

MMALE numerical simulation for multi-material large deformation fluid flows

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Abstract. Multi-material arbitrary Lagrangian Eulerian (MMALE) method, coupled with moment of fluid (MOF) interface reconstruction, was studied and applied to multi-material large deformation flow problems. In MMALE method, the mesh lines are allowed to cross the material interfaces and mixed cells are introduced. In mixed cells, the MOF method is used to reconstruct the interfaces. The numerical examples show the high accuracy and resolution of MOF-MMALE, it is validated that MOF-MMALE method is an effective way to simulate flow problems of multi-material large deformation.

1. Introduction

Multi-material large deformation fluid flows exist frequently in astrophysics, weapon physics and inertial confinement fusion (ICF) fields. There are two important characteristics in these kinds of flow phenomena. One is the violent movement of the fluid, which leads to large deformation of fluid field, the other is the existence of multi-material and the distortion of the interface between different materials. Up to now, numerical simulation is one of the major ways to study these problems. In numerical simulation of multi-material large deformation fluid flows, the most important thing is tracking the material interfaces accurately while dealing with the large deformation of fluid flows simultaneously.

The numerical methods for multi-material large deformation fluid flows are Lagrangian method, Eulerian method or arbitrary Lagrangian-Eulerian (ALE) method. In these methods, such-and-such difficulties are exist. Lagrangian method can track the material interfaces sharply, but it can't deal with the large deformation of computational mesh. Eulerian method can hold the large deformation of fluid flows, but it will bring large numerical diffusion of physical variables. If the deformation of fluid is small, ALE method is the best selection, but if the deformation is large, ALE method is helpless.

To alter this predicament of numerical simulation of multi-material large deformation fluid flows, many research teams (LLNL, LANL, AWE, CEA, IAPCM, etc.) start to develop newly numerical frame to overcome this difficulty and multi-material ALE (MMALE) method[1-3] is presented. In MMALE, mixed cells are introduced and the material interfaces are permitted to cross computational cells. Here mixed cells are cells including two or more kinds of materials. The introduction of mixed cells make the computational code robust while keep the computational results as accurate as possible. To handle the material interfaces in mixed cells, moment of fluid (MOF) interface reconstruction method[4-6] is used in MMALE simulations. MMALE method is employed widely in the computation of multi-material and large deformation fluid flows.

The MMALE method coupled with MOF interface reconstruction (MOF-MMALE) was studied, and applied to multi-material large deformation flow problems. This paper is organized as follows. In section



2, we present the theoretical system of MMALE numerical simulation. The theoretical system is consisted of single velocity multi-material model, Lagrangian computing, rezoning, remapping, closure model and MOF interface reconstruction. Next, some numerical examples include more than two materials to emphasize key properties of MMALE method in Section 3. Finally, conclusions and perspectives about future works are given in Section 4.

2. MMALE method

Because of the introduction of mixed cells in MMALE, extra steps are needed to accomplish this framework, such as capturing the interface, closing the system of equations, and computing the equation of state in mixed cell.

The flowchart of MMALE method is shown in figure 1. First, the Lagrangian computing is performed, in this step the velocity, mesh, density variables are updated. Then the closure model is called to update the volume fraction. Next, the mesh is rezoned to obtain new mesh with good quality. Subsequently, MOF interface reconstruction is employed to determine the position of material interfaces. Finally, the physical variables are remapped to transfer the old variables from old mesh to new mesh. Hereto, one step of MMALE method is finished.

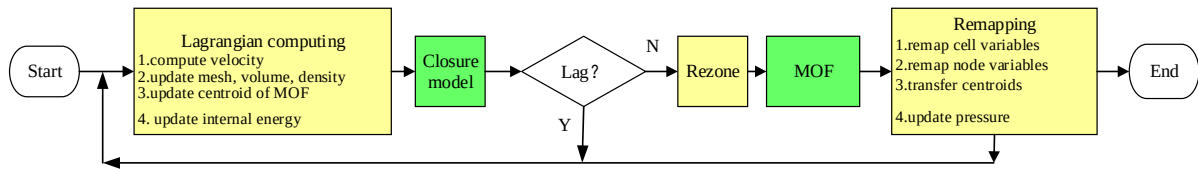


Figure 1. The flowchart of MMALE method.

2.1. Single Velocity multi-material model

In mixed cell, single velocity multi-material model[7] is adopted. In this model, different materials in one mixed cell have same velocity but different thermodynamic state, as shown in figure 2.

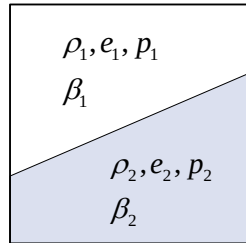


Figure 2. Mixed cell.

The system of equations of single velocity multi-material model can be written as

$$\begin{aligned}
 \frac{d\mathbf{u}}{dt} &= -\frac{1}{\rho} \nabla p \\
 \frac{d\rho_i}{dt} &= -\rho_i \nabla \cdot \mathbf{u}_i \\
 \frac{d\beta_i}{dt} &= \beta_i (\nabla \cdot \mathbf{u}_i - \nabla \cdot \mathbf{u}) \\
 \frac{de_i}{dt} &= -\frac{p_i}{\rho_i} \nabla \cdot \mathbf{u}_i \\
 \frac{d\mathbf{x}}{dt} &= \mathbf{u}
 \end{aligned} \tag{1}$$

Here $\rho_i, \mathbf{u}_i, \beta_i, e_i$ and p_i are density, velocity, volume fraction, specific internal energy and pressure of the i th material, respectively. $\mathbf{u}$ is the velocity, ρ is the average density and p is the average pressure. the equation of state of the material is given by

$$p_i = p_i(\rho_i, e_i) \quad (2)$$

The system of equation (1) for a multi-material medium is not closed and one needs to use some closing relations in mixed cells. The closure model will be discussed in subsection 2.4.

2.2. Lagrangian computing

Lagrangian computing is performed in staggered mesh. In staggered mesh, the coordinate and velocity are defined at cell nodes and state variables, such as density, pressure, are defined at cell centers. For space discretization, compatible hydrodynamic algorithms are used and extended to multi-material case in our MMALE method. Compatible hydrodynamic algorithms[8] are classical algorithms to solve the system of hydrodynamic equations in staggered mesh, and applied in many large scientific code. Predictor-corrector algorithms are employed for time discretization, which can reach two order accuracy in time.

2.3. Rezoning and remapping

Rezoning is an important step in MMALE to get new mesh with good quality. In current implementation of our MMALE method, only simple rezoning strategy is used, for example, rezoning to initial mesh or Winslow rezoning algorithm. Small adjustment is applied according to actual problems. More refined rezoning algorithms will be integrated into our code to improve the robustness and capacity of our code in future works.

The remapping must be split into two steps, one for cell variables and the other for node variables. For cell variables remapping, Sutherland-Hodgman polygon intersection algorithm is used. For node variables remapping, the subcell remapping algorithm[9] is used.

2.4. Closure model

In Lagrangian computing step, not only the mesh, velocity, density, but also the volume fraction are needed to update. After remapping step, the average pressure in mixed cell is also resolved. Extra assumptions are added to compute the material divergence and average pressure in mixed cell.

Currently, equal compressibility is provided. Equal compressibility model is based on assumption of that the compressibility of each material in mixed cell is equal, and the different material divergence is equal each other.

$$\nabla \cdot \mathbf{u}_i = \nabla \cdot \mathbf{u} \quad (3)$$

We can deduce easily that

$$\frac{d\beta_i}{dt} = 0 \quad (4)$$

Which shows that the volume fraction is not changed in equal compressibility model. The average pressure is given by

$$p = \sum_i \beta_i p_i \quad (5)$$

2.5. MOF interface reconstruction

MOF interface reconstruction method was suggested by Dyadechko in 2005[4], many features of which are similar to VOF. In figure 3, MOF interface reconstruction in a mixed cell including two materials is shown. The curve segment is true interface between materials and the straight is

reconstructed interface. The region Ω with shadow is reference material, Φ is angle between the interface and the x-axis, $0 \leq \Phi < 2\pi$. $(n_x, n_y) = (\cos\Phi, \sin\Phi)$ is the direction of interface, which points from the interface to the inside of reference material. (x_c, y_c) is centroid of the reference material.

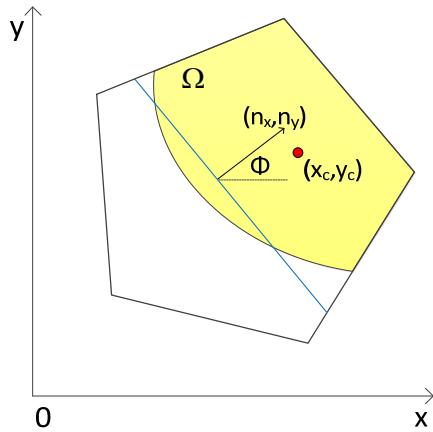


Figure 3. MOF interface reconstruction.

MOF achieves second-order accuracy by tracking and using the volume fractions and first moments or centroid of each material region in a computational cell. In plane coordinates, centroid is defined as

$$x_c = A_\Omega^{-1} \int_\Omega x dx dy, \quad y_c = A_\Omega^{-1} \int_\Omega y dx dy \quad (6)$$

Here $A_\Omega = \int_\Omega dx dy$ is the area of region Ω .

The location of the linear interface in each mixed cell is chosen to preserve the volumes and provide the best possible approximation to the material centroids. The object function is minimized using a optimizing process to obtain the direction of interface

$$E(\phi) = [x_c^{\text{comp}}(\phi) - x_c]^2 + [y_c^{\text{comp}}(\phi) - y_c]^2 \quad (7)$$

Here $(x_c^{\text{comp}}, y_c^{\text{comp}})$ is computational centroid.

3. Numerical examples

All the numerical results presented in this section are performed in plane geometry. The material are characterized by a perfect gas equation of state which writes $p = \rho e(\gamma - 1)$ where γ stands for the specific heat ratio of the gas.

3.1. Two-material shock tube problem

Consider a two-material shock tube problem. The computational domain is $[0,1]$ with an interface initially located at $x=0.5$. The initial state for left material are $(\rho_l, p_l, \mathbf{u}_l, \gamma_l) = (1, 1, 0, 1.4)$ and $(\rho_r, p_r, \mathbf{u}_r, \gamma_r) = (0.125, 0.1, 0, 5/3)$ for the right material. This is a true multi-material problem because of the different specific heat ratio.

We set all the physical boundaries as solid walls, and paved 200, 400 cells on the computational domain. The problem is simulated by MMALE method and Lagrangian method. In rezoning step of MMALE simulation, the new mesh is rezoned back to initial mesh which is actually equivalent with Eulerian method. We compared the MMALE numerical results with exact solution and Lagrangian results in figure 4. We have found from these figures that not only MMALE results but also Lagrangian results are both shown good agreement with exact solutions. Some inaccuracy appears in specific

internal energy figure near the contact discontinuity for Lagrangian results, but doesn't for MMALE results.

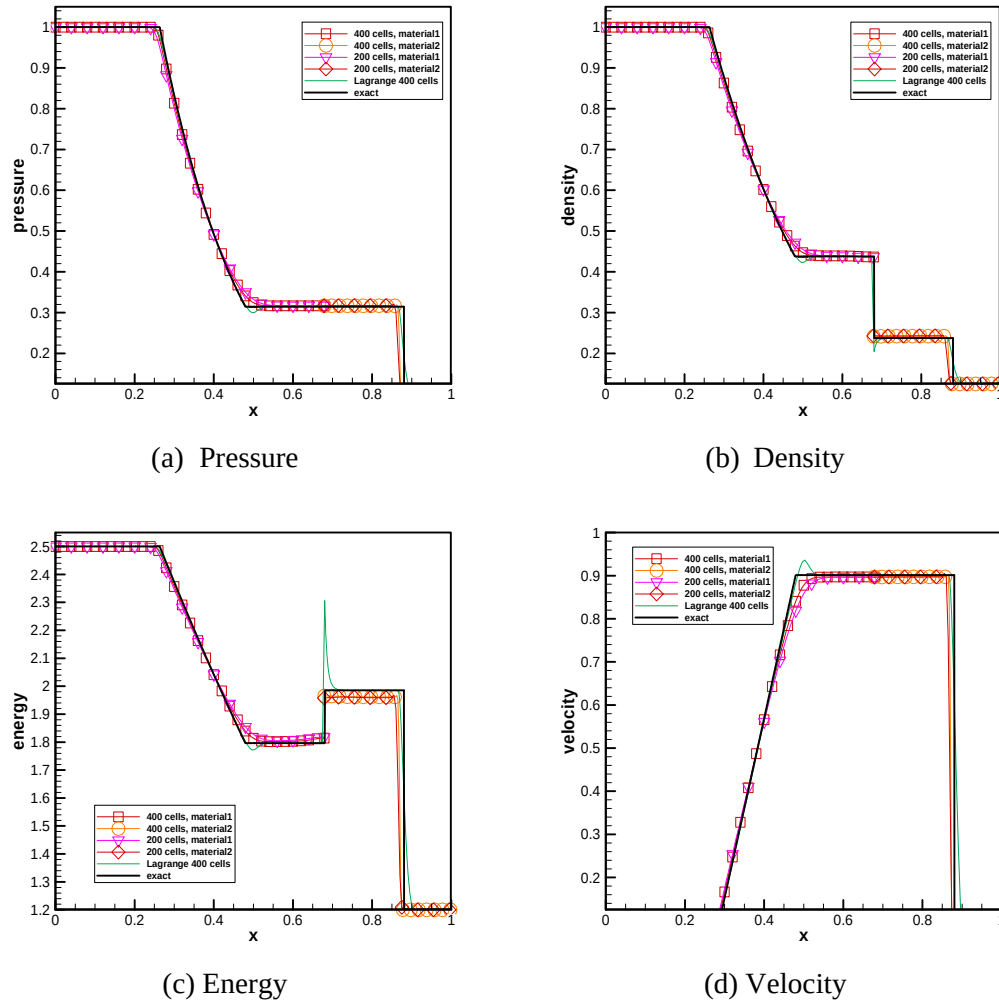


Figure 4. Two-material shock tube problem. Comparison of MMALE results with exact solutions and Lagrangian results.

3.2. Rayleigh-Taylor instability

This test case deals with the well-known Rayleigh-Taylor instability. The computational domain is the rectangular box $[0,1/3] \times [0,1]$ which is paved with 34×100 cells. The initial set up consists of two immiscible fluids which are separated by a perturbed interface, whose equation writes $y_i(x) = 0.5 + a_0 \cos(6\pi x)$, $a_0 = 0.01$. The heavy fluid is located above the light one. The densities of the two fluids are $\rho_h = 2$ and $\rho_l = 1$. The same polytropic index $\gamma_h = \gamma_l = 1.4$ is shared by the two fluids. A downward gravity field is applied, $\mathbf{g} = (g_x, g_y)^t = (0, -0.1)^t$.

This configuration is not stable, the heavy fluid will sink and light fluid will rise. We set all the physical boundaries as solid walls and set time step $dt=0.001$. Mixed cells are existed at initial time. The MMALE numerical results for ten moments from time 1 to 10 is shown in figure 5, the time evolution of the instability can be seen clearly from these ten figures. It can also be seen from these figures that MOF-MMALE can identify small or tiny structure, for example, the “hook” structure near the edge of

the heavy fluid “mushroom” is reconstructed successfully by MOF-MMLAE. This capacity of high resolution is attributed to MOF interface reconstruction.

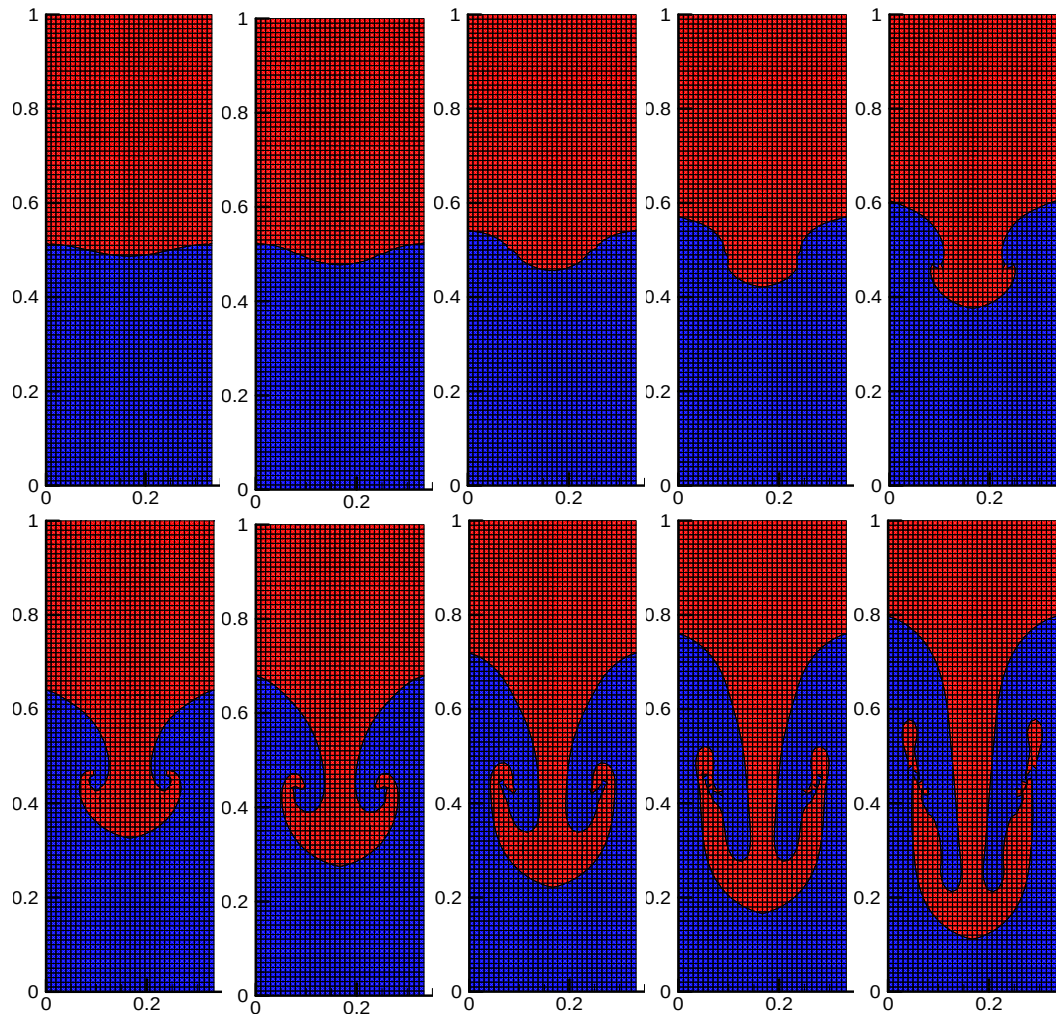


Figure 5. MMALE numerical results of Rayleigh-Taylor instability problem for ten moments from time 1 to 10.

3.3. Interaction of shock wave with Helium bubble

This test case corresponds to the interaction of shock wave with a cylindrical Helium bubble surrounded by air at rest. Consider a rectangular domain of dimensions $[0,0.65] \times [-0.089,0.089]$ initially full of air of data $(\rho_a, p_a, \mathbf{u}_a, \gamma_a) = (1, 10^5, 0, 1.4)$ displayed in figure 6. The cylindrical bubble is represented by a disk characterized by its center $(x, y) = (0.32, 0)$ and its radius $r = 0.025$. The initial data of Helium bubble are $(\rho_h, p_h, \mathbf{u}_h, \gamma_h) = (0.182, 10^5, 0, 1.648)$. We set all boundary conditions as solid wall except at the right end where we impose a piston boundary condition defined by the inward velocity $u^* = -124.824$. The moving of the piston will produce a shock wave, and the shock wave will interact with the Helium bubble at time $t_i = 668.153 \times 10^{-6}$. MOF-MMALE method is used to simulate this problem.

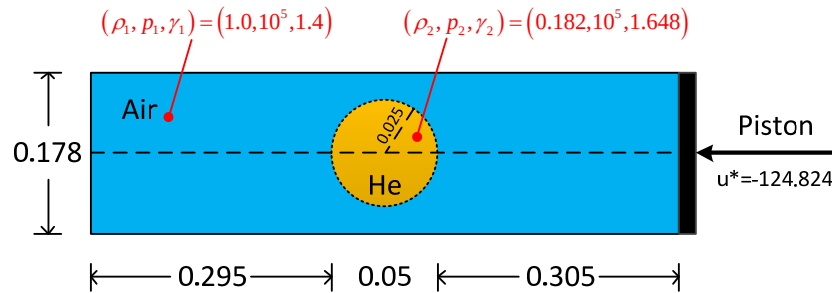


Figure 6. Interaction of shock wave with Helium bubble.

To compute this problem, we paved the computational domain with 260×72 cells and fixed the time step $dt = 10^{-7}$. In this case, the initialization of the volume fraction is performed by computing the intersection between the circle, which corresponds to the bubble boundary, and the initial mesh. The last time of computation is set to 1342×10^{-6} . We have performed computations with MMALE method and displayed in figure 7 the time evolution of the bubble at three different moments of 800×10^{-6} , 1100×10^{-6} and 1342×10^{-6} . At each step, we distribute the cells equally in the computational domain compressed by the right end piston.

The comparison of an experimental image[10] and the numerical results of interface at the final time has been displayed in figure 8. It shows a good agreement that validates our MOF-MMALE method from a qualitative point of view.

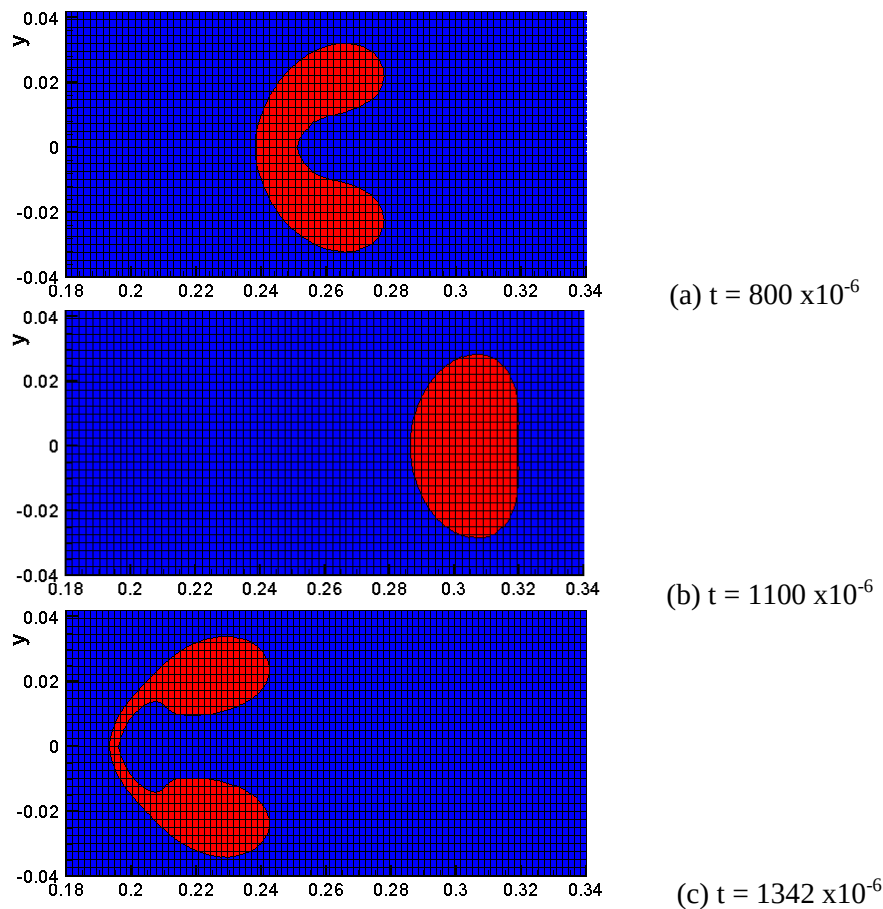


Figure 7. Interface of Helium bubble at three different moments.

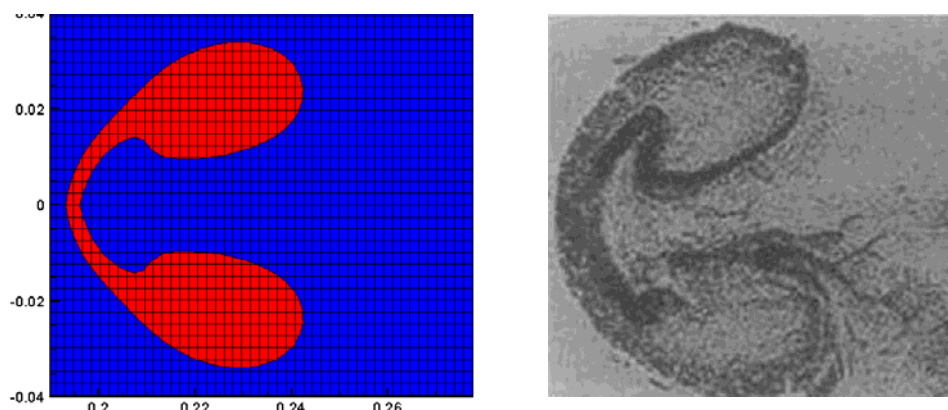


Figure 8. Comparison of MOF-MMALE interface (left) with experiment (right) at final time 1342×10^{-6} .

4. Conclusions and future works

We have described MOF-MMALE method devoted to the numerical simulation of multi-material large deformation fluid flows. The basic ideal of MOF-MMALE is to introduce mixed cells based on traditional ALE method. The introduction of mixed cells can increase the freedom of mesh rezoning and reduce the deformation of computational mesh, which make the MMALE method deal with the large deformation of fluid flows easily. On the other hand, MOF interface reconstruction is employed to determine the material interface in mixed cell.

Though some models used in current MOF-MMALE method are simple, the numerical results have shown the outstanding capacity, accuracy and efficiency in simulation of multi-material large deformation fluid flows. MOF-MMALE method is an effective way to simulate flow problems of multi-material large deformation.

The future works include improving the thermodynamic closure model, increasing mesh scale and performing large-scale parallel computing.

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