A very robust MMALE method based on a novel VoF method for compressible fluid flows

Bojiao Sha

sepervisor：Prof. Zupeng Jia

Graduate School of China Academy of Engineering Physics

Institute of Applied Physics and Computational Mathematics

Outline

- Research background
- Review of VoF algorithm
- Review of MoF algorithm
- A novel SVoF algorithm
- MMALE method based on SVoF algorithm
- Example of 2D SVoF algorithm and its application in MMALE
- Example of 3D SVoF algorithm and its application in MMALE
- Conclusion

Research background

- In the practical problems of implosion dynamics and ICF, the large deformation of multi-material and interface instability caused by strong shearing deformation pose challenges to the numerical methods.
- In the last two decades, the Multi-Material ALE method (MMALE) have been developed for the simulation of such problems.

J.S. Peery, D.E. Carroll, Comput. Methods Appl. Mech. Eng. 187 (2000) 591–619.

S. Galera, P.-H. Maire, J. Breil, J. Comput. Phys. 229 (2010) 5755–5787.

S. Galera, J. Breil, P.-H. Maire, Comput. Fluids 229 (2010) 5755–5787.

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- Characteristics of MMALE method :
  1) By introducing mixed cells that allow multiple materials within a cell, material interfaces can cross the cell
  2) Handling large deformation of mesh by rezoning and remapping
  3) Handling large deformation of interface with interface capturing methods(VoF, MoF)
- The interface reconstruction algorithm is an important part of the MMALE method.
- In practical applications, the accuracy and robustness of VoF methods need further improvement.

- Review of VoF algorithm

1) geometric VoF

SLIC, W. F. Noh, 1976

PLIC, D. L. Youngs, 1982

LVIRA, J. E. Pilliod, E. G. Puckett, 2004

2) algebraic VoF

FCT-VoF, M. Rudman, 1997

CICSAM, C. Ubbink, R.I. Issa, 1999

3) algebraic-geometric VoF

THINC, F. Xiao, 2005

TVD-VoF, S. Pirozzoli, 2019

Steps (take the least squares VoF method as an example) :

- Determine the normal of the linear interface $\boldsymbol{n} = \nabla f / |\nabla f|$——solving the minimal problem :

$$min \sum_{c' \in N(c)} [f_{c'} - f_c - \nabla f_c \cdot (\boldsymbol{x}_{c'} - \boldsymbol{x}_c)]^2 \omega_{c'}$$

where f is volume fraction, $\omega_{c'} = 1/|\boldsymbol{x}_{c'} - \boldsymbol{x}_c|^2$

- Determine the intercept of the linear interface d——solving nonlinear equations : $g(d) = V(d) - V = 0$

where V is the given area of reference material in mixed cell, $V(d)$ is its area of the intercepted polygon by the linear interface $\boldsymbol{n} \cdot \boldsymbol{x} + d = 0$ in mixed cell

- Advantages of VoF algorithm :

only need volume fraction, don’t need other data(eg: material centroid)

- Disadvantages of VoF algorithm :
  - ✓ information of neighboring cells are needed to compute the normal of the linear interface, 2D case : 8 neighboring cells; 3D case : 26 neighboring cells
  - ✓ poor continuity of the interfaces
- Need to develop more accurate and robust 2D and 3D VoF methods in practical applications.

- Review of MoF algorithm

1） analytical reconstruction — high efficiency, high accuracy

Lemoine，2017，J.C.P. ；   Lemoine，2020，J.C.P.

Cheng Wang, 2021, Journal of Beijing Institute of Technology

2） local optimization— efficient, accurate, less robust

Dyadechko，2005，LA-UR-05-7571

Ahn，2007，J.C.P.

Chen，2017，J.C.P.

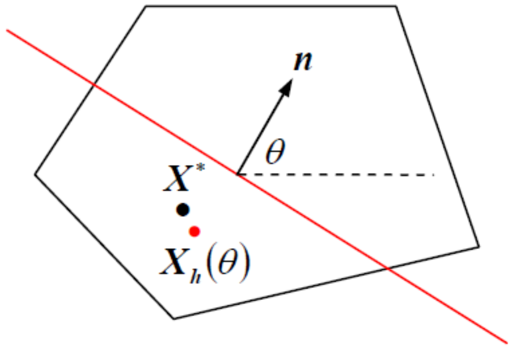
3） global optimization— less efficient, accurate, robust

Qing，2019， J.C.P.

MoF algorithm (2D case)

- Condition : material volume fraction f^*, material centroid $\boldsymbol{X}^*$
- Determine the normal $\boldsymbol{n}(\theta)$ and intercept of the linear interface, satisfying that the volume fraction of material polygon intercepted by the linear interface equals to f^*, and centroid $\boldsymbol{X}_h(\theta)$ as close as possible to $\boldsymbol{X}^*$, that is

$$\min f(\theta) = \|\boldsymbol{X}_h(\theta) - \boldsymbol{X}^*\|_2^2, \quad 0 \le \theta \le 2\pi$$

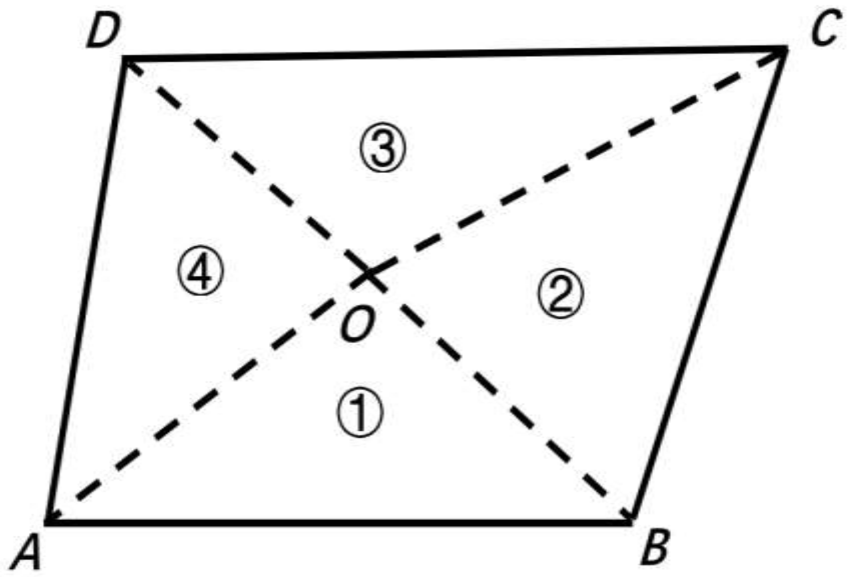


Schematic of MoF algorithm

- Advantages of MoF algorithm :
  - ✓ No need of information from neighboring cells
  - ✓ Higher accuracy than VoF, better interface continuity
  - ✓ No dependence on reconstruction order in three-material interface reconstruction
- Disadvantages of MoF algorithm :
  - ✓ Its accuracy and robustness deteriorate when the material centroids are incompatible with the volume fraction, such as large aspect ratio cell, accumulation of errors in long-time calculations

Novel SVoF algorithm

- Take a 2D quadrilateral cell $\Omega\ (ABCD)$ as an example, let O be its center.
- Fitst dissect Ω by connecting the center O to each of the four vertices, and divide the cell Ω into four subcells $\Omega_k (k = 1, \ldots, 4)$.
- Assume that the volume fraction of each material in each subcell is given. Then the volume fraction of each material in the mixed cell Ω can be obtained by a simple calculation.



mixed cell Ω and its dissection

- The desired linear interface must satisfy two conditions :

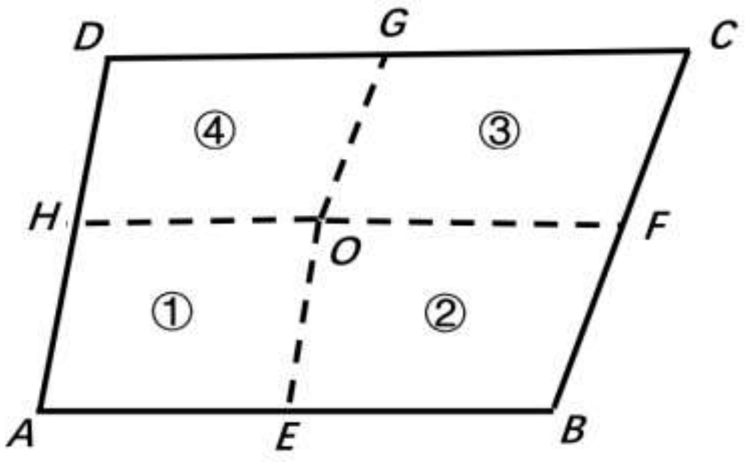
(1) Exactly meet the volume fraction of the specified material in the cell Ω

(2) Minimize the following functional : min $g(\theta) = \sum_{k=1}^{4}(f_k(\theta) - f_k^*)^2$

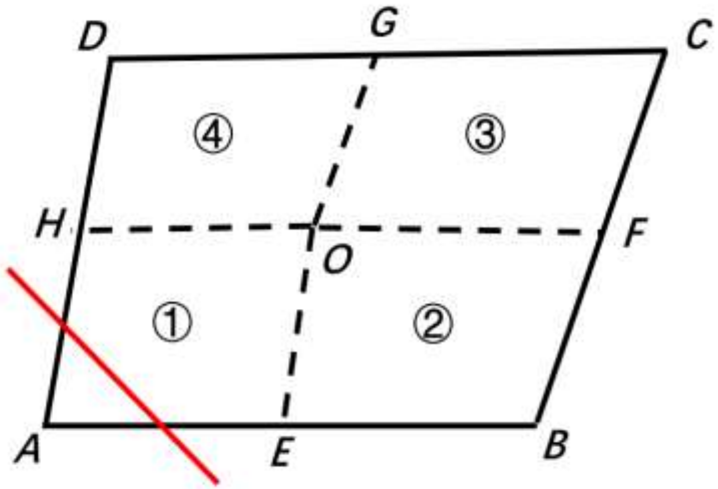
where f_k^* is the given volume fraction of the specified material in Ω_k, $f_k(\theta)$ is obtained as follows : first give the normal $\boldsymbol{n}(\theta) = (\cos(\theta), \sin(\theta))$, find the linear interface that satisfies condition (1) , then use it to intercept each Ω_k to obtain the volume fraction $f_k(\theta)$ of the specified material in Ω_k.

- An improved quadratic fit golden section algorithm is used to solve the above minimization problem.

- There is another dissection for quadrilateral cells, as shown in the left figure. Under this dissection, the minimization procedure fails in some cases.
- Suppose the interface is located at one corner of the cell, as shown in the right figure. In this case the linear interface cannot be uniquely determined.



another dissection



the interface is located at one corner of the cell

- Under the second dissection, the objective function is shown in the left figure, it is constant in an interval. This leads to the failure of the minimization.
- While under the first dissection, the objective function has a unique minimum, as shown in the right figure.

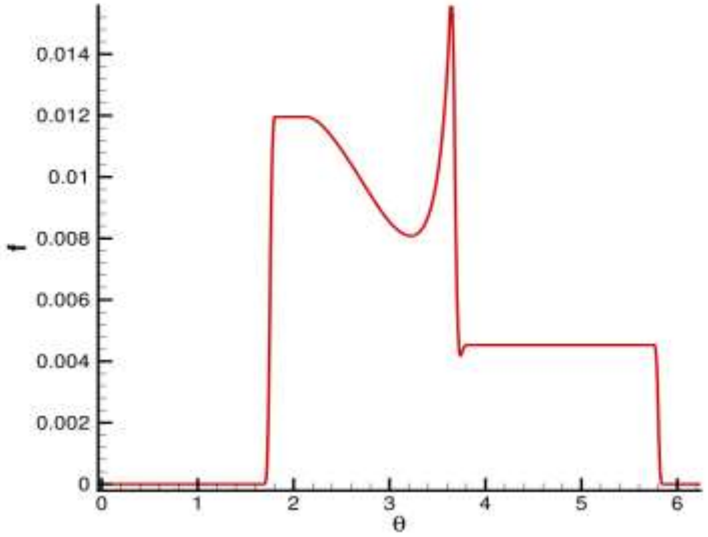


image of the objective function under second dissection

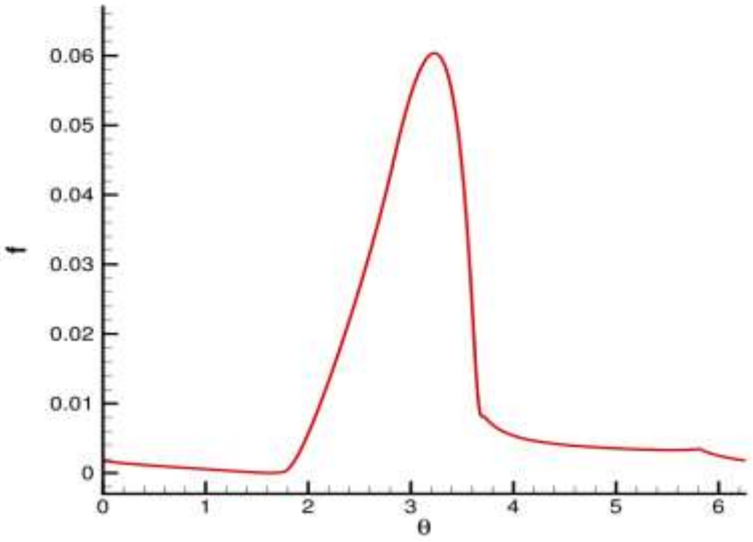
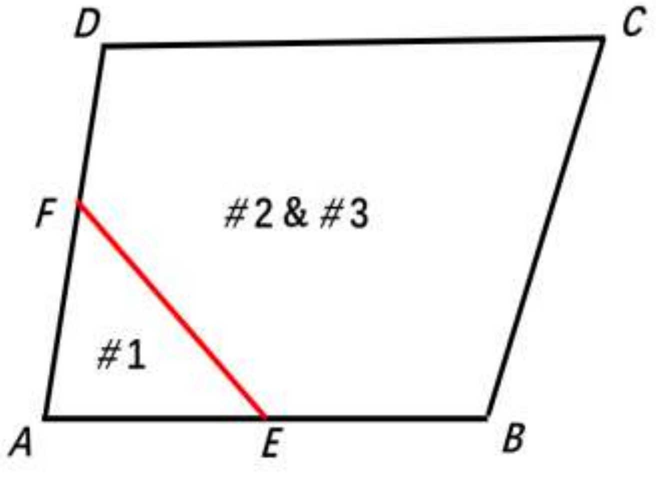
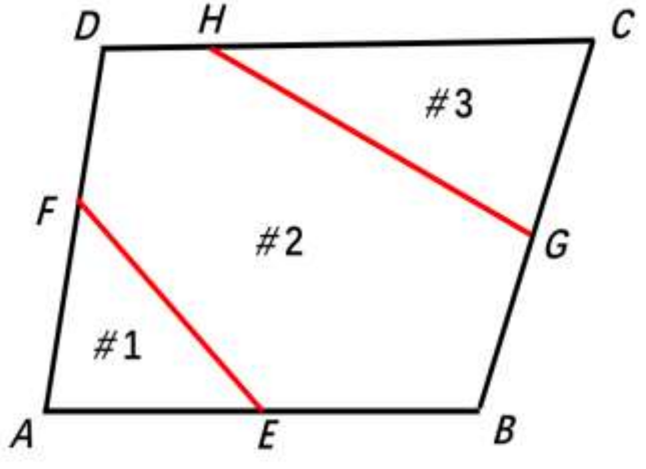


image of the objective function under first dissection

- Three-material interface reconstruction of MoF
- Cut the cell sequentially in a specified order (nested dissection), referred to as the ND algorithm.
- There are 6 possible reconstruction orders, taking (#1, #2, #3) as an example, as shown in the figure.
- 1) cut #1 out of the mixed cell; 2) cut #2 out of the union of #2 and #3
- For each order, calculate a value based on the given data and reconstruction results. Select the reconstruction order corresponding to the smallest value.

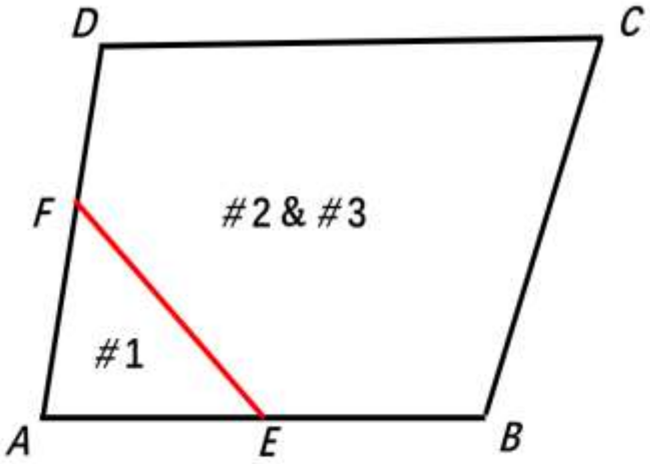


first step

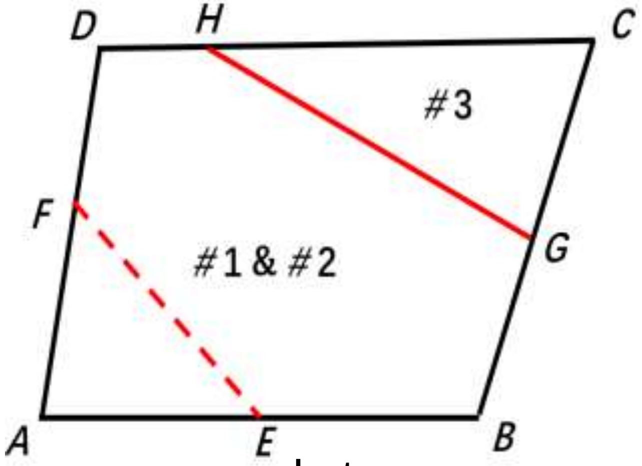


second step

- Our algorithm differs from the ND algorithm.
- Suppose : the area $volf(k)$ of each material k is given; the material centroid $\boldsymbol{x}_{c,k}^{*}$ of each material is also given.
- Taking (#1, #2, #3) as an example, the procedure is shown in the figure.
- 1) cut #1 out of the mixed cell; 2) cut the union of #1 and #2 out of the mixed cell to get the polygon of #3.



first step



second step

- We obtain reconstructed centroids $\boldsymbol{x}_{c,1}$, $\boldsymbol{x}_{c,3}$, $\boldsymbol{x}_{c,12}$ of #1, #3 and the union of #1 and #2, respectively . The reconstructed centroid $\boldsymbol{x}_{c,2}$ of #2 can be calculated by :

$$\boldsymbol{x}_{c,2} = (\boldsymbol{x}_{c,12} \cdot \big(volf(1) + volf(2)\big) - \boldsymbol{x}_{c,1} \cdot volf(1))/volf(2)$$

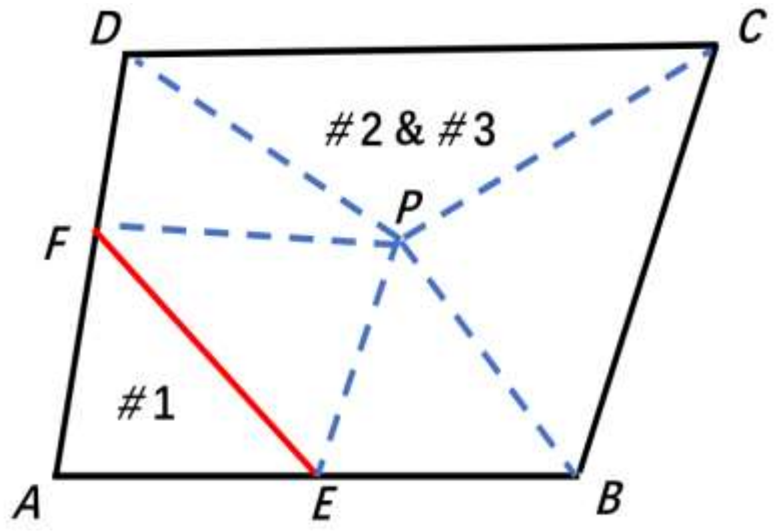
- For each order $m(m = 1, \ldots 6)$, introduce a value $fv(m)$:

$$fv(m) = \left\|\boldsymbol{x}_{c,1} - \boldsymbol{x}_{c,1}^{*}\right\|^2 + \left\|\boldsymbol{x}_{c,2} - \boldsymbol{x}_{c,2}^{*}\right\|^2 + \left\|\boldsymbol{x}_{c,3} - \boldsymbol{x}_{c,3}^{*}\right\|^2$$

- Let the smallest of them be $fv(m_0)$, select the reconstruction order corresponding to it.

- In SVoF algorithm, the material centroids are only used to determine the reconstruction order in three-material interface reconstruction.

- If the ND algorithm is used, we need to cut #2 from the union of #2 and #3.
- First, the union of #2 and #3 is dissected, as shown on the right, and the volume fraction of each material in the subcells need to be given.
- It is difficult to give the volume fraction of each material in these subcells. So we use the above algorithm rather than ND in three-material interface reconstruction.



second step of ND algorithm

MMALE method based on SVoF algorithm

- Lagrangian step

    Maire’s cell-centered scheme(2D), The compatible scheme(3D)

    Tipton’s pressure relaxation closure model

- Rezoning step

    Winslow’s algorithm , knupp’s algorithm

- Interface reconstruction step

    novel SVoF algorithm

- Remapping step

    integral conservative remapping method based on a polygon-intersection algorithm

    the volume fractions of all materials in each of the subcells are also remapped for any multi-material Lagrangian cell

- Update the physical quantities of the mixed cell with the Tipton's pressure relaxation closure model.
- At time moments $t^n, t^{n+\frac{1}{2}}, t^{n+1}$, $\boldsymbol{x}^n, \boldsymbol{x}^{n+\frac{1}{2}}, \boldsymbol{x}^{n+1}$ are the coordinates, $V^n, V^{n+\frac{1}{2}}, V^{n+1}$ are the volumes of the cell. The characteristic length of the cell is denoted by L^n.
- $\Delta V^{n+\frac{1}{2}} = V^{n+\frac{1}{2}} - V^n$, $\Delta V^{n+1} = V^{n+1} - V^n$. The index l is used to identify specific materials.
- Suppose $p_l^{n+\frac{1}{2}} + R_l^{n+\frac{1}{2}} = \hat{p}^{n+\frac{1}{2}}$, where $R_l^{n+\frac{1}{2}} = -\rho_l^n c_l^n \frac{L^n}{\Delta t} \frac{1}{V_l^n} \Delta V_l^{n+\frac{1}{2}}$ is the relaxation term that emulates bulk viscosity.
- The pressure $p_l^{n+\frac{1}{2}}$ is obtained by the isentropic assumption,

$$p_l^{n+\frac{1}{2}} = p_l^n - \rho_l^n (c_l^n)^2 \Delta V_l^{n+\frac{1}{2}} / V_l^n.$$

- Get a system of linear equations about $\hat{p}^{n+\frac{1}{2}}$ and $\Delta V_l^{n+\frac{1}{2}}$

$$p_l^n - \frac{\rho_l^n (c_l^n)^2 \left[1+\frac{L^n}{c_l^n \Delta t}\right] \Delta V_l^{n+\frac{1}{2}}}{V_l^n} = \hat{p}^{n+\frac{1}{2}}, \quad \sum_l \Delta V_l^{n+\frac{1}{2}} = \Delta V_l^{n+\frac{1}{2}}$$

- It has an explicit solution

$$\hat{p}^{n+\frac{1}{2}} = \bar{p}^n - \bar{B}^n \frac{\Delta V^{n+\frac{1}{2}}}{V^n}, \quad \Delta V_l^{n+\frac{1}{2}} = \frac{V_l^n}{B_l^n}\left[(p_l^n - \bar{p}^n) + \bar{B}^n \frac{\Delta V^{n+\frac{1}{2}}}{V^n}\right]$$

where $B_l^n, \bar{B}^n$ and $\bar{p}^n$ are defined by

$$B_l^n = \rho_l^n (c_l^n)^2 \left[1 + \frac{L^n}{c_l^n \Delta t}\right], \qquad \bar{p}^n = \sum_l \frac{f_l^n p_l^n}{B_l^n} \Big/ \sum_l \frac{f_l^n}{B_l^n}$$

$$\bar{B}^n = 1 \Big/ \sum_l \frac{f_l^n}{B_l^n} = \sum_l f_l^n \Big/ \sum_l \frac{f_l^n}{B_l^n} \quad \text{where } f_l^n = V_l^n / V^n$$

- The equation for $\Delta f_l^{n+\frac{1}{2}}$ can be written as

$$\Delta f_l^{n+\frac{1}{2}} = \frac{f_l^n(p_l^n - \bar{p}^n)}{B_l^n} + f_l^n\left(\frac{\bar{B}^n}{B_l^n} - 1\right)\Delta V^{n+\frac{1}{2}}/V^n$$

- Suppose $\Delta f_l^{n+1} = 2\Delta f_l^{n+\frac{1}{2}}$, then we have $f_l^{n+1} = f_l^n + \Delta f_l^{n+1}$, $V_l^{n+1} = f_l^{n+1} V^{n+1},\ \rho_l^{n+1} = m_l / V_l^{n+1}$
- Update the specific internal energy of each material

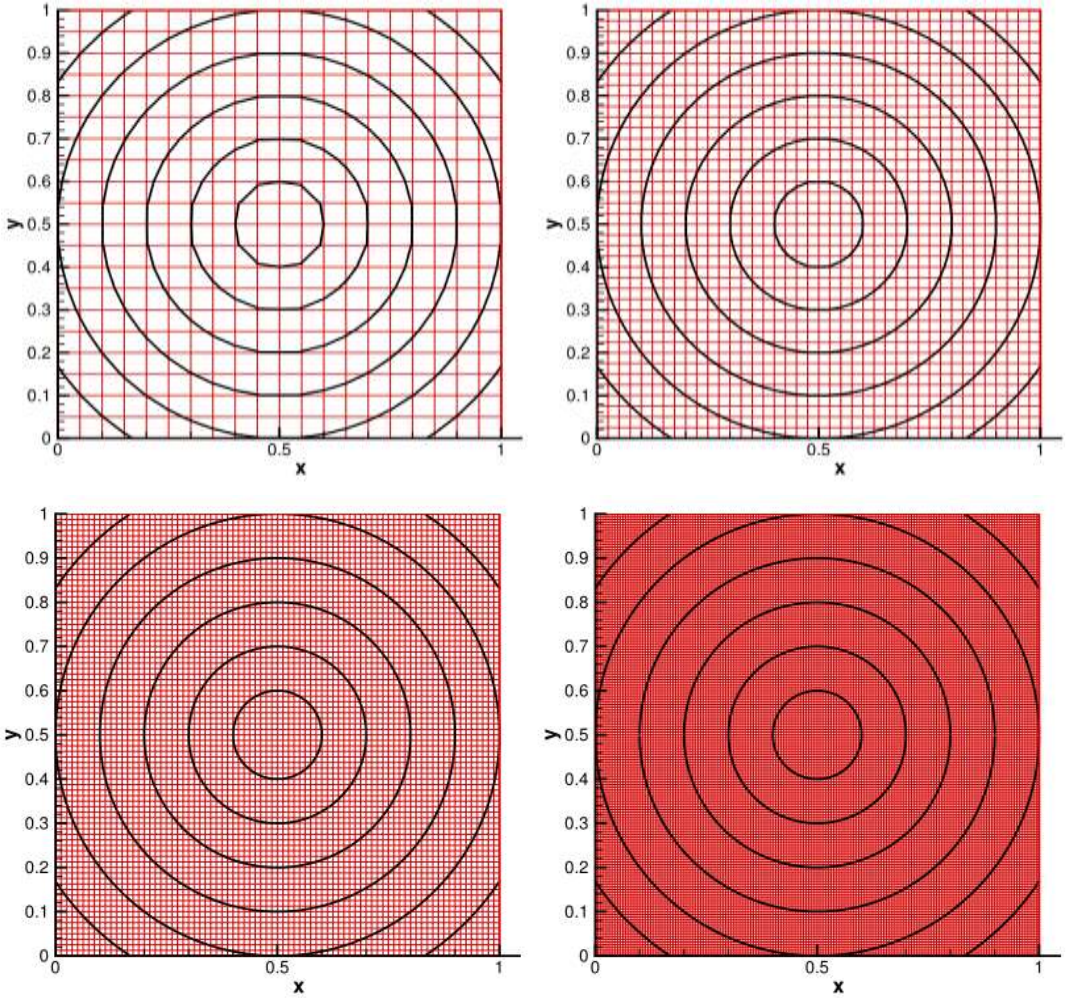
$$m_l\left(e_l^{n+1} - e_l^n\right) = -\hat{p}^{n+\frac{1}{2}}(V_l^{n+1} - V_l^n)$$

- $p_l^{n+1}$and c_l^{n+1} are obtained from EoS of material l.
- For the subcell volume fractions $f_{l,k}^n$, suppose $f_{l,k}^{n+1} = f_{l,k}^n + 2\Delta f_l^{n+\frac{1}{2}}$

Example of 2D SVoF algorithm and its application in MMALE

- Accuracy test
- Reconstruct circular interfaces on random polygonal meshes
- 2D Rayleigh-Taylor instability problem
- Bubble Shock interaction problem
- 2D Triple point problem
- Impact problem

- Accuracy test——Reconstruct circular interfaces on uniform square meshes



Reconstruct six circles using SVoF

$Nx \times Ny$	20×20	40×40	80×80	160×160	320×320
$E(L^1)$	8.808E-08	3.154E-08	1.285E-08	1.877E-09	9.425E-10
order		1.481632	1.295414	2.775268	0.9938641

convergence order of original MoF

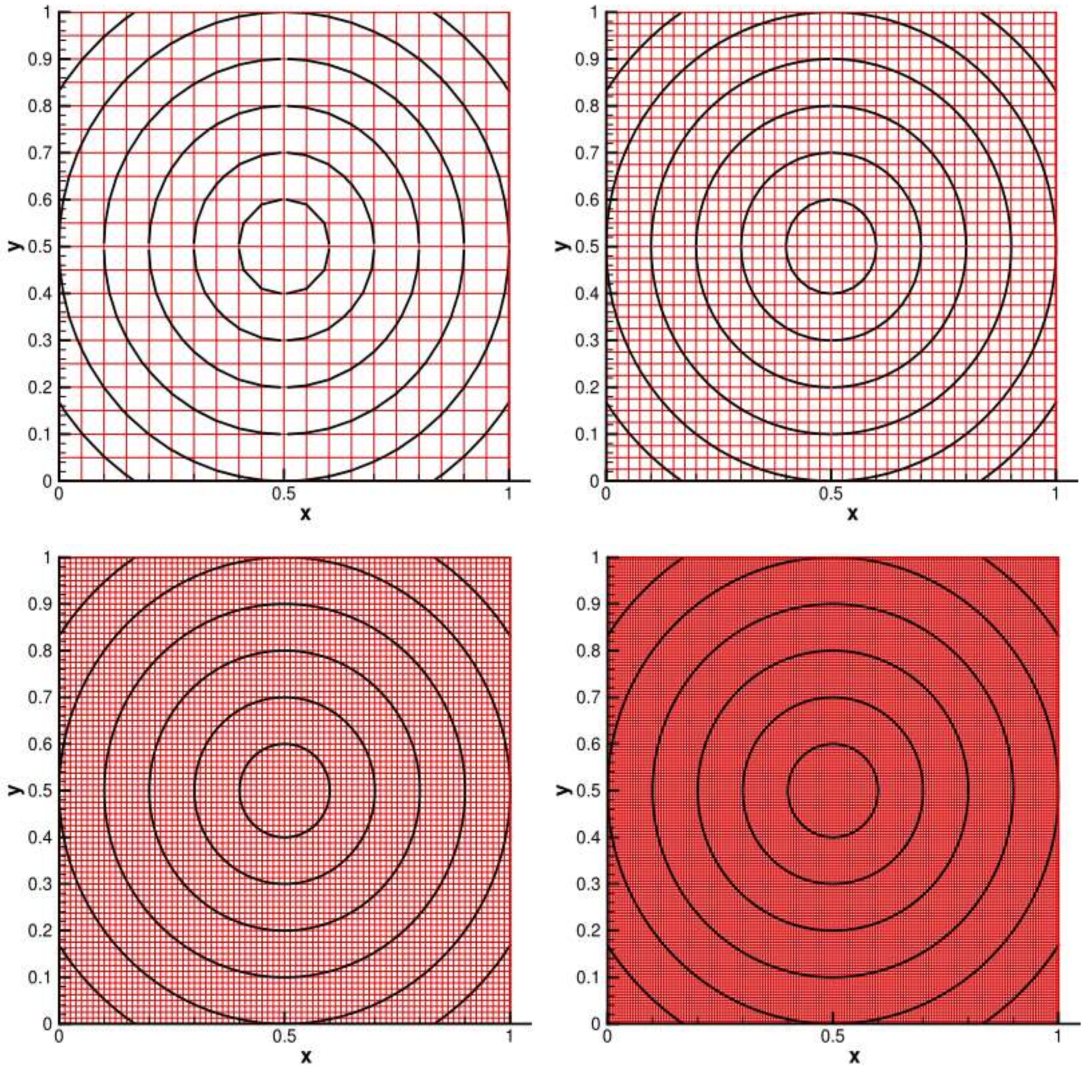
$Nx \times Ny$	20×20	40×40	80×80	160×160	320×320
$E(L^1)$	5.880E-08	1.744E-08	7.711E-09	1.414E-09	9.260E-10
order		1.753423	1.177402	2.447002	0.6109245

convergence order of robust MoF

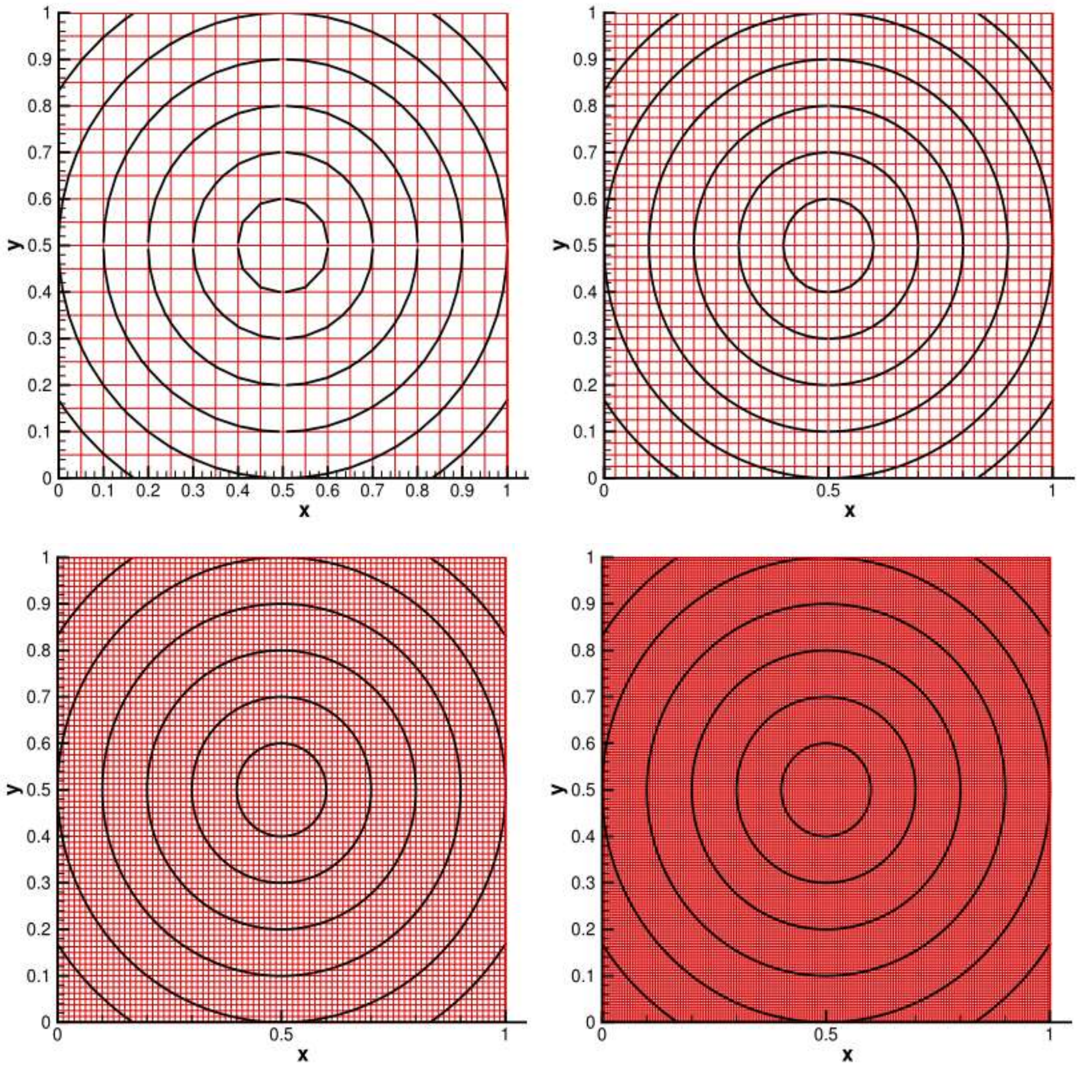
$Nx \times Ny$	20×20	40×40	80×80	160×160	320×320
$E(L^1)$	1.400E-07	5.434E-08	1.531E-08	4.740E-09	1.367E-09
order		1.365340	1.827540	1.691515	1.793874

convergence order of SVoF

The convergence order of SVoF is nearly second-order, and remains stable with mesh refinement.

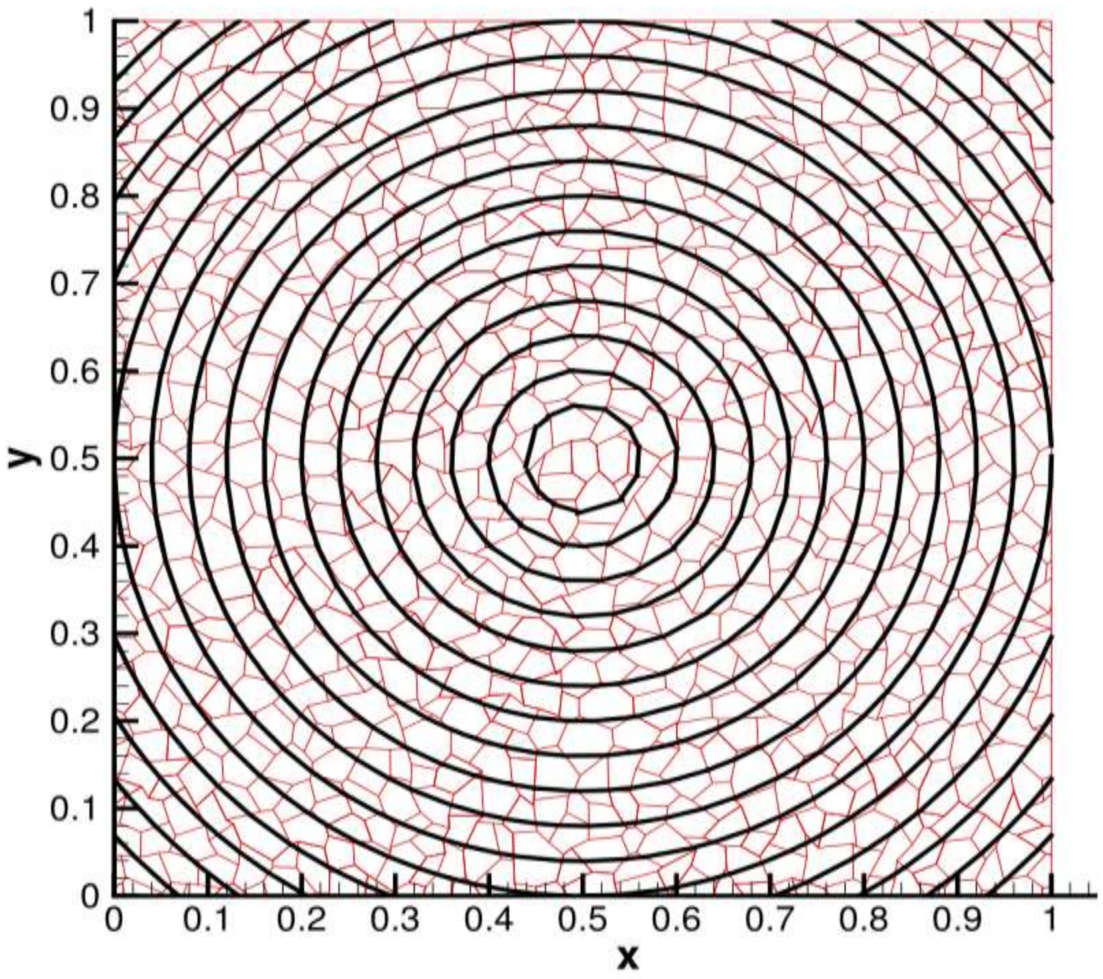


Reconstruct six circles using original MoF



Reconstruct six circles using robust MoF

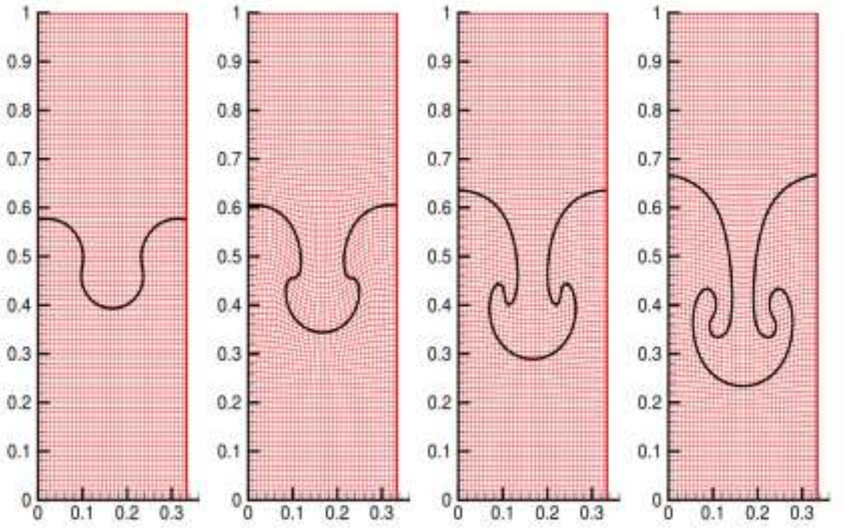
- Reconstruct circular interfaces on random polygonal meshes (There are many three-material cells)



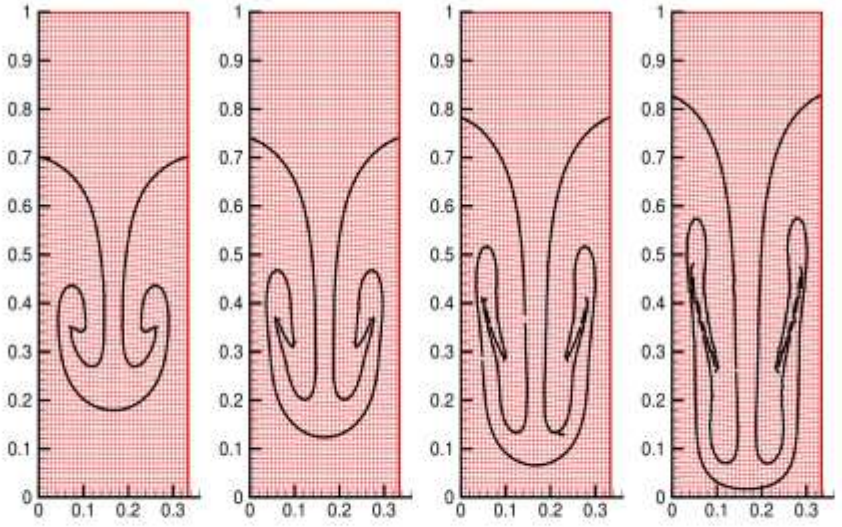
It can be seen that the SVoF algorithm is accurate and effective for reconstruction of three-material cells.

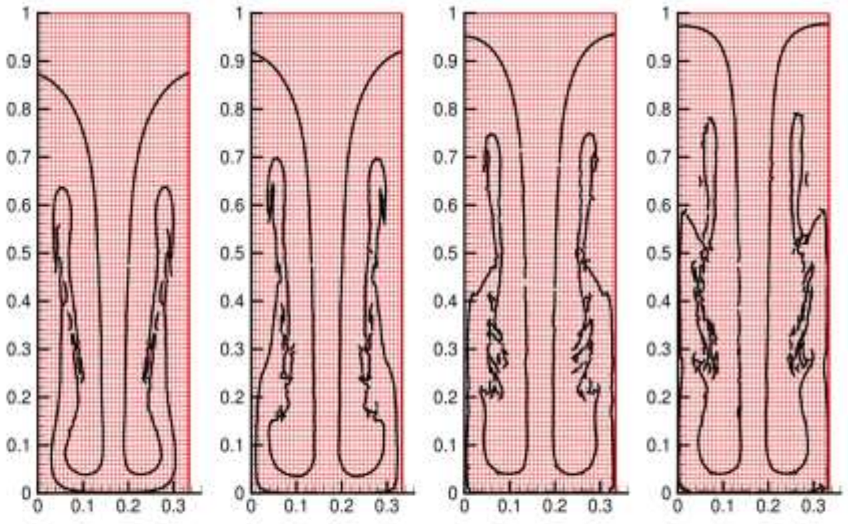
- 2D Rayleigh-Taylor instability problem

T=5,6,7,8 meshes and interfaces



T=9,10,11,12 meshes and interfaces



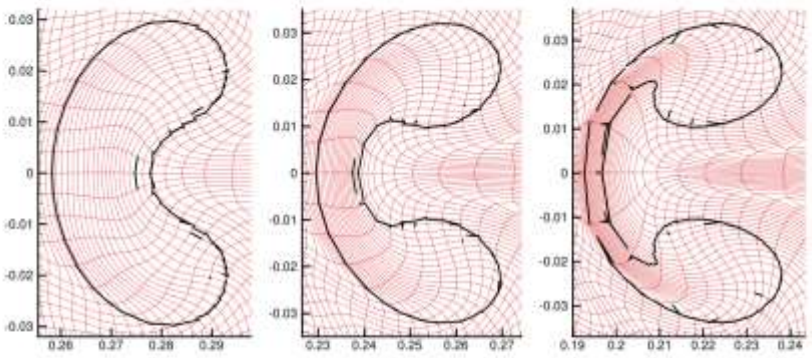


T=13,14,15,16 meshes and interfaces

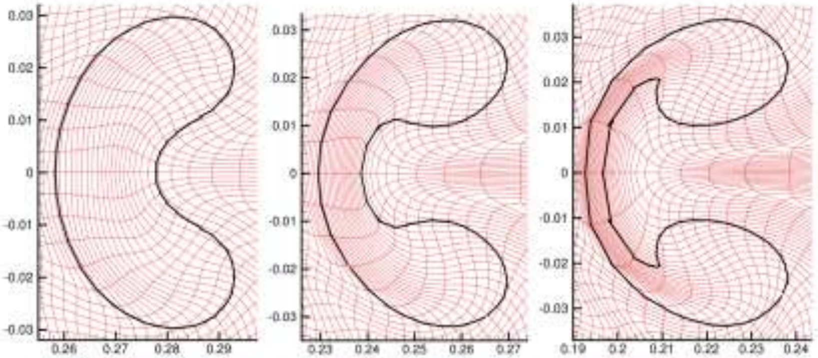
MoF-MMALE(Qing, 2020, CICP) runs to T=12; SVoF-MMALE runs to T=16, and is much more robust.

- Bubble Shock interaction problem

MoF
(Qing, 2020, CICP)

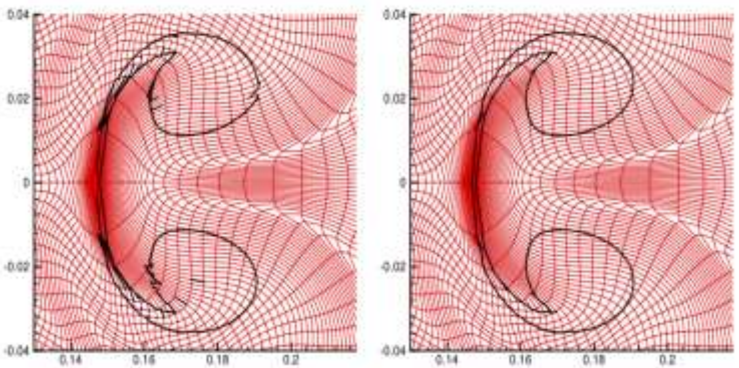


SVoF

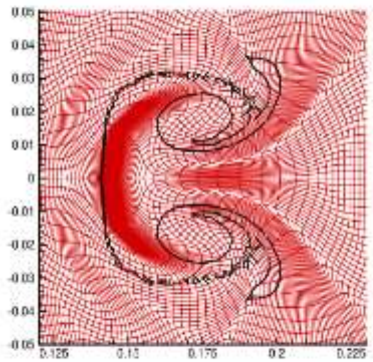


Schlieren images from experimental data

T1=913.153×10^{-6}, T2=1095.153×10^{-6},
T3=1342.153×10^{-6} meshes and interfaces



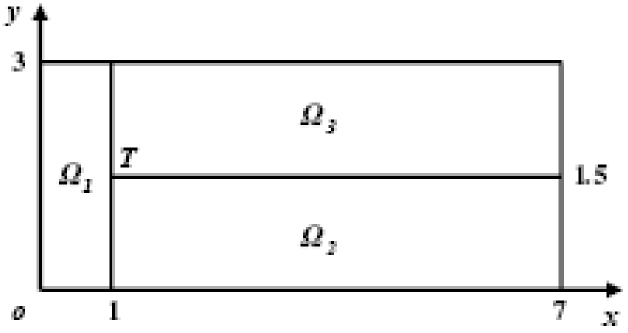
T4=1700.0×10^{-6} meshes and interfaces
left: MoF right: SVoF the interface is clearer



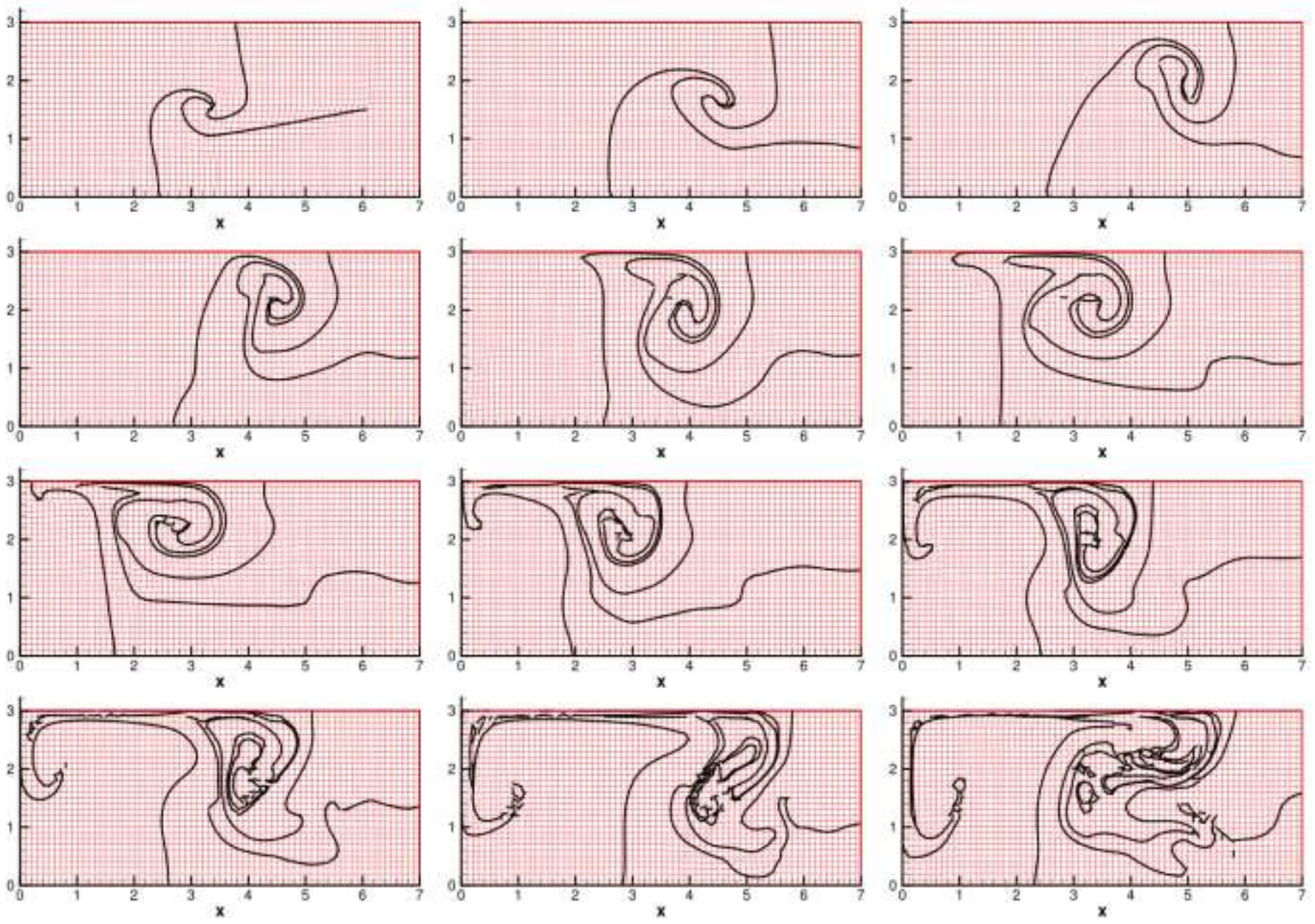
T5=2300.0×10^{-6} meshes and interfaces
SVoF

MoF-MMALE(Qing, 2020, CICP) runs to T4；
SVoF-MMALE runs to T5, and is much more robust.

- 2D Triple point problem



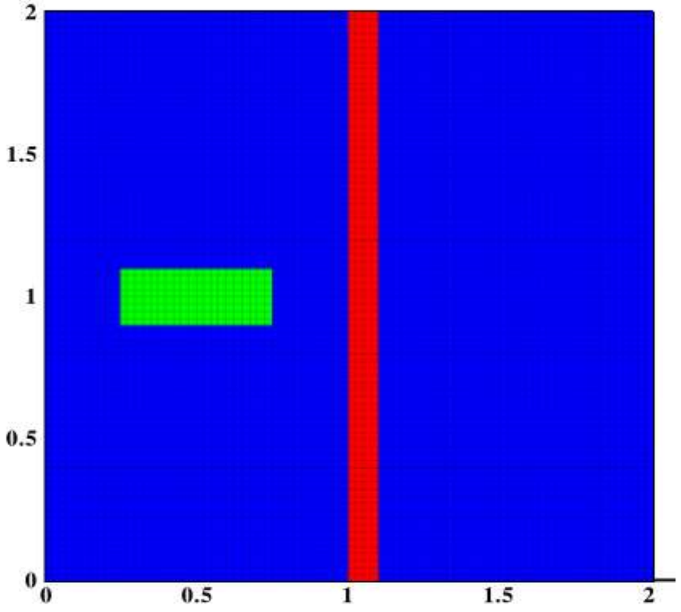
Initial configuration



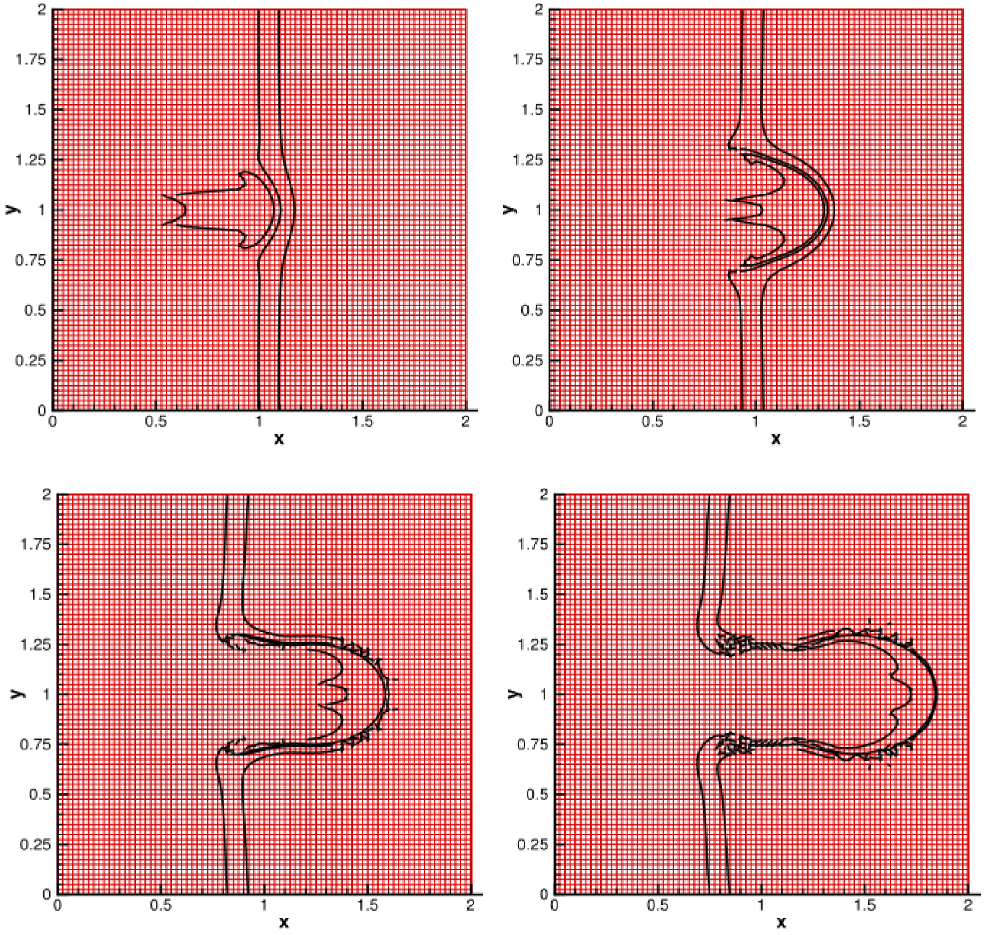
T=3,5,8,10,12,14,16,18,20,22,26,30
meshes and interfaces (from the upper left to the lower right)

MoF-MMALE(Qing, 2020, CICP) runs to T=9；
SVoF-MMALE runs to T=30, and is much more robust.

- Impact problem



Initial configuration

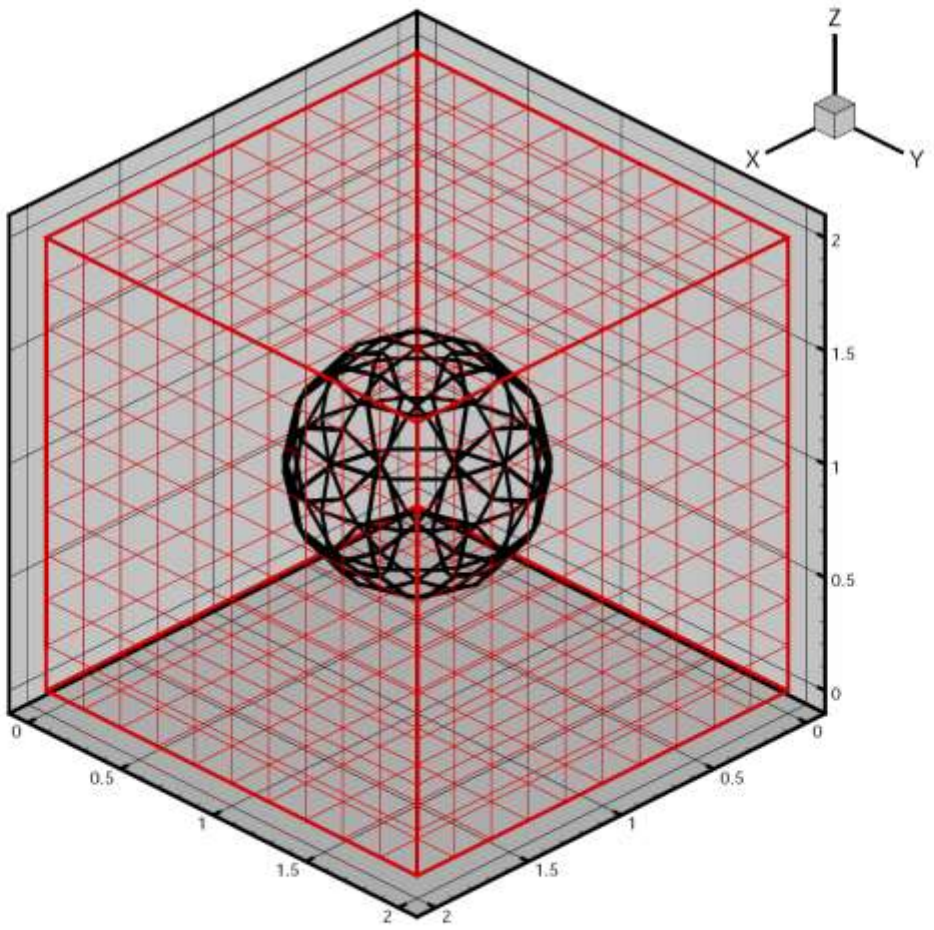


T=2,4,6,8 meshes and interfaces
(from the upper left to the lower right)

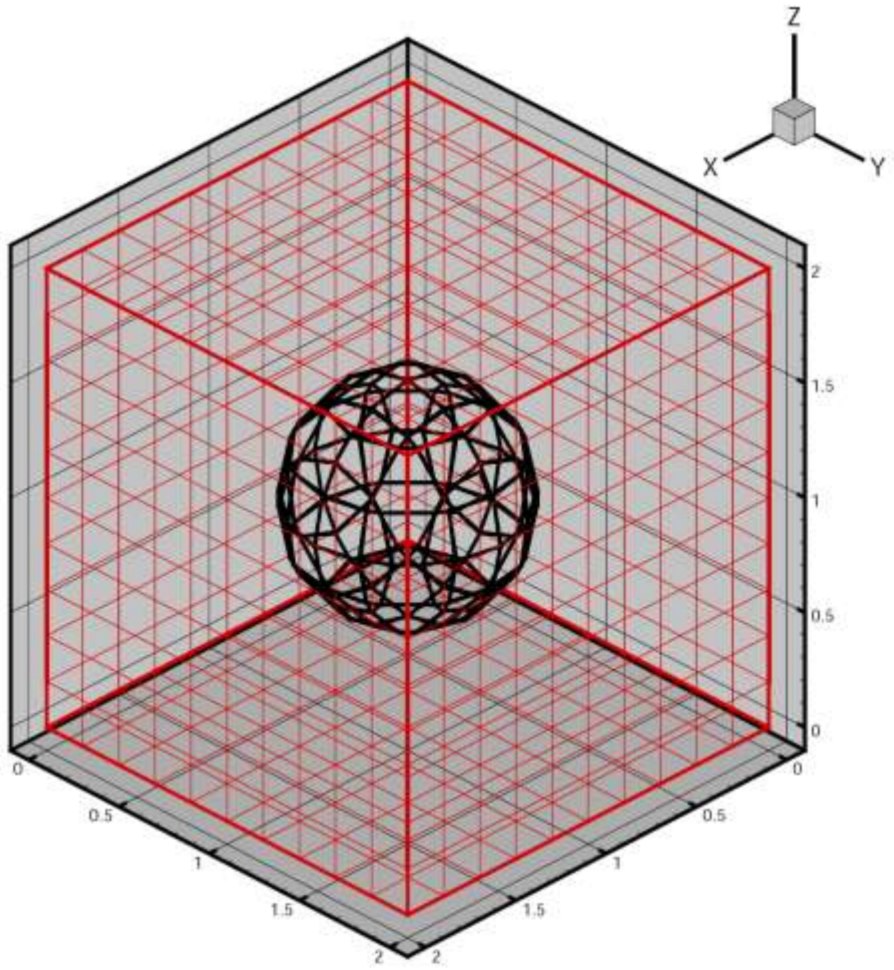
Example of 3D SVoF algorithm and its application in MMALE

- Reconstruct a sphere on orthogonal meshes
- Three-material reconstruction
- 3D Rayleigh-Taylor instability problem

- Reconstruct a sphere on orthogonal meshes

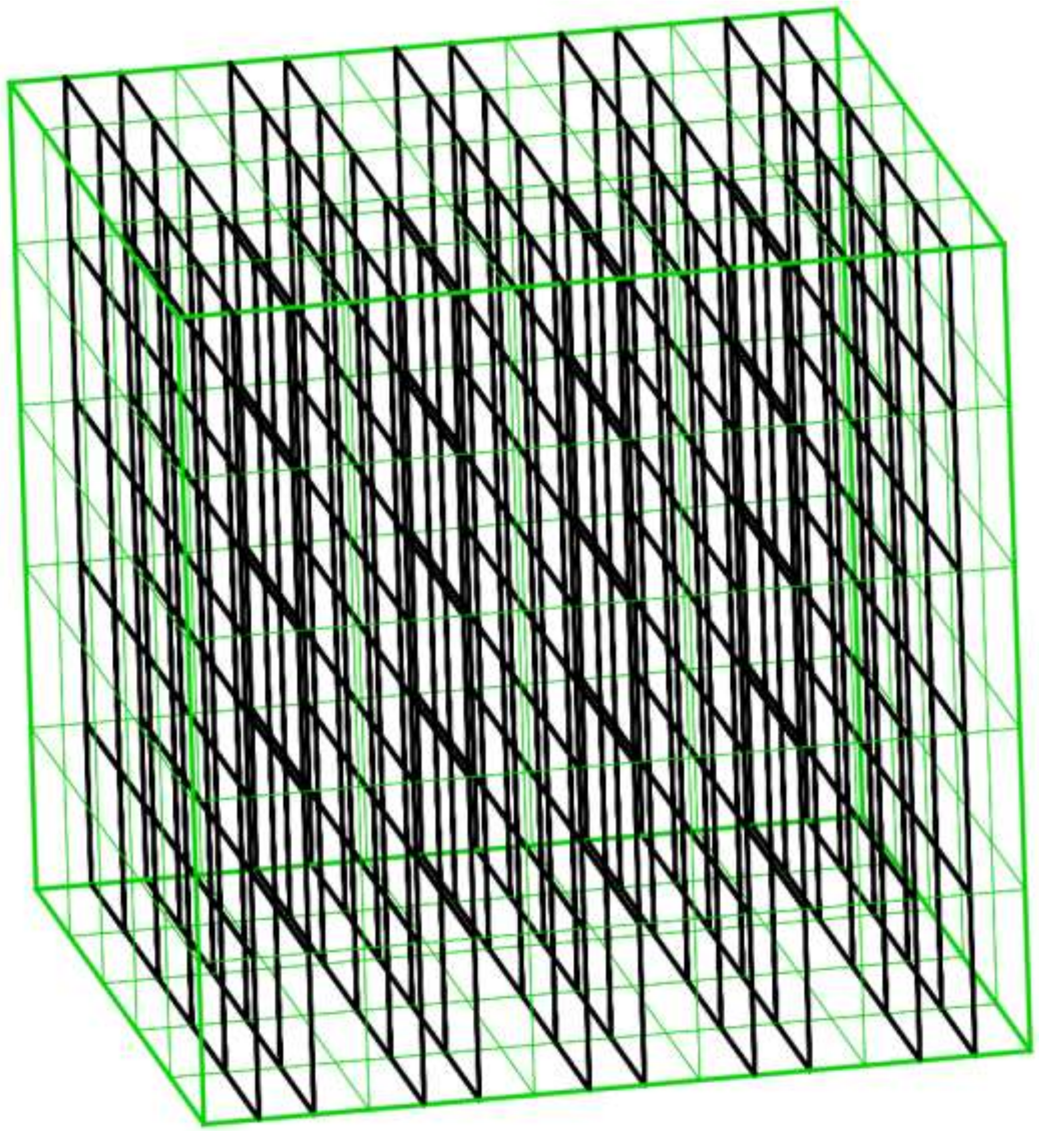


MoF algorithm



SVoF algorithm

- Three-material reconstruction



- Reconstruct parallel planes on a $5 \times 5 \times 5$ mesh, with two interfaces in each cell

- The reconstruction results are correct and verify the correctness of the program

- 3D Rayleigh-Taylor instability problem

T=9, MoF

T=9, SVoF

T=12, SVoF

T=13, SVoF

At T=9, the results of SVoF-MMALE and MoF-MMALE are comparable.

SVoF-MMALE is more robust than MoF-MMALE.

Conclusion

- A novel VoF algorithm (SVoF), which does not need information of neighboring cells, is proposed for the first time. Its accuracy is comparable to that of the MoF algorithm.
- A MMALE method based on the SVoF algorithm is proposed, which is much more robust than existing MoF-based MMALE methods.

[1] **Bojiao Sha, Zupeng Jia ， A very robust MMALE method based on a novel VoF method for two-dimensional compressible fluid flows ， to be submitted.**

[2] **Bojiao Sha, Zupeng Jia ， A very robust MMALE method based on a novel VoF method for three-dimensional compressible fluid flows ， prepared.**

Thank you all !