Oral presentation | Multi-phase flow
Multi-phase flow-I
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[1-D-04] A Low-dissipation Numerical Method for Capturing Gas-liquid Interfaces in Phase Change Simulation

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A Low-dissipation Numerical Method for Capturing Gas-liquid Interfaces in Phase Change Simulation

Session: Multi-phase flow-I

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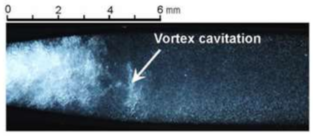
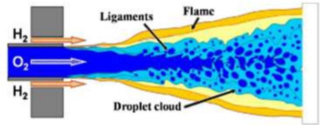
Introduction

- Compressible multiphase flows occur in various engineering situations,
  e.g., cavitation, droplet atomization, bubbly flows.
- Complex flow structures are created due to the interference between shock waves and gas-liquid interfaces.
- **Phase change** makes the flow structures more complex due to newly generated interfaces.
- For accurate simulation, numerical schemes should have both **computational stability** and **discontinuity-capturing ability**.
- We conducted phase-change simulation using stable and low-dissipation numerical methods based on **Boundary Variation Diminishing (BVD) principle**.



Vortex cavitation in venturi tube (Soyama, 2021)



Coaxial subcritical combustion of cryogenic O2/H2 (Murrone et al., 2019)

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Six-equation model

- Advection of VOF

$$\partial_t \alpha_1 + \boldsymbol{u} \cdot \nabla \alpha_1 = \mu(p_1 - p_2).$$

- Mass conservation law

$$\partial_t(\alpha_1 \rho_1) + \nabla \cdot (\alpha_1 \rho_1 \boldsymbol{u}) = 0,$$
$$\partial_t(\alpha_2 \rho_2) + \nabla \cdot (\alpha_2 \rho_2 \boldsymbol{u}) = 0.$$

- Momentum conservation law

$$\partial_t(\rho \boldsymbol{u}) + \nabla \cdot (\rho \boldsymbol{u} \otimes \boldsymbol{u} + p\mathbb{I}) = \boldsymbol{0}.$$

- Energy conservation law

$$\partial_t(\alpha_1 E_1) + \nabla \cdot (\alpha_1 (E_1 + p_1) \boldsymbol{u}) + \Sigma = -\mu p_{\mathrm{I}}(p_1 - p_2),$$
$$\partial_t(\alpha_2 E_2) + \nabla \cdot (\alpha_2 (E_2 + p_2) \boldsymbol{u}) - \Sigma = \mu p_{\mathrm{I}}(p_1 - p_2),$$

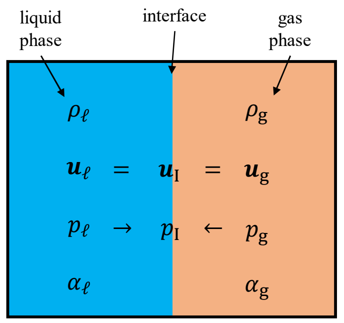
where

$$\Sigma = -\boldsymbol{u} \cdot (Y_2 \nabla(\alpha_1 p_1) - Y_1 \nabla(\alpha_2 p_2)).$$

- Stiffened gas equation of state

$$p_k = (\gamma_k - 1)(\mathcal{E}_k - \eta_k \rho_k) - \gamma_k \pi_k \quad (k = 1, 2).$$

α_k: volume fraction
ρ_k: density
u: velocity
E_k: total energy
p_k: pressure
Y_k: mass fraction
γ_k: heat capacity ratio
$\mathcal{E}_k$: internal energy
π_k, η_k: material dependent parameters



Control volume

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Six-equation model

Compact form and extended model:

$$\partial_t \boldsymbol{q} + \nabla \cdot \boldsymbol{f}(\boldsymbol{q}) + \boldsymbol{\sigma}(\boldsymbol{q}, \nabla \boldsymbol{q}) = \boldsymbol{\psi}_{\mathrm{p}}(\boldsymbol{q}) + \boldsymbol{\psi}_{\mathrm{T}}(\boldsymbol{q}) + \boldsymbol{\psi}_{\mathrm{g}}(\boldsymbol{q}),$$

advection term | non-conservative term | pressure relaxation term | temperature relaxation term | Gibbs-energy relaxation term

where,

$$\boldsymbol{q} = \begin{bmatrix} \alpha_1 \\ \alpha_1 \rho_1 \\ \alpha_2 \rho_2 \\ \rho \boldsymbol{u} \\ \alpha_1 E_1 \\ \alpha_2 E_2 \end{bmatrix}, \quad \boldsymbol{f}(\boldsymbol{q}) = \begin{bmatrix} 0 \\ \alpha_1 \rho_1 \boldsymbol{u} \\ \alpha_2 \rho_2 \boldsymbol{u} \\ \rho \boldsymbol{u} \otimes \boldsymbol{u} + p\mathbb{I} \\ \alpha_1 (E_1 + p_1) \boldsymbol{u} \\ \alpha_2 (E_2 + p_2) \boldsymbol{u} \end{bmatrix}, \quad \boldsymbol{\sigma}(\boldsymbol{q}, \nabla \boldsymbol{q}) = \begin{bmatrix} \boldsymbol{u} \cdot \nabla \alpha_1 \\ 0 \\ 0 \\ \boldsymbol{0} \\ \Sigma(\boldsymbol{q}, \nabla \boldsymbol{q}) \\ -\Sigma(\boldsymbol{q}, \nabla \boldsymbol{q}) \end{bmatrix},$$

$$\boldsymbol{\psi}_{\mathrm{p}}(\boldsymbol{q}) = \begin{bmatrix} \mu(p_1 - p_2) \\ 0 \\ 0 \\ \boldsymbol{0} \\ -\mu p_{\mathrm{I}}(p_1 - p_2) \\ \mu p_{\mathrm{I}}(p_1 - p_2) \end{bmatrix}, \boldsymbol{\psi}_{\mathrm{T}}(\boldsymbol{q}) = \begin{bmatrix} \frac{\theta(T_2 - T_1)}{\kappa} \\ 0 \\ 0 \\ \boldsymbol{0} \\ \theta(T_2 - T_1) \\ -\theta(T_2 - T_1) \end{bmatrix}, \boldsymbol{\psi}_{\mathrm{g}}(\boldsymbol{q}) = \begin{bmatrix} \frac{\nu(g_2 - g_1)}{\rho_{\mathrm{I}}} \\ \nu(g_2 - g_1) \\ -\nu(g_2 - g_1) \\ \boldsymbol{0} \\ \nu e_{\mathrm{I}}(g_2 - g_1) \\ -\nu e_{\mathrm{I}}(g_2 - g_1) \end{bmatrix}.$$

Thermal and chemical relaxation terms are added to consider phase change.

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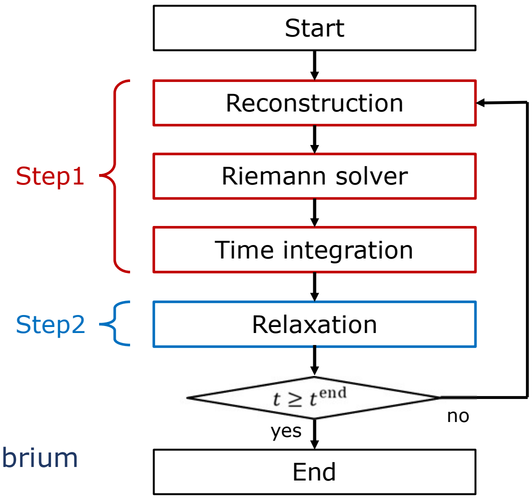
Calculation procedure

$$\partial_t \boldsymbol{q} + \nabla \cdot f(\boldsymbol{q}) + \sigma(\boldsymbol{q}, \nabla \boldsymbol{q}) = \psi_{\mathrm{p}}(\boldsymbol{q}) + \psi_{\mathrm{T}}(\boldsymbol{q}) + \psi_{\mathrm{g}}(\boldsymbol{q})$$

advection term | non-conservative term | pressure relaxation term | temperature relaxation term | Gibbs-energy relaxation term

Step1: Solve homogeneous part of the model with FVM,
$\partial_t \boldsymbol{q} + \nabla \cdot f(\boldsymbol{q}) + \sigma(\boldsymbol{q}, \nabla \boldsymbol{q}) = \boldsymbol{0}$.

Step2: Solve the ODE systems including the relaxation terms,
- $\partial_t \boldsymbol{q} = \psi_{\mathrm{p}}(\boldsymbol{q})$,
- $\partial_t \boldsymbol{q} = \psi_{\mathrm{p}}(\boldsymbol{q}) + \psi_{\mathrm{T}}(\boldsymbol{q})$,
- $\partial_t \boldsymbol{q} = \psi_{\mathrm{p}}(\boldsymbol{q}) + \psi_{\mathrm{T}}(\boldsymbol{q}) + \psi_{\mathrm{g}}(\boldsymbol{q})$.



p-relaxation: only mechanical equilibrium
p-pT-relaxation: mechanical and thermal equilibrium
p-pT-pTg-relaxation:
mechanical, thermal, and chemical equilibrium

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2. Two-phase numerical model
3. BVD scheme
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5. Summary

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BVD principle

The numerical flux at $x = x_{i+\frac{1}{2}}$:

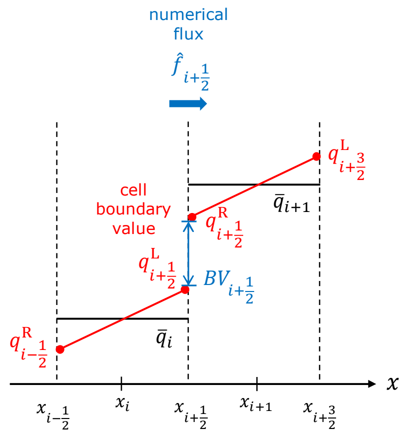
$$\hat{f}_{i+\frac{1}{2}} = \underbrace{\frac{1}{2}\left(f\left(q^{\mathrm{L}}_{i+\frac{1}{2}}\right) + f\left(q^{\mathrm{R}}_{i+\frac{1}{2}}\right)\right)}_{\text{central-difference term}} - \underbrace{\frac{1}{2}\left|\alpha_{i+\frac{1}{2}}\right|\left(q^{\mathrm{R}}_{i+\frac{1}{2}} - q^{\mathrm{L}}_{i+\frac{1}{2}}\right)}_{\text{artificial-viscosity term}}$$

where,

$q^{\mathrm{L/R}}$: left/right cell-boundary value,

α: characteristic speed.

Boundary Variation $BV_{i+\frac{1}{2}} \equiv \left|q^{\mathrm{R}}_{i+\frac{1}{2}} - q^{\mathrm{L}}_{i+\frac{1}{2}}\right|$ should be Diminishing for suppressing the numerical dissipation error.



Boundary Variation Diminishing principle

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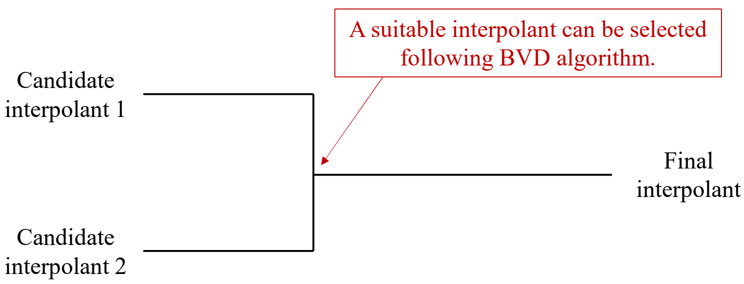
Hybrid-type BVD scheme

Candidate interpolant 1:

stable, non-oscillation scheme (MUSCL, WENO, upwind, etc.)

Candidate interpolant 2:

discontinuity-capturing scheme (THINC, downwind, etc.)



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MUSCL scheme

Reconstruction function:

$$Q_i^{\mathrm{MUSCL}}(x) = \bar{q}_i + \Phi(r)(\bar{q}_{i+1} - \bar{q}_i)X_i(x),$$

where,

$$r = \frac{\bar{q}_i - \bar{q}_{i-1}}{\bar{q}_{i+1} - \bar{q}_i},\ X_i(x) = \frac{x - x_i}{\Delta x}.$$

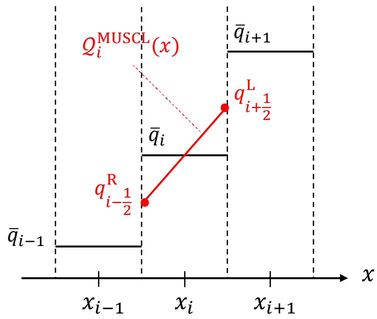
$\Phi(r)$: slope limiter function

Harmonic limiter: $\Phi(r) = \frac{r + |r|}{1 + |r|}$

The boundary values are found as,

$$q_{i+\frac{1}{2}}^{\mathrm{L,MUSCL}} = Q_i^{\mathrm{MUSCL}}\left(x_{i+\frac{1}{2}}\right) = \bar{q}_i + \frac{1}{2}\Phi(r)(\bar{q}_{i+1} - \bar{q}_i),$$

$$q_{i-\frac{1}{2}}^{\mathrm{R,MUSCL}} = Q_i^{\mathrm{MUSCL}}\left(x_{i-\frac{1}{2}}\right) = \bar{q}_i - \frac{1}{2}\Phi(r)(\bar{q}_{i+1} - \bar{q}_i).$$



MUSCL scheme

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THINC scheme

Reconstruction function:

$$Q_i^{\mathrm{THINC}}(x) = q_{\mathrm{a}} + q_{\mathrm{d}} \tanh\big(\beta(X_i(x) - d_i)\big),$$

where,

$$q_{\mathrm{a}} = \frac{\bar{q}_{i-1} + \bar{q}_{i+1}}{2},\ q_{\mathrm{d}} = \frac{\bar{q}_{i+1} - \bar{q}_{i-1}}{2},\ X_i(x) = \frac{x - x_i}{\Delta x}.$$

The boundary values are found as

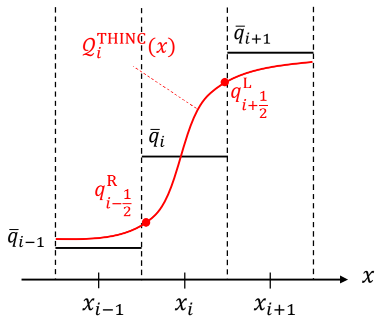
$$q_{i+\frac{1}{2}}^{\mathrm{L,THINC}} = Q_i^{\mathrm{THINC}}\left(x_{i+\frac{1}{2}}\right) = q_{\mathrm{a}} + q_{\mathrm{d}} \frac{T_1 + T_2/T_1}{1 + T_2},$$

$$q_{i-\frac{1}{2}}^{\mathrm{R,THINC}} = Q_i^{\mathrm{THINC}}\left(x_{i-\frac{1}{2}}\right) = q_{\mathrm{a}} - q_{\mathrm{d}} \frac{T_1 - T_2/T_1}{1 - T_2},$$

$$\left(T_1 = \tanh\left(\frac{\beta}{2}\right),\ T_2 = \tanh\left(\frac{\alpha_i \beta}{2}\right),\ \alpha_i = \frac{\bar{q}_i - q_{\mathrm{a}}}{q_{\mathrm{d}}}\right).$$

The steepness parameter β determines the characteristics of the THINC scheme:

- ✓ Small β (≈ 1.1): stable, suppressing numerical oscillation.
- ✓ Large β ($\approx 1.6 \sim 3.0$): suitable for capturing discontinuity.



THINC scheme

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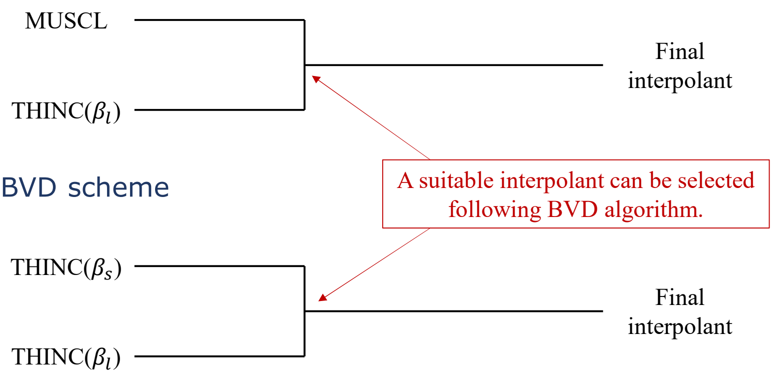
Hybrid-type BVD scheme

- MUSCL-THINC-BVD scheme
- Adaptive THINC-BVD scheme



BVD algorithm

Procedure for selecting a suitable interpolant for cell Ω_i in the MUSCL-THINC-BVD scheme:

A) Calculate total BV (TBV),

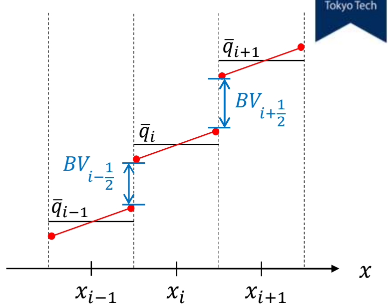
$$TBV_i^m = BV_{i-\frac{1}{2}}^m + BV_{i+\frac{1}{2}}^m,$$

for all possible patterns ($m = 1 \sim 8$).

B) Select the final interpolant function as

$$Q_i(x) = \begin{cases} Q_i^{\mathrm{MUSCL}}(x) & \text{if } \underset{m}{\operatorname{argmin}}\, TBV_i^m \in \{1,2,3,4\}, \\ Q_i^{\mathrm{THINC}}(x) & \text{if } \underset{m}{\operatorname{argmin}}\, TBV_i^m \in \{5,6,7,8\}. \end{cases}$$

Same procedure can be applied for the adaptive THINC-BVD scheme.



m	cell $i-1$	cell i	cell $i+1$
1	MUSCL	MUSCL	MUSCL
2	MUSCL	MUSCL	THINC
3	THINC	MUSCL	MUSCL
4	THINC	MUSCL	THINC
5	MUSCL	THINC	MUSCL
6	MUSCL	THINC	THINC
7	THINC	THINC	MUSCL
8	THINC	THINC	THINC

Contents

- Riemann solver:
  HLLC (wave-propagation method)
- Time integration: 3rd-order RK
- CFL: 0.5

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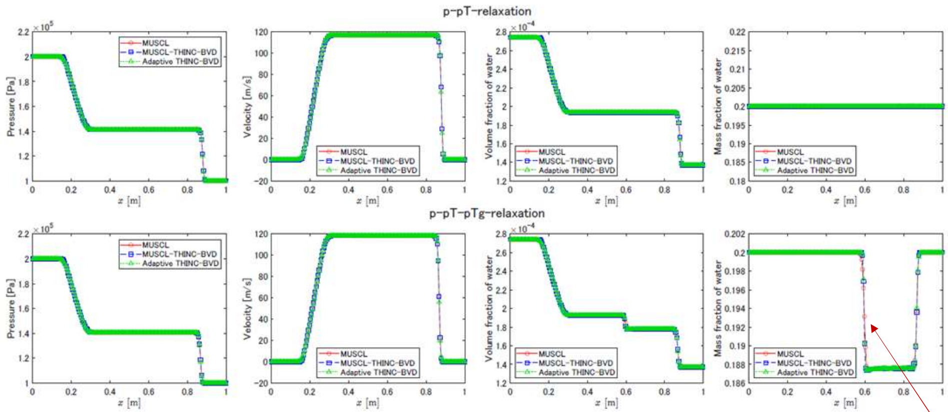
1D water shock tube problem

Numerical results

without phase change

with phase change



The BVD method shows captured the interface within 3 - 4 cells.

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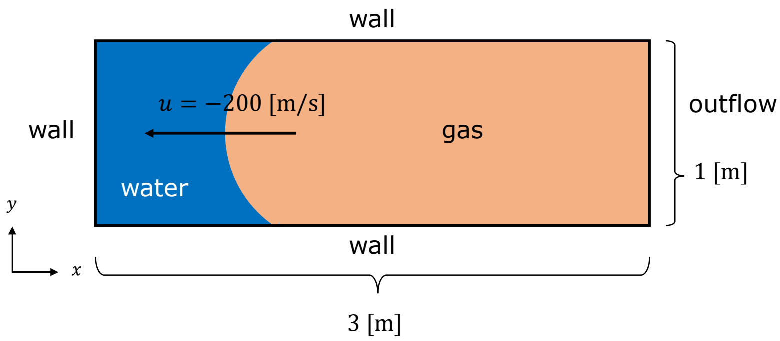
2D cavitating RMI problem

Conceptual diagram of the problem



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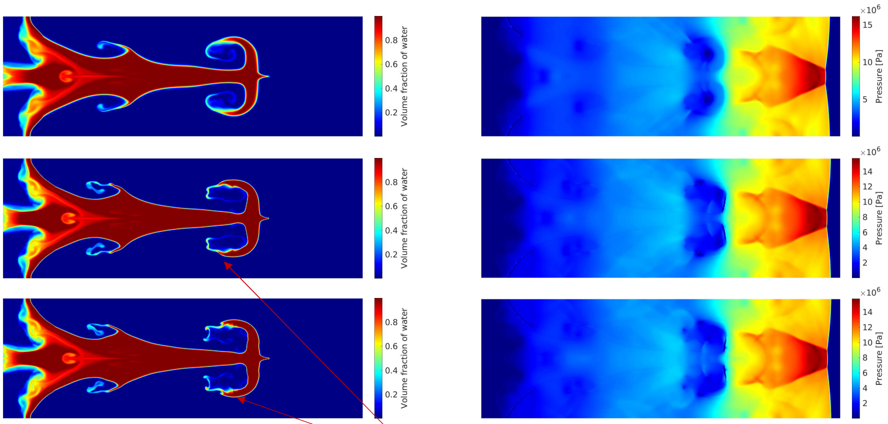
2D cavitating RMI problem

Numerical results (without phase change)

MUSCL

MUSCL-THINC-BVD

Adaptive THINC-BVD



Volume fraction of water

The BVD method shows more developed instability.

Pressure

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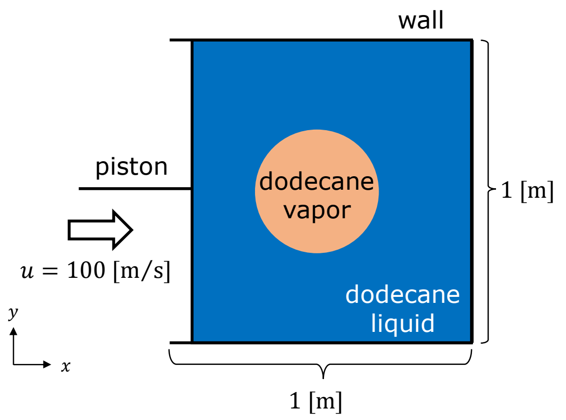
2D vapor bubble compression problem

Conceptual diagram of the problem



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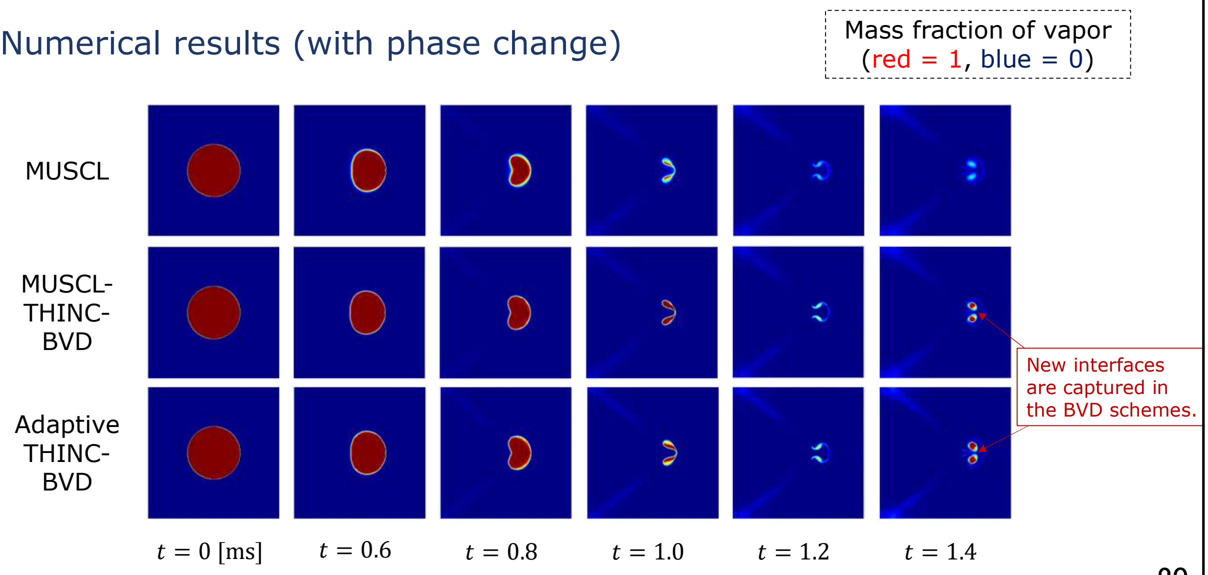
2D vapor bubble compression problem

Numerical results (with phase change)



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Summary

- We introduced MUSCL-THINC-BVD and adaptive THINC-BVD scheme for the accurate simulation of the compressible multiphase flows with phase change.
- Following the Boundary Variation Diminishing principle, a suitable interpolant was selected from two kinds of candidate interpolants.
- The numerical results showed that the BVD schemes can capture both continuous and discontinuous solutions more accurately than the existing scheme.
- Future work:
  - Unstructured grids
  - Other candidate interpolants
  - High-order scheme for turbulent flows

Thank you for your attention!