Oral presentation | Data science and AI

Data science and AI-IV

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[13-C-03] A low-dissipation reconstruction scheme for compressible single- and multi-phase flows based on the artificial neural network

*Minsheng Huang[1], Lidong Cheng[1,2], Wenjun Ying[1,3] (1. Shanghai Jiao Tong University, 2. Sichuan Research Institute, Shanghai Jiao Tong University, 3. School of Mathematical Sciences, MOE-LSC and Institute of Natural Sciences, Shanghai Jiao Tong University)

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A low-dissipation reconstruction scheme for compressible single- and multi-phase flows based on artificial neural network

Speaker: Minsheng Huang

Shanghai Jiao Tong University

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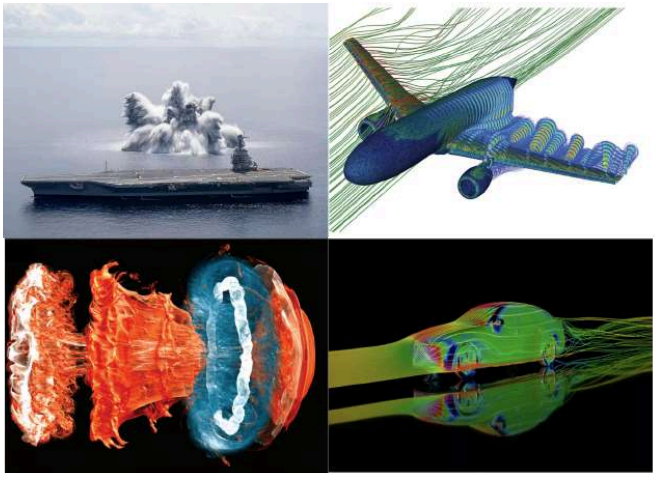
Overview

- **Introduction**
- MUSCL-THINC-BVD
- Deep-MUSCL-THINC-BVD(DeepMTBVD)
- Numerical Method
- Numerical Result
- Conclusion

Background



Compressible fluid dynamics is one of the most active and challenging research areas in CFD, with applications in **aerospace engineering**,**the automotive** and **the defense industries**, etc.

Numerical method of resolving discontinuty in compressible flow

- Multi-moment Constrained finite Volume method(MCV)
- High order Discontinuous Galerkin (DG)
- Flux Reconstruction (FR)/Correction Procedure via Reconstruction (CPR)
- Conventional Finite Volume Method (FVM)
- Deep Learning Method (PINNs, DeepONet)

Reconstrcution in FVM

Piecewise constant

Pros:

- Simple implementation

Cons:

- Low accuracy
- Excessive dissipation

TVD Scheme (MUSCL)

Pros:

- Second order in smooth region
- Simple implementation

Cons:

- Excessive disspation especially around discontinuities and extrema

(W/T)ENO and its variants

Pros:

- High-order accuracy and resolution
- Parallelizable
- Robust

Cons:

- Wide stencils
- Complexibility of choosing admissible stencils

Boundary variation diminishing (BVD) scheme

BVD Scheme

- Discontinous region: THINC scheme
  - Gibbs phenomenon is inevitable
  - Sigmoid functions performs better
- Smooth region: Polynomial-based scheme

- High accuracy in smooth region
- High resolution of discontinuty, material interface
- Robustness and adaptivity
- Prepare all candidate reconstruction functions

BVD scheme in structured grid:

- One-stage: Z. Sun, 2016, X.Deng 2018a, Z. Hou, 2021, C. Pan, 2024
- Two-stage: X. Deng, 2019
- Multi-stage: X. Deng, 2020a, X. Deng, 2020b, X. Deng, 2022c

BVD scheme in unstructured grid:

- Single-phase flow: X. Deng, 2017a, X.Deng, 2017b
- Multi-phase flow: L. Cheng, 2021, L. Cheng, 2022

Deep Learning

Deep Learning Method

- Directly Solving PDEs:
  - DeepONet
  - FNO
  - PINNs
  - Deep Ritz Method
  - The Weak Adversarial Network (WAN)

- Supplement to traditional methods:
  - Trouble cell detector
  - Flow structure detector
  - Reconstruction based on neural network

Keeps framework of codes

Extracting physical information from data

Simplifying complex processes

MUSCL-THINC-BVD

- Introduction
- **MUSCL-THINC-BVD**
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Consider the invisid single- and two-phase compressible flows:

$$\frac{\partial \mathbf{U}}{\partial t} + \nabla \cdot \mathbf{F} = \mathbf{S}.$$

- Inviscid Euler equation:

$$\boldsymbol{U} = \begin{pmatrix} \rho \\ \rho \boldsymbol{V} \\ E \end{pmatrix}, \quad \boldsymbol{F}(\boldsymbol{U}) = \begin{pmatrix} \rho \boldsymbol{V} \\ \rho \boldsymbol{V} \otimes \boldsymbol{V} + p\boldsymbol{I} \\ (E+p)\boldsymbol{V} \end{pmatrix}, \quad \boldsymbol{S} = \begin{pmatrix} 0 \\ 0 \\ 0 \end{pmatrix}.$$

- The five-equation model for two-phase inviscid compressible flow:

$$\boldsymbol{U} = \begin{pmatrix} \rho_1\alpha_1 \\ \rho_2\alpha_2 \\ \rho \boldsymbol{V} \\ E \\ \alpha_1 \end{pmatrix}, \boldsymbol{F}(\boldsymbol{U}) = \begin{pmatrix} \rho_1\alpha_1 \boldsymbol{V} \\ \rho_2\alpha_2 \boldsymbol{V} \\ \rho \boldsymbol{V} \otimes \boldsymbol{V} + p\boldsymbol{I} \\ (E+p)\boldsymbol{V} \\ \alpha_1 \boldsymbol{V} \end{pmatrix}, \boldsymbol{S} = \begin{pmatrix} 0 \\ 0 \\ \mathbf{0} \\ 0 \\ \alpha_1 \nabla \cdot \boldsymbol{V} \end{pmatrix}.$$

For close the system, we apply the stiffened equation of state (EOS):

- Inviscid Euler equation:

$$p(\rho, e) = (\gamma - 1)\rho\left(e - e_\infty\right) - \gamma p_\infty,$$

- The five-equation model for two-phase inviscid compressible flow:

$$p_k(\rho_k, e_k) = (\gamma_k - 1)\rho_k\left(e_k - e_{k,\infty}\right) - \gamma p_{k,\infty},$$

we need to determin an additional EOS of the mixture:

$$p\left(\rho, e, \alpha_1, \alpha_2\right) = \left(\rho e - \sum_{k=1}^{2} \alpha_k \rho_k e_{\infty,k} + \sum_{k=1}^{2} \frac{\alpha_k p_{\infty,k}}{\gamma_k - 1}\right) / \sum_{k=1}^{2} \frac{\alpha_k}{\gamma_k - 1},$$

where

$$\rho e = \alpha_1\rho_1 e_1 + \alpha_2\rho_2 e_2.$$

Admissible reconstruction scheme

- The MUSCL scheme

$$Q_i^M(x) = \bar{u}_i + \sigma_i \frac{x - x_i}{\Delta x_i}, \quad x \in [x_{i-1/2}, x_{i+1/2}],$$

where $\bar{u}_i$ is the cell-average value, and σ_i is the slope defined in cell C_i, accompied by proper slope limiter $\tilde{\Delta}$:

$$\sigma_i = \tilde{\Delta}(\bar{u}_i - \bar{u}_{i-1}, \bar{u}_{i+1} - \bar{u}_i).$$

- The THINC scheme

$$Q_i(x)_i^T = \bar{u}_{\min} + \frac{\bar{u}_{\max} - \bar{u}_{\min}}{2}\left(1 + \theta \tanh\left(\beta \frac{x - x_{i-1/2}}{x_{i+1/2} - x_{i-1/2}} - \tilde{x}_i\right)\right), \quad x \in [x_{i-1/2}, x_{i+1/2}],$$

where $\bar{u}_{\min} = \min(\bar{u}_{i-1}, \bar{u}_{i+1}), \bar{u}_{\max} = \max(\bar{u}_{i-1}, \bar{u}_{i+1})$ and $\theta = sgn(\bar{u}_{i+1} - \bar{u}_{i-1})$. β is selected to control the thickness of the jump, which is always valued from 1.4 to 2.0.

The BVD scheme

Assume that left- and right-side values of an arbitrary cell boundary I_i are U^L and U^R, the approximate Rimenan solver in the canonical formulation is given:

$$F(U^L, U^R) = \frac{1}{2}\underbrace{(F(U^L) + F(U^R))}_{\text{Central part}} - \underbrace{A(U^L, U^R)(U^R - U^L)}_{\text{Dissipative part}}.$$

Here, $F(U^L, U^R)$ denotes the numerical flux between the I_i and $A(U^L, U^R)$ is the matrix computed from U^L, U^R.

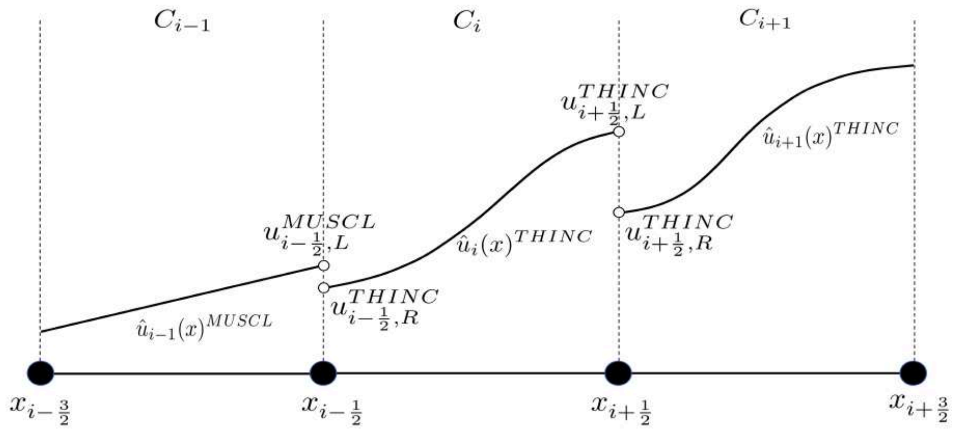
The BVD scheme is designed to select the reconstruction function from multiple candidates so as to minimize the dissipation term.

$$\Xi := \left\{Q_i^{\xi_1}(x), Q_i^{\xi_2}(x), \cdots, Q_i^{\xi_N}(x)\right\} \xrightarrow{\text{BVD scheme}} Q_i^{\xi_{opt}}(x), \quad \text{on } C_i.$$

$$\hat{u}_i(x)^{BVD} = \begin{cases} \hat{u}_i(x)^{THINC}, \text{ if } \delta < C < 1-\delta, \text{ and } (\bar{u}_{i+1}-\bar{u}_i)(\bar{u}_i-\bar{u}_{i-1}) > 0, \\ \qquad \text{and } TBV_{i,\min}^{THINC} < TBV_{i,\min}^{MUSCL}, \\ \hat{u}_i(x)^{MUSCL}, \text{ otherwise} . \end{cases}$$

$$TBV_{i,\min}^{s} = \min\left\{f(M,M,s), f(T,T,s), f(M,T,s), f(T,M,s)\right\},$$

$$f(s_1,s_2,s) = \left|\hat{u}_{i-1/2}^{L,s1} - \hat{u}_{i-1/2}^{R,s}\right| + \left|\hat{u}_{i+1/2}^{L,s} - \hat{u}_{i+1/2}^{R,s_2}\right|, \quad s, s_1, s_2 \in \{MUSCL, THINC\}.$$



The BVD scheme is summarized as following steps:

```
// 1. Reconstruct all admissible reconstructions
  for cell in all cells:
    for scheme in admissible set:
      reconstruct and save scheme in the cell

// 2. Select optimal canditate reconstruction
  for cell in all cells:
    for scheme in candidate set:
      find minimal boundary variation of all schemes

// 3. Calculate the cell boundary value
  for cell in all cells:
    using selected scheme from (2) to reconstruct
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Deep MUSCL-THINC-BVD

- Introduction
- MUSCL-THINC-BVD
- **Deep-MUSCL-THINC-BVD(DeepMTBVD)**
- Numerical Method
- Numerical Result
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DeepMTBVD

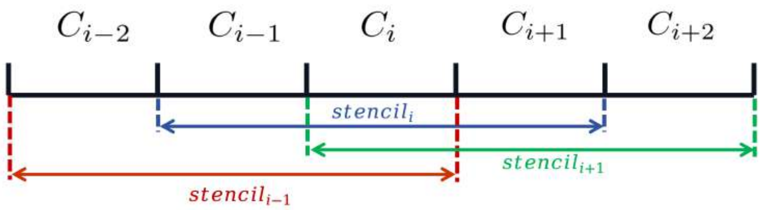
- MUSCL-THINC-BVD
  - Reconstruct all candidate schemes
  - Calculate the total boundary variation (TBV)
  - Select the scheme leading to minimum TBV

Pros:
- reduce the dissipative error
- Directly extend to the multi candidate reconstructions

Cons:
- Every cell needs to reconstruct all possible scheme
- Encountered with multi candidate reconstructions is cost expensively

- DeepMTBVD
  - Select the scheme by Neural network
  - Reconstruct the selected scheme in each cell

Pros:
- Reduce the dissipative error same to MUSCL-THINC-BVD
- Extend to the multi-candidates without expensive cost



Observation:

1. The stencils of BVD scheme consists of $\{C_{i-2}, C_{i-1}, C_i, C_{i+1}, C_{i+2}\}$.
3. The BVD scheme describes the discontinuity which the relative value among the neighboring cells.
2.

$$\frac{\bar{u}^s - \bar{u}_{\min}}{\bar{u}_{\max} - \bar{u}_{\min}} \in [0,1], \quad s \in \{\text{MUSCL}, \text{THINC}\}.$$

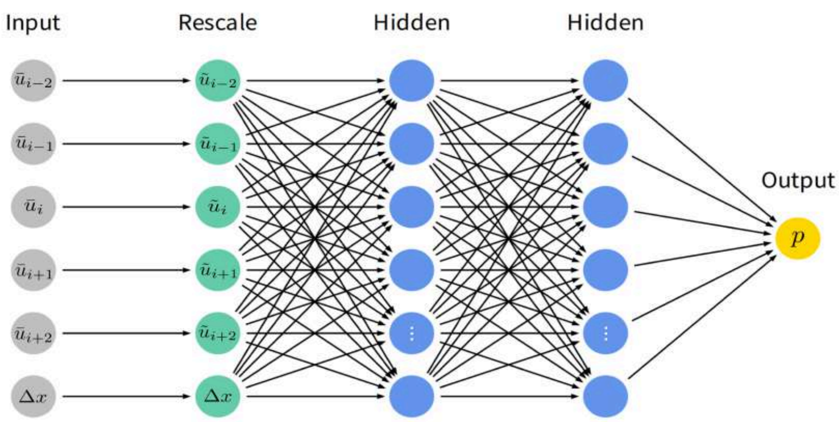
Here, $\bar{u}_{\min} = \min(\bar{u}_{i-1}, \bar{u}_{i+1}), \bar{u}_{\max} = \max(\bar{u}_{i-1}, u_{\bar{i}+1})$.

Normalization formualtion:

$$\tilde{u}_i = \begin{cases} \frac{\bar{u}_i - \bar{u}_{\min}}{\bar{u}_{\max} - \bar{u}_{\min}}, & \bar{u}_{\max} \neq \bar{u}_{\min}, \\ 0, \quad \bar{u}_{\max} = \bar{u}_{\min} < 10^{-15}, \\ 1, \quad \bar{u}_{\max} = \bar{u}_{\min} > 10^{-15}. \end{cases}$$

Sturcture of the Neural Network

The DeepMTBVD $\mathcal{N}(\tilde{u}_{i-2}, \tilde{u}_{i-1}, \tilde{u}_i, \tilde{u}_{i+1}, \tilde{u}_{i+2}, \Delta x; \Theta)$ with two hidden layers is described as following:



In the figure abovce the output p is probability of the THINC scheme.

Loss function

Let the label and probability (p_y) of the THINC scheme and MUSCL scheme

$$p_y = \begin{cases} p, & y = 1, \\ 1 - p, & y = 0. \end{cases} \quad y = \begin{cases} 1, & \text{THINC} \\ 0, & \text{MUSCL} \end{cases}$$

Let loss function is reformulated as:

$$loss = \sum_{i=1}^{N} FL(p_y^i),$$
$$FL(p_y) = -\omega_t (1 - p_y)^\gamma log(p_y).$$

Remark:

- Loss learn the features from the imbalanced data.
- The weight ω_0 for MUSCL is larger than ω_1 for THINC.

Data generation

1. Set different mesh size Δx.

2. Randomly set up the initial data at x = 0.5 in a sod tube.

$$(\rho_i^{(0)}, u_i^{(0)}, p_i^{(0)}) = \begin{cases} (\rho_i^L, u_i^L, p_i^L), & x \leq 0.5, \\ (\rho_i^R, u_i^R, p_i^R), & x \geq 0.5. \end{cases}$$

3. Calculate several time steps (about 10) by third-order SSP Runge-Kutta.

4. Given target cell C_i, we mark it as "1" if it is reconstructed by THINC, otherwise it is marked as "0". we record the $(\bar{u}_{i-2}, \bar{u}_{i-1}, \bar{u}_i, \bar{u}_{i+1}, \bar{u}_{i+2}, \Delta x, y)$ as one sample.

5. Change the mesh size and initial data and proceed to the next round.

Numerical Method

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Numerical Method

Dividing the computational domain into N cells, and denotes i^{th} cell $C_i = [x_{i-1/2}, x_{i+1/2}], i = 1, \cdots, N$. Assume that grid size is $\Delta x_i = x_{i+1/2} - x_{i-1/2}$ and cell center locates at $x_{i+1/2}$, the general integral formulation of conservative variable $\mathbf{U}$ over a finite volume cell C_i, which follows the cell-average values:

$$\overline{\boldsymbol{U}}_i = \frac{1}{\Delta x_i} \int_{x_{i-1/2}}^{x_{i+1/2}} \boldsymbol{U} dx.$$

The Euler equation or five-equation model is reformulated as:

$$\frac{d}{dt}\overline{\boldsymbol{U}}_i = -\frac{1}{\Delta x_i}\left(\underbrace{\mathcal{A}^+ \Delta \boldsymbol{U}_{i-1/2}}_{\text{right-moving fluctuations}} + \underbrace{\mathcal{A}^- \Delta \boldsymbol{U}_{i+1/2}}_{\text{left-moving fluctuations}} + \underbrace{\mathcal{A} \Delta \boldsymbol{U}_i}_{\text{total fluctuation}} \right),$$

where $\mathcal{A}^+ \Delta \boldsymbol{U}_{i-1/2}, \mathcal{A}^- \Delta \boldsymbol{U}_{i+1/2}, \mathcal{A} \Delta \boldsymbol{U}_i$ is calculated by wave-propgation method.

$$\mathcal{A}^{\pm}\Delta\boldsymbol{U}_{i\mp1/2}=\sum_{k=1}^{K}\left[s^k\left(\boldsymbol{U}^L_{i-1/2},\boldsymbol{U}^R_{i+1/2}\right)\right]^{\pm}\boldsymbol{W}^k\left(\boldsymbol{U}^L_{i-1/2},\boldsymbol{U}^R_{i+1/2}\right),$$

$$\mathcal{A}\Delta\boldsymbol{U}_{i}=\sum_{k=1}^{K}\left[s^k\left(\boldsymbol{U}^R_{i-1/2},\boldsymbol{U}^L_{i+1/2}\right)\right]^{\pm}\boldsymbol{W}^k\left(\boldsymbol{U}^R_{i-1/2},\boldsymbol{U}^L_{i+1/2}\right),$$

where K, s^k and W^k are the number of waves, moving speeds, and jumps of three propagation discontinuities solved by Riemann solvers such as HLL/HLLC.

Once given spatial discretization, we apply the two-stage second-order SSP Runge-Kutta for temporal evolution

$$\overline{\boldsymbol{U}}^{*}=\overline{\boldsymbol{U}}^{n}+\Delta t\mathcal{L}\left(\overline{\boldsymbol{U}}^{n}\right),$$

$$\overline{\boldsymbol{U}}^{n+1}=\frac{1}{2}\overline{\boldsymbol{U}}^{n}+\frac{1}{2}\left(\overline{\boldsymbol{U}}^{*}+\Delta t\mathcal{L}\left(\overline{\boldsymbol{U}}^{*}\right)\right).$$

Algorithm of DeepMTBVD

```
1. // Select input stencil for each cell
  for i in all cells:
    stencil[i][0] = u[i-2]
    stencil[i][1] = u[i-1]
    stencil[i][2] = u[i]
    stencil[i][3] = u[i+1]
    stencil[i][4] = u[i+2]
    stencil[i][5] = dx

2. // Inferrenced neural network
  prediction = network→inferrence(stencil)

3. // Recontructed by prediction
  for i in all cells:
    if prediction[i] < p0:
      cell i is reconstructed by MUSCL
    else
      cell i is reconstructed by THINC

4. // Advance to next sub-time step
```

- We perform inference on all cells at once, rather than one cell at a time. In practice, inferrencing one by one is not as fast and efficient as inferrencing together.
- p_0 is a parameter, which is depend on problem. Generally we will take 0.5, unless otherwise specified in the numerical example.
- Conservative quantities and characteristic quantities can also be trained under this framework.

Numerical Results

- Introduction
- MUSCL-THINC-BVD
- Deep-MUSCL-THINC-BVD(DeepMTBVD)
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Sod's Problem

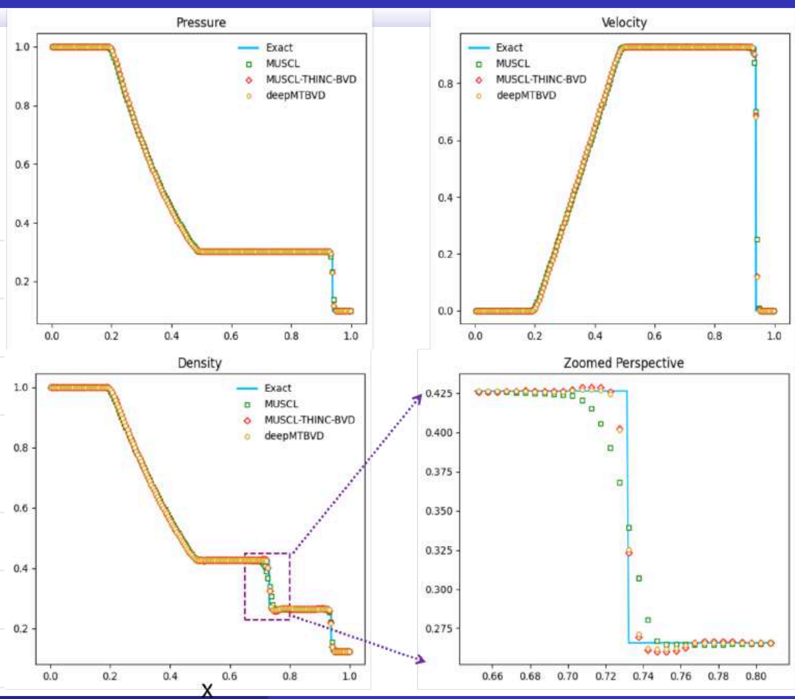
$$(\rho_0, v_0, p_0) = \begin{cases} (1,0,1), & 0 \leqslant x \leqslant 0.5 \\ (0.125, 0, 0.1), & \text{otherwise} \end{cases}.$$

- N = 10000

Time(s)	MUSCL-THINC-BVD	DeepMTBVD
Reconstruction Time	48.6	11.8
Selection Time	4.4	36.2
Total Time	53.0	48.0

- N = 100000

Time(s)	MUSCL-THINC-BVD	DeepMTBVD
Reconstruction Time	4951.3	1139.1
Selection Time	650.1	3734.6
Total Time	5601.4	4873.7



Blast wave

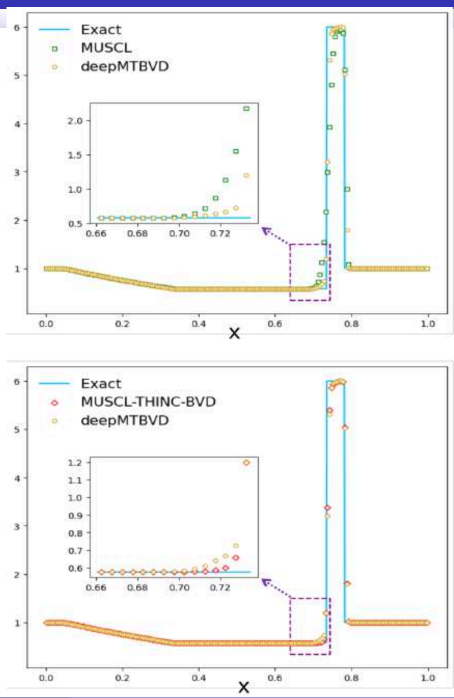
$$(\rho, u, p) = \begin{cases} (1.0, 0.0, 1000.0) & \text{if } x < 0.5 \\ (1.0, 0.0, 0.01) & \text{otherwise} \end{cases}$$

- N = 10000

Time(s)	MUSCL-THINC-BVD	DeepMTBVD
Reconstruction Time	60.0	12.6
Selection Time	5.1	42.2
Total Time	65.1	54.8

- N = 100000

Time(s)	MUSCL-THINC-BVD	DeepMTBVD
Reconstruction Time	4746.5	782.9
Selection Time	600.8	2655.2
Total Time	5347.3	3438.1



Simple interface problem

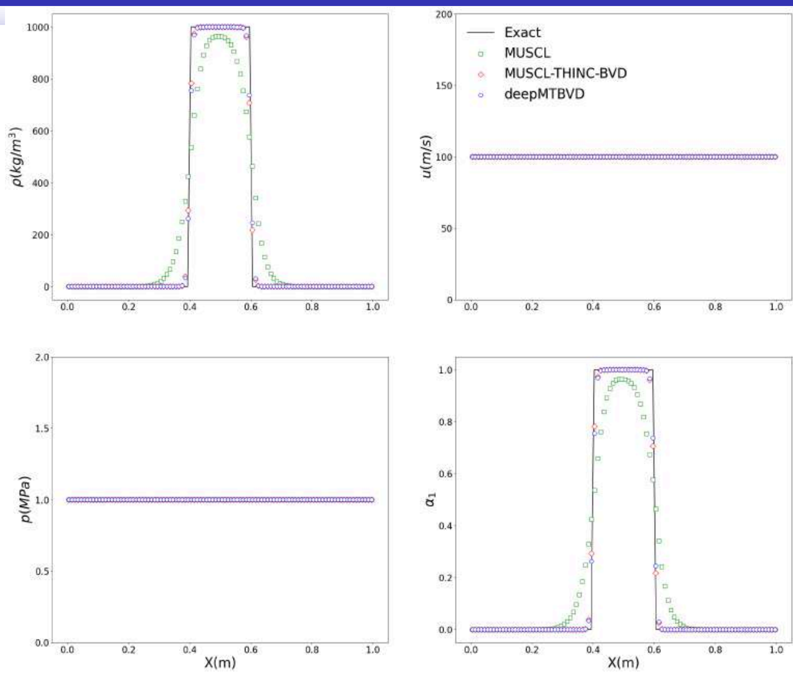
if $x < 0.4$ or $x > 0.6$:

$$(\alpha_1, \rho, u, p) = (10^{-8}, 1, 1000, 100000),$$

if $0.4 \leq x \leq 0.6$.

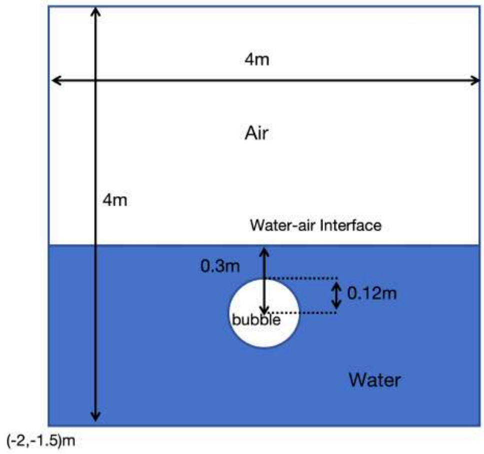
$$(\alpha_1, \rho, u, p) = (1 - 10^{-8}, 1000, 1000, 100000).$$

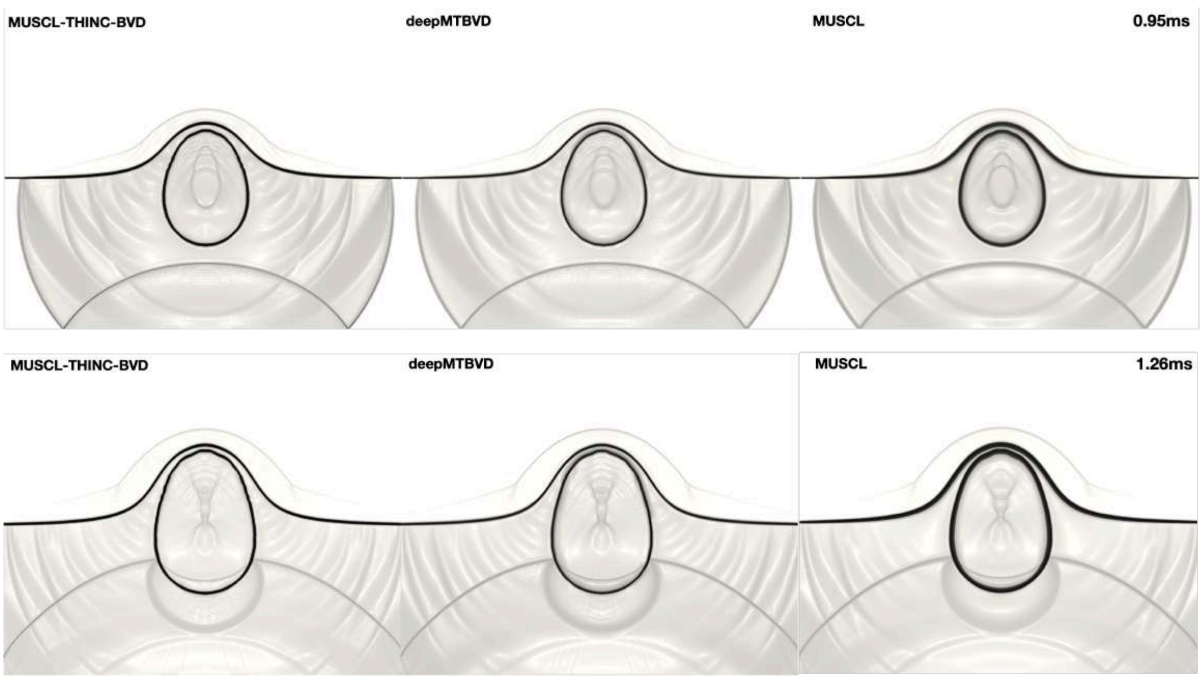
The parameters of stiffened EOS are : $\gamma_1 = 4.4, p_{\infty,1} = 6 \times 10^8, e_{\infty,1} = 0 \gamma_2 = 1.4, p_{\infty,2} = 0, e_{\infty,2} = 0.$ In this example, p_0 is set to be 0.4.

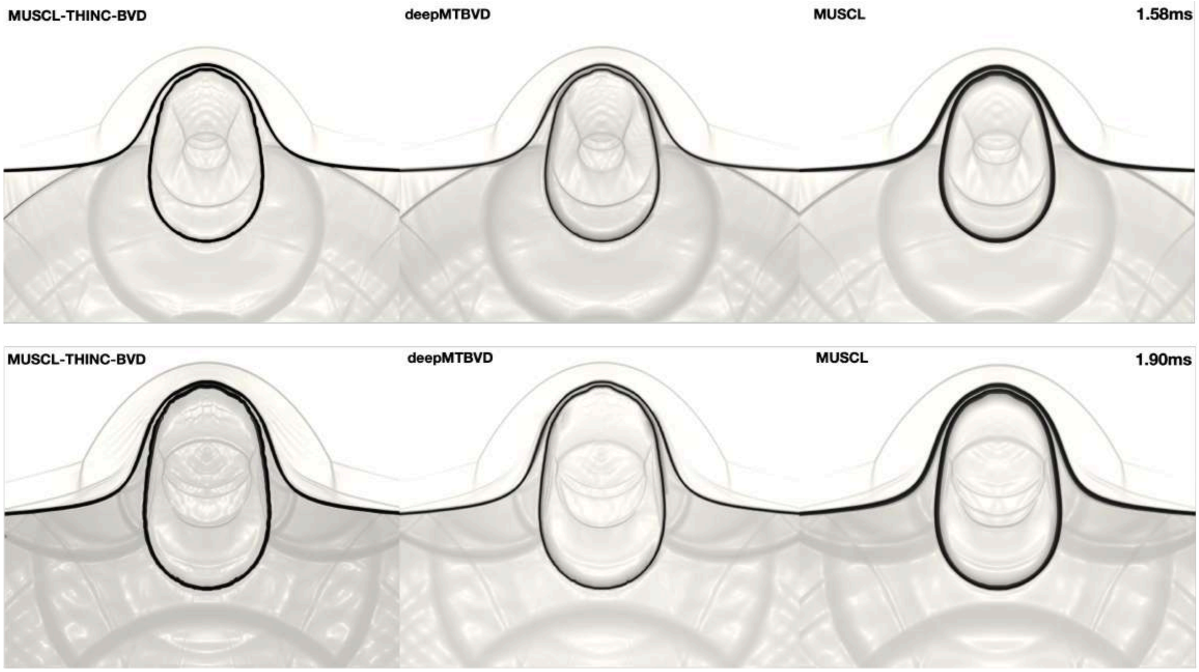


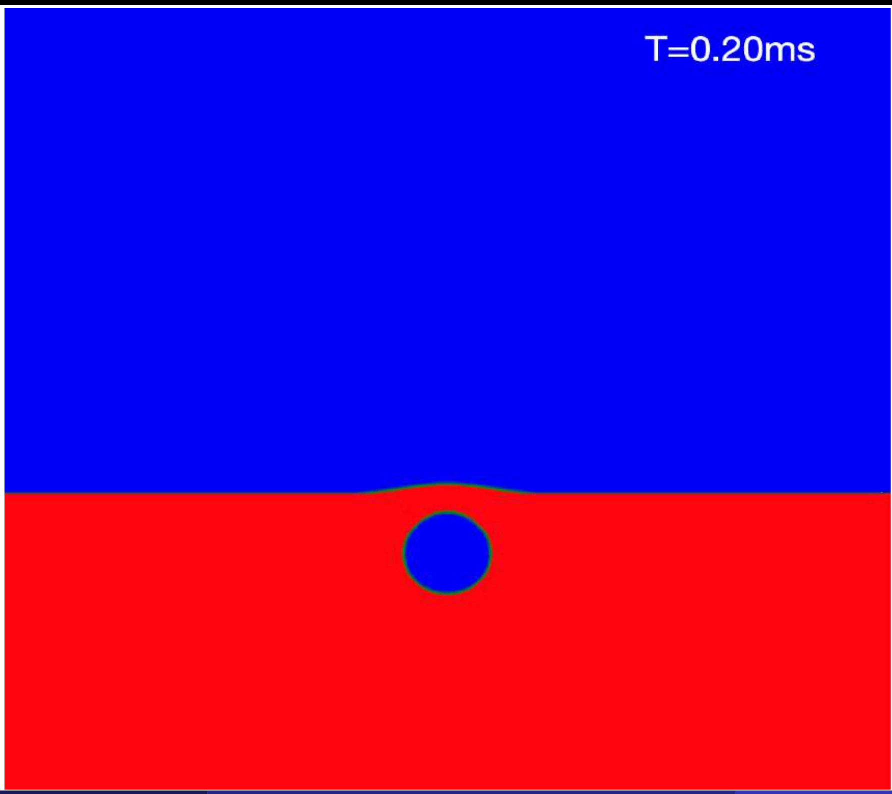
Underwater explosion

The computation domain is $[-2\mathrm{m}, 2\mathrm{m}] \times [-1.5\mathrm{m}, 2.5\mathrm{m}]$. The diameter of cylindrical air cavity is $0.24\mathrm{m}$ which initially centered at $(0, -0.3)\mathrm{m}$ with high pressure 10^9 Pa and high density $1250\mathrm{kg/m}^3$. The planar water-air interface is located at $y = 0\mathrm{m}$. Both water and air mediums are under standard atmospheric conditions and stay stationary initially. Under this assumption, The density of pure water is $1000\mathrm{kg/m}^3$ and pure air is $1\mathrm{kg/m}^3$. In water medium, the volume fraction of air $\alpha_1 = 10^{-8}$ and vice versa in air.

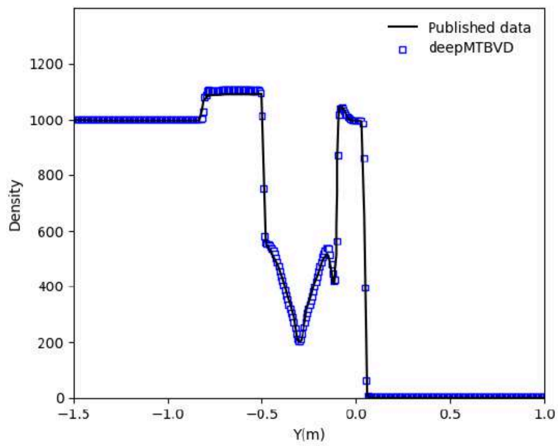




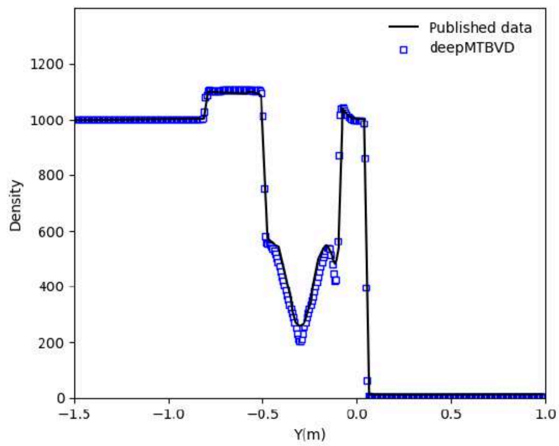

MUSCL-THINC-BVD
deepMTBVD
MUSCL
1.58ms
MUSCL-THINC-BVD
deepMTBVD
MUSCL
1.90ms


T=0.20ms

Compare with the result from Shukla [1] among $x = 0$ at $t = 0.2ms$



Compare with the result from Hu[2] among $x = 0$ at $t = 0.2ms$



1. R. K. Shukla, C. Pantano, and J. B. Freund. An interface capturing method for the simulation of multi-phase compressible flows. Journal of Computational Physics, 229(19):7411–7439, 2010.

2. X. Y. Hu, N. A. Adams, and G. Iaccarino. On the hllc riemann solver for interface interaction in compressible multi-fluid flow. Journal of Computational Physics, 228(17):6572–6589, 2009.

Two-dimensional shock–R22-cylinder interaction

In the R22 bubble,

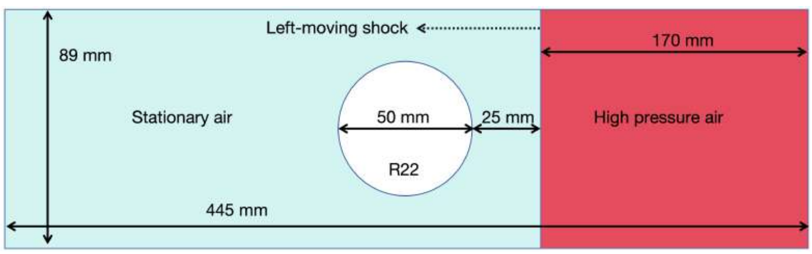
$$(\rho_1, \rho_2, u_1, u_2, p, \alpha_1) = \left(3.869 \text{ kg/m}^3, 1.225 \text{ kg/m}^3, 0.0, 0.0, 1.01325 \times 10^5 \text{ Pa}, 1.0 - 10^{-8}\right),$$

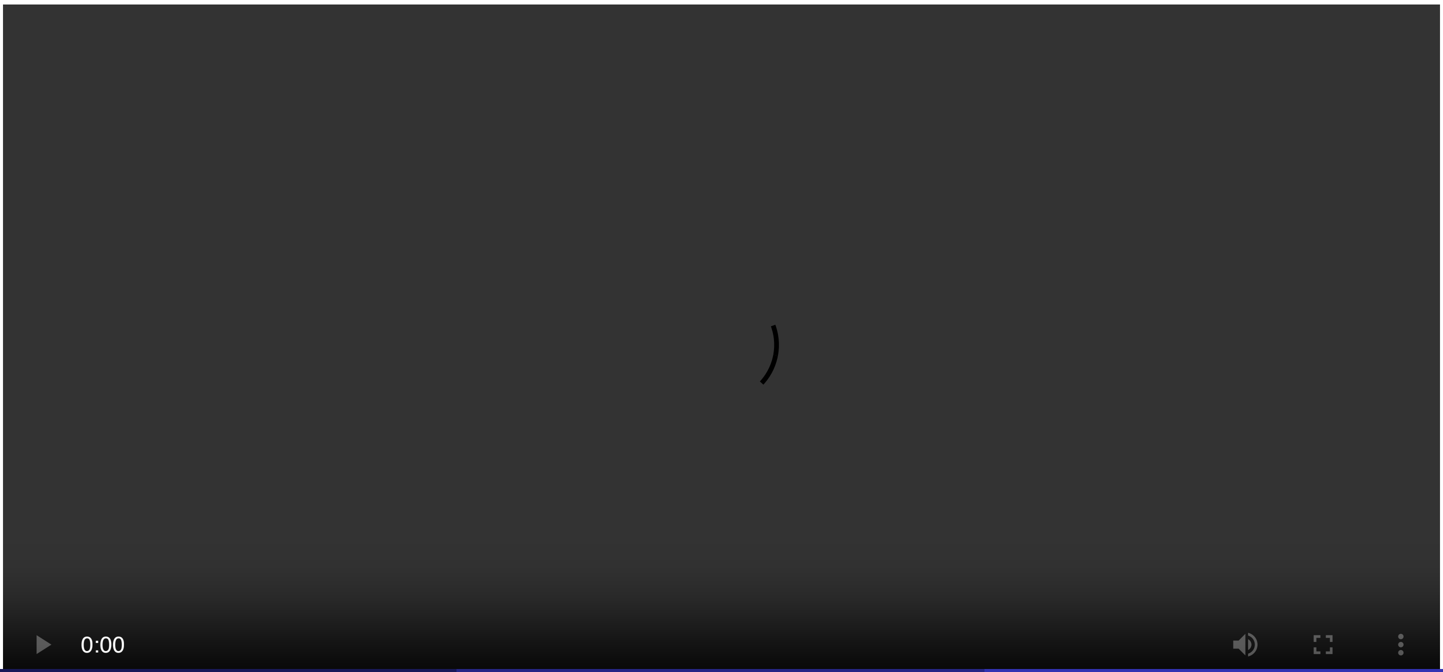
while outside the bubble, the parameters in the pre-shock are:

$$(\rho_1, \rho_2, u_1, u_2, p, \alpha_1) = \left(3.869 \text{ kg/m}^3, 1.225 \text{ kg/m}^3, 0.0, 0.0, 1.01325 \times 10^5 \text{ Pa}, 10^{-8}\right),$$

and the corresponding parameters in the post-shock are:

$$(\rho_1, \rho_2, u_1, u_2, p, \alpha_1) = \left(3.869 \text{ kg/m}^3, 1.686 \text{ kg/m}^3, -113.5 \text{ m/s}, 0.0, 1.59 \times 10^5 \text{ Pa}, 10^{-8}\right)$$

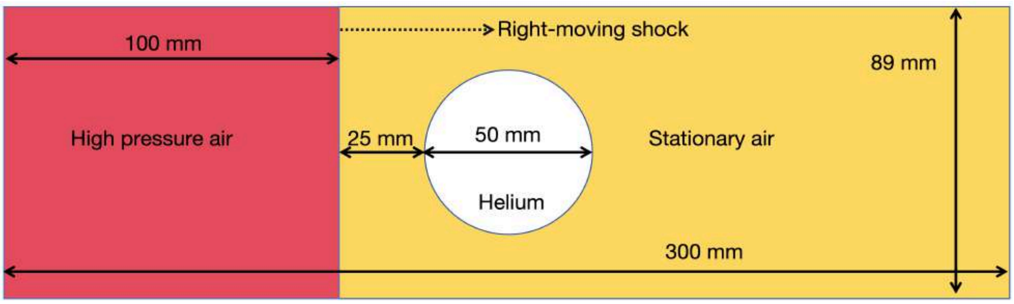


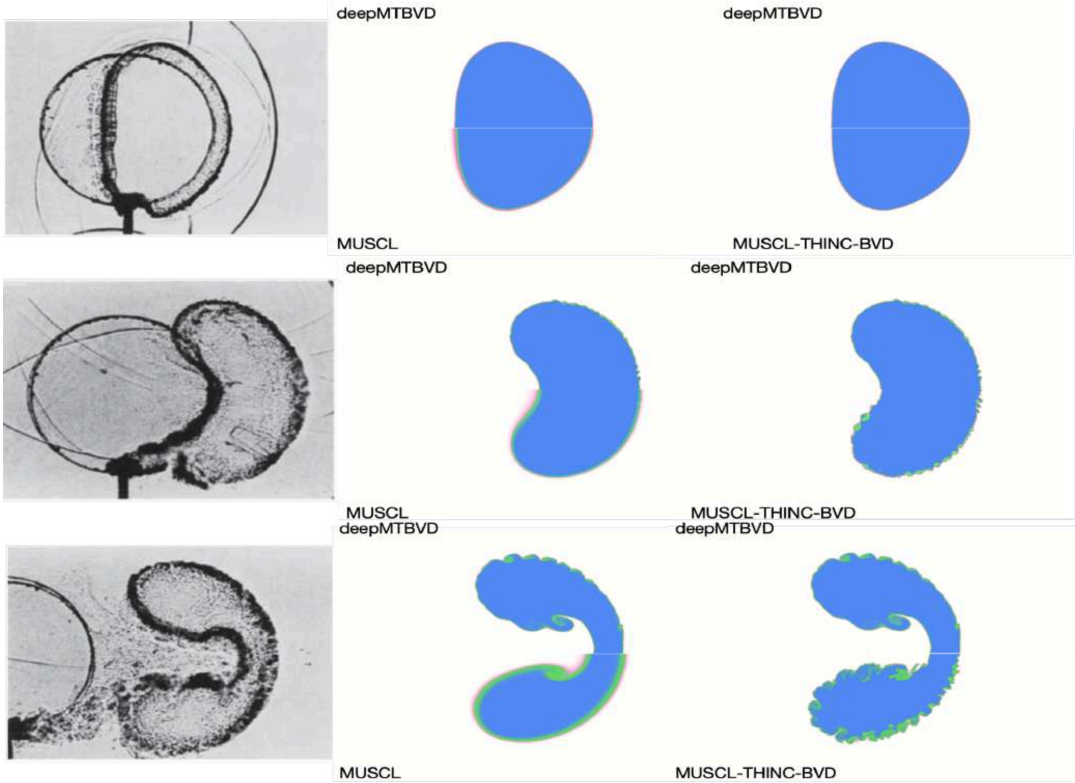


Two-dimensional shock-helium-bubble interaction

$$(\alpha_1, \rho, u, v, p) = \begin{cases} (10^{-8}, 0.167\ \mathrm{kg/m^3}, 0.0, 0.0, 1.01325 \times 10^5\ \mathrm{Pa}) & \text{Helium bubble ,} \\ (1.0 - 10^{-8}, 1.686\ \mathrm{kg/m^3}, 113.5\ \mathrm{m/s}, 0.0, 1.59 \times 10^5\ \mathrm{Pa}) & \text{Post-shock ,} \\ (1.0 - 10^{-8}, 1.225\ \mathrm{kg/m^3}, 0.0, 0.0, 1.01325 \times 10^5\ \mathrm{Pa}) & \text{Otherwise.} \end{cases}$$

The corresponding parameters of EOS are $\gamma_1 = 1.4, p_{\infty,1} = e_{\infty,1} = 0$ and $\gamma_2 = 1.667, p_{\infty,2} = e_{\infty,2} = 0$




deepMTBVD
deepMTBVD
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MUSCL-THINC-BVD
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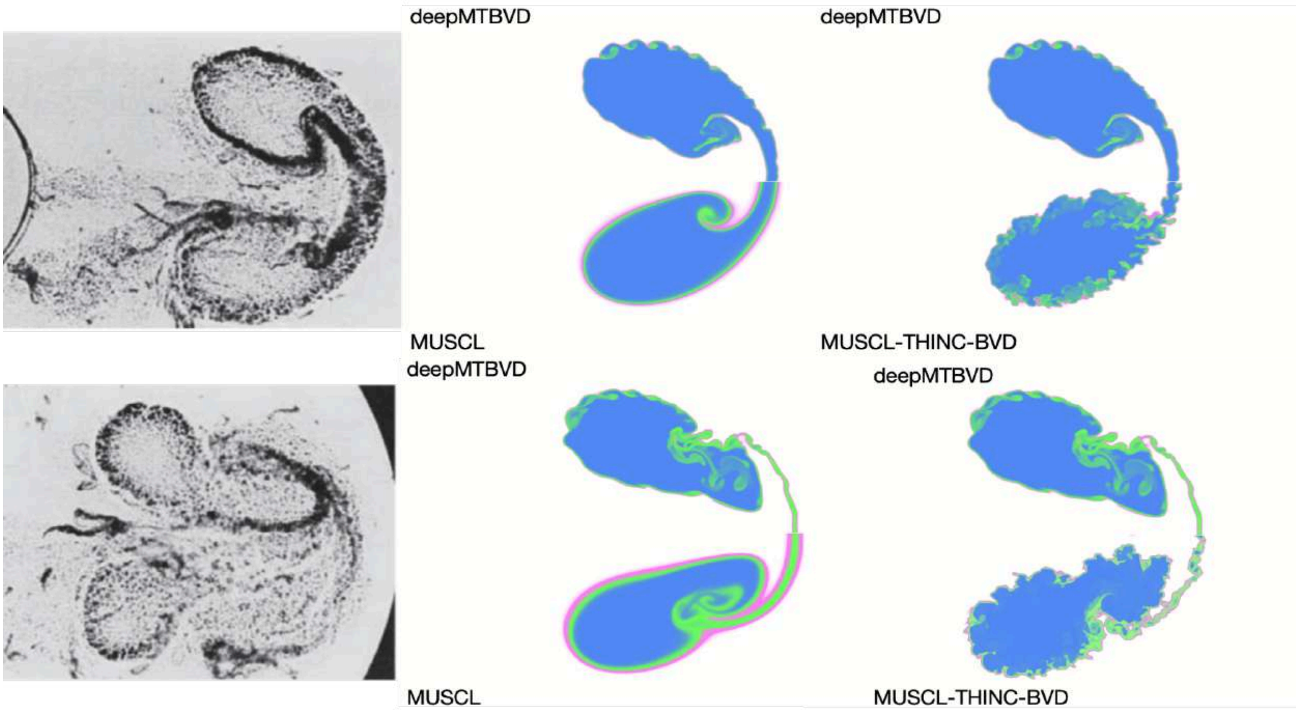
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Numerical Results

- Introduction
- MUSCL-THINC-BVD
- Deep-MUSCL-THINC-BVD(DeepMTBVD)
- Numerical Method
- Numerical Result
- **Conclusion**

Conclusion

- A novel low-dissipative scheme is proposed, DeepMTBVD, which is based on BVD scheme and the artificial neural network.
- The DeepMTBVD is trained from the data obtained by 1D Euler equation, and then is successfully extended to multi-dimensional and two-phase flow.
- Compared with MUSCL scheme, the DeepMTBVD shows the lower dissipaiton, while compared to MTBVD, the DeepMTBVD achieves comparable results with less computational time.
- In the future, we will extend this method into multi-candidate reconstructions and into unstructured grid.

Thank you for listening!