}	0

3.2 *Shearing flow test*

Since there is not any topological change in the Zalesak rotation test, it can not evaluate the comprehensive performance of an advection scheme. Because of the existence of the fluid shear, it is more complicated for realistic fluid flow. The present shearing flow test is performed to examine the complicated performance of the ULA scheme. The following two-dimensional velocity field is chosen:

$$U = \cos(x)\sin(y) \tag{26a}$$

$$V = -\sin(x)\cos(y) \tag{26b}$$

with $x, y \in [0, \pi]$. The mesh size is 100×100 and the initial free surface has a circle shape of radius $\pi/5$ with its center at $[\pi/2, \pi/3]$ as shown in Figs.4-6(a). The time step is $\pi/400$ and a total 2000 steps calculation is carried out, in which the first 1000 steps is performed before the signs of the velocity field change and the next 1000 steps is performed after the signs change. The calculation results of the ULA scheme, FCT-VOF method and the SLA scheme after 1000 steps and 2000 steps are shown in Figs.4-6. The corresponding fractional errors and percentage error results of the three advection schemes are listed in Table 2.

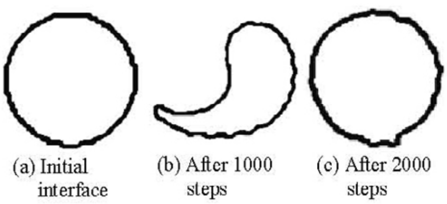

Fig.4 The simulation results with the FCT-VOF method

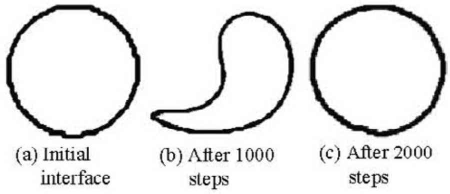

Fig.5 The simulation results with the SLA scheme

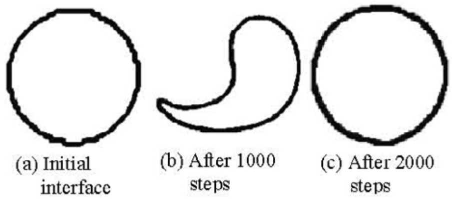

Fig.6 The simulation results with the ULA scheme

It can be seen from Figs.4 to 6 that after 2000 time steps, the SLA scheme and the ULA scheme exhibit the best performance, maintaining a sharp interface and also retaining the initial configuration. There are some burrs after 1000 time steps in the FCT-VOF calculation as shown in Fig.4(b). However it still retains the initial configuration with tiny unevenness after 2000 time steps as shown in Fig.4(c). Table 2 gives the progression of fractional errors and percentage errors at the 1000 and 2000 time steps. The errors for the ULA scheme are clearly lower than the other two schemes. The percentage error for the ULA scheme is still zero, consistent with the Zalesak rotation test.

Table 2 The fractional error and percentage error of the FCT-VOF method, SLA scheme and ULA scheme in shearing flow test

Errors		FCT-VOF	SLA	ULA
E_1	$N = 1000$	0.0255	0.0249	0.0121
	$N = 2000$	0.0540	0.0286	0.0150
E_2	$N = 1000$	3.56×10^{-4}	4.89×10^{-5}	0
	$N = 2000$	7.36×10^{-4}	9.69×10^{-5}	0

3.3 *Rayleigh-Taylor instability test*

The Rayleigh-Taylor instability is a good example to test the effect of coupled volume of fraction f and momentum transport, because the flow is density-driven and errors in the f field will lead to errors in the momentum solution. In the present Rayleigh-Taylor instability test, a higher density liquid is placed over a lower density liquid in a rectangular domain of 1 m $\times$ 4 m with a mesh resolution of 64$\times$256. The top half of the domain is filled with fluid of density $\rho_1 = 1.225\text{kg/m}^3$ and the bottom half with a fluid of density $\rho_2 = 0.1694\text{kg/m}^3$. The viscosity of both the fluids is taken as 3.13×10^3 kg/ms. Initially a perturbation given by the function $y = 0.05\cos(2\pi x)$ is applied at the interface, which results in a density driven flow. No-slip boundary conditions are used on all the wall boundaries. A constant time step of 0.0002 is used which approximately corresponds to the Courant number of 0.06.

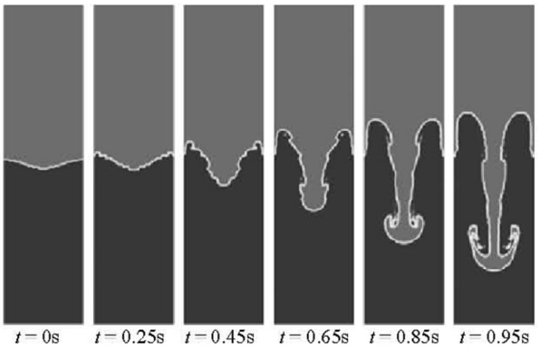

Fig.7 The evolution of Rayleigh-Taylor instability with time using FCT-VOF method

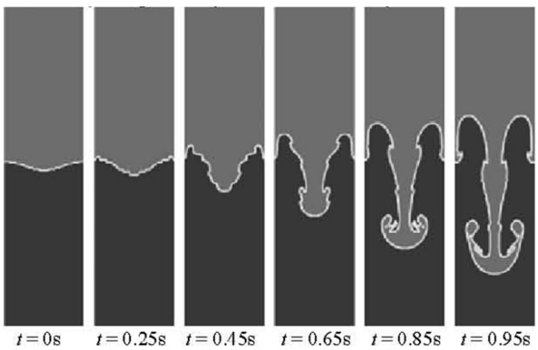

Fig.8 Theevolution of Rayleigh-Taylor instability with time using SLA scheme

Figures 7-9 show the evolution of the Rayleigh-Taylor instability using the FCT-VOF, SLA and ULA schemes at six different moments. From a qualitative point of view, the results from different schemes have simillar characteristics up to 0.45 s. From the moment 0.65 s on, the situation becomes different. The FCT-VOF method shows the formation of jetsam below the peak on both sides close to the wall and also close to the filament connected to the blob at the center as shown in Fig.7. The formation of the blob at the center is seen to have some burrs at the interface in the case of FCT-VOF compared to SLA scheme (Fig.8) and ULA scheme (Fig.9). Finally, the interface at the center takes some kind of an inverted mushroom shape, with smaller secondary filaments forming at the inner circumference of the mushroom. The formations of these secondary instabilities are more pronounced with the SLA and ULA schemes compared to more diffused solution of FCT-VOF.

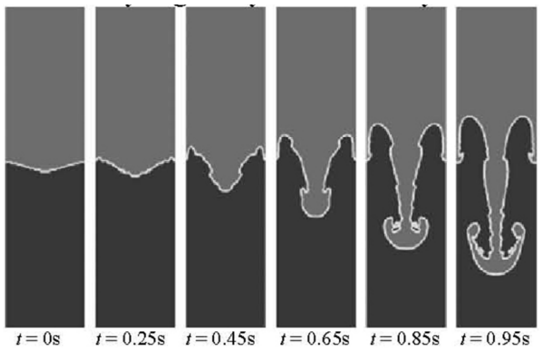

Fig.9 The evolution of Rayleigh-Taylor instability with time using ULA scheme

Table 3 shows the percentage errors of the schemes at different time steps. It can be clearly seen that the FCT is the most diffusive scheme with a largest mass loss relative to the SLA and ULA schemes, which explains the diffusive solution obtained by the FCT-VOF. The ULA scheme is superior with 100% mass conservation.

4. Conclusion

A new advection scheme based on PLIC scheme, named as the ULA scheme, for VOF method has been developed in this article. This method can be used to calculate the flux through tracking the new position of the interfaces in cells. If the new interface from one cell goes into the neighboring cells, then the flux between these cells can be calculated based on geometric tools. In the ULA scheme the outflow flux for one cell is the inflow flux for another cell. In this way, the mass conservation can be kept exactly without any amendment algorithm. The performance of the ULA scheme is tested using three typical advection calculation examples and the comparison with the FCT-VOF method and the SLA scheme is made. A reasonable interface can be achieved for all the three advection schemes. The ULA scheme can reach a higher accuracy for flux calculation than the other two schemes and can keep the mass conservation exactly. The ULA scheme presented in this article is based on structural mesh and its unstructural application needs further research.

Table 3 The fractional error and percentage error of the FCT-VOF method, SLA scheme and ULA scheme in Rayleigh-Taylor instability test

Times	Errors	FCT	SLA ($\times 10^{-3}$)	ULA ($\times 10^{-3}$)
0.25 s	E_1	0.201	0.2412	0.05022
	E_2	0.0151	0.01225	0
0.45 s	E_1	1.052	0.137	0.07217
	E_2	0.15	0.0637	0
0.65 s	E_1	4.015	9.236	0.9156
	E_2	0.6876	0.8946	0
0.85 s	E_1	8.214	89	1.565
	E_2	1.5167	44	0
0.95 s	E_1	9.089	38.2	1.565
	E_2	2.6791	17.4	0

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