

# Hybrid Multifluid Algorithms Based on the Path-Conservative Central-Upwind Scheme

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*joint work with*

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February 25, 2022

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## Multicomponent Flows

- Consider flow models describing the dynamics of fluids consisting of several immiscible and compressible fluids
- Assume
  - All fluid components can be described by a single velocity  $(u, v)$  and a single pressure  $p$  and the governing equations in 2-D are:

$$\rho_t + (\rho u)_x + (\rho v)_y = 0$$

$$(\rho u)_t + (\rho u^2 + p)_x + (\rho uv)_y = 0$$

$$(\rho v)_t + (\rho uv)_x + (\rho v^2 + p)_y = 0$$

$$E_t + [u(E + p)]_x + [v(E + p)]_y = 0$$

Here:  $\rho$  is the density of the fluid mixture and  $E$  is the total energy

- The fluid components are separated by interfaces, and each fluid component is equipped with its own equation of state (EOS):

$$p = (\gamma - 1) \left[ E - \frac{\rho}{2}(u^2 + v^2) \right] - \gamma p_\infty$$

i.e., have different specific heat ratios  $\gamma$  and stiffness parameters  $p_\infty$

## Multicomponent Flows

$$\begin{pmatrix} \rho \\ \rho u \\ \rho v \\ E \end{pmatrix}_t + \begin{pmatrix} \rho u \\ \rho u^2 + p \\ \rho uv \\ u(E + p) \end{pmatrix}_x + \begin{pmatrix} \rho v \\ \rho uv \\ \rho v^2 + p \\ v(E + p) \end{pmatrix}_y = \mathbf{0}$$



$$\mathbf{U}_t + \mathbf{F}(\mathbf{U})_x + \mathbf{G}(\mathbf{U})_y = \mathbf{0}$$

$$\mathbf{EOS:} \quad p = (\gamma - 1) \left[ E - \frac{\rho}{2}(u^2 + v^2) \right] - \gamma p_\infty$$

A multifluid problem with several components:

$$\gamma = \gamma_I, \quad p_\infty = p_{\infty,I}$$

$$\gamma = \gamma_{II}, \quad p_\infty = p_{\infty,II}$$

$$\gamma = \gamma_{III}, \quad p_\infty = p_{\infty,III}$$

...

# Multicomponent Flows

- Fluid components are usually identified by a variable  $\phi$  that propagates with the fluid velocity:

$$\phi_t + u\phi_x + v\phi_y = 0$$

or

$$(\rho\phi)_t + (\rho u\phi)_x + (\rho v\phi)_y = 0$$

- *Various models — various choices of  $\phi$* 
  - a state variable, say,  $\gamma$  or any function of it<sup>1</sup>
  - the mass fraction of the fluid component in the fluid mixture<sup>2</sup>
  - a level-set function, whose zero level-set defines the interface between the fluid components<sup>3</sup>

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<sup>1</sup>Roe, 1982; Karni, 1994.

<sup>2</sup>Abgrall, 1998; Abgrall, 1996; Saurel and Abgrall, 1999a; Larroutourou, 1991.

<sup>3</sup>Fedkiw, Aslam, Merriman, and Osher, 1999; Mulder, Osher, and Sethian, 1992.

## What May Go Wrong? – 1-D Example

$$\begin{pmatrix} \rho \\ \rho u \\ E \\ \rho\phi \end{pmatrix}_t + \begin{pmatrix} \rho u \\ \rho u^2 + p \\ u(E + p) \\ \rho u\phi \end{pmatrix}_x = \mathbf{0} \quad \Leftrightarrow \quad \mathbf{U}_t + \mathbf{F}(\mathbf{U})_x = \mathbf{0}$$

**EOS:**  $p = (\gamma - 1) \left[ E - \frac{\rho}{2} u^2 \right] - \gamma p_\infty$

**Example:** A multifluid problem with two components

$$\gamma = \gamma_I, \quad p_\infty = p_{\infty,I}$$

$$\gamma = \gamma_{II}, \quad p_\infty = p_{\infty,II}$$

## Finite-Volume Framework – 1-D

$$U_t + F(U)_x = 0$$

- $\bar{U}_j(t) \approx \frac{1}{\Delta x} \int_{C_j} U(x, t) dx$ : cell averages over  $C_j := [x_{j-\frac{1}{2}}, x_{j+\frac{1}{2}})$
- $U_{j+\frac{1}{2}}^-(t)$  and  $U_{j+\frac{1}{2}}^+(t)$ : reconstructed point values at  $x_{j+\frac{1}{2}}$
- Semi-discrete FV method:

$$\frac{d}{dt} \bar{U}_j(t) = - \frac{H_{j+\frac{1}{2}} \left( U_{j+\frac{1}{2}}^-, U_{j+\frac{1}{2}}^+ \right) - H_{j-\frac{1}{2}} \left( U_{j-\frac{1}{2}}^-, U_{j-\frac{1}{2}}^+ \right)}{\Delta x}$$

$$H_{j\pm\frac{1}{2}} \approx F(U_{j\pm\frac{1}{2}}(t)): \text{numerical fluxes}$$

# Finite-Volume Framework – 1-D

$$\{\bar{U}_j(t)\} \rightarrow \{U_{j+\frac{1}{2}}^\pm\} \rightarrow \{H_{j+\frac{1}{2}}\} \rightarrow \{\bar{U}_j(t + \Delta t)\}$$

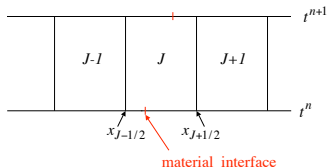
A piecewise-linear reconstruction (**conservative**, **second-order** accurate, **non-oscillatory** provided the slopes are computed by a **nonlinear limiter**):

$$\tilde{U}_j(x) = \bar{U}_j + (U_x)_j(x - x_j), \quad x \in C_j$$

$$(U_x)_j = \text{minmod} \left( \theta \frac{\bar{U}_j - \bar{U}_{j-1}}{\Delta x}, \frac{\bar{U}_{j+1} - \bar{U}_{j-1}}{2\Delta x}, \theta \frac{\bar{U}_{j+1} - \bar{U}_j}{\Delta x} \right)$$

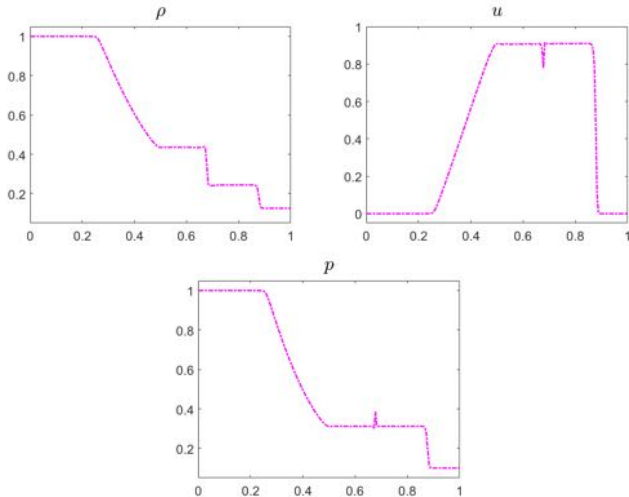
$$U_{j+\frac{1}{2}}^+ := \bar{U}_j + \frac{\Delta x}{2} (U_x)_j$$

$$U_{j+\frac{1}{2}}^- := \bar{U}_j - \frac{\Delta x}{2} (U_x)_j$$



$$\frac{d\bar{U}_j}{dt} = - \frac{H_{j+\frac{1}{2}}(U_{j+\frac{1}{2}}^-, U_{j+\frac{1}{2}}^+) - H_{j-\frac{1}{2}}(U_{j-\frac{1}{2}}^-, U_{j-\frac{1}{2}}^+)}{\Delta x}$$

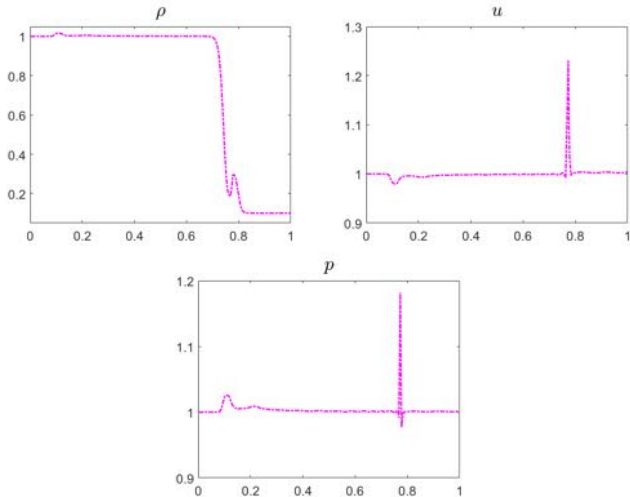
## 1-D Example – Shock Tube Problem



$$(\rho, u, p, \gamma, p_\infty)^T = \begin{cases} (1.000, 0, 1.0, 1.6, 0)^T, & \text{if } x < 0.25 \\ (0.125, 0, 0.1, 1.4, 0)^T, & \text{if } x > 0.25 \end{cases}$$

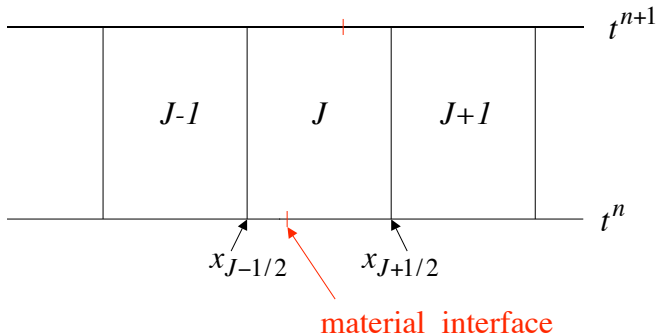


# 1-D Example – Contact Wave Problem



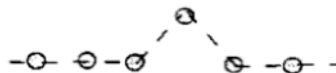
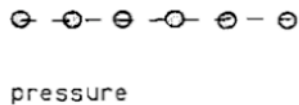
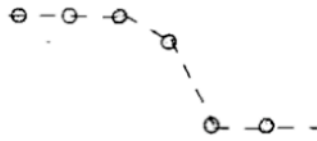
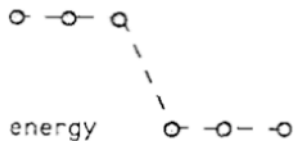
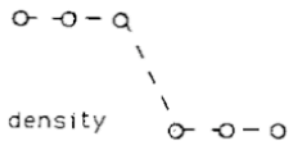
$$(\rho, u, p, \gamma, p_\infty)^T = \begin{cases} (1.0, 1.0, 1.0, 1.6, 0)^T, & \text{if } x < 0.25 \\ (0.1, 1.0, 1.0, 1.4, 0)^T, & \text{if } x > 0.25 \end{cases}$$

## Multicomponent Flows – What may go wrong?



- Fluxes are computed using the information in the "mixed" cell.
- No valid EOS in mixed cells.

## Multicomponent Flows – What may go wrong?<sup>4</sup>



<sup>4</sup>Karni, 1994.

# Multicomponent Flows – Numerical Methods

- Front-capturing algorithms:
  - *Fluid-mixture type algorithms*<sup>5</sup>
  - *Five-equation model*<sup>6</sup>
  - *Pressure evolution method*<sup>7</sup>
  - *A simple fully conservative algorithm*<sup>8</sup>
  - *Ghost-fluid methods*<sup>9</sup>
  
- Front-tracking algorithms:
  - *Moving-mesh techniques*<sup>10</sup>
  - *Interface tracking methods*<sup>11</sup>

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<sup>5</sup>Abgrall and Saurel, 2003; Shyue, 1998.

<sup>6</sup>Allaire, Clerc, and Kokh, 2002; Cheng, Zhang, and Liu, 2020.

<sup>7</sup>Karni, 1994.

<sup>8</sup>Saurel and Abgrall, 1999b.

<sup>9</sup>Fedkiw, Aslam, Merriman, and Osher, 1999; Abgrall and Karni, 2001.

<sup>10</sup>Harten and Hyman, 1983; Chertock and Kurganov, 2005.

<sup>11</sup>Davis, 1992; Chertock, Karni, and Kurganov, 2008; Wang and Shu, 2010.

# Interface Tracking Method – 1-D<sup>12</sup>

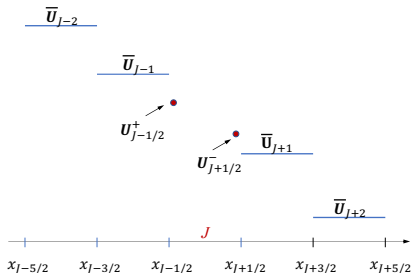
$$U_t + F(U)_x = 0$$

$$\frac{d}{dt} \bar{U}_j(t) = - \frac{H_{j+\frac{1}{2}}(U_{j+\frac{1}{2}}^-, U_{j+\frac{1}{2}}^+) - H_{j-\frac{1}{2}}(U_{j-\frac{1}{2}}^-, U_{j-\frac{1}{2}}^+)}{\Delta x}, \quad j \neq J$$

Don't use unreliable "mixed" cell data!

$$U_{j-\frac{1}{2}}^+ = \mathcal{D}(\bar{U}_{j-2}, \bar{U}_{j-1}, \bar{U}_j)$$

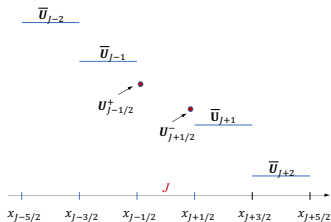
$$U_{j+\frac{1}{2}}^- = \mathcal{D}(\bar{U}_{j-1}, \bar{U}_j, \bar{U}_{j+1})$$



<sup>12</sup>Chertock, Karni, and Kurganov, 2008.

## Interface Tracking Method – Main Idea<sup>13</sup>

Don't use unreliable "mixed" cell data!



- **Instead**

- Use the reliable single fluid data from the both sides of the interface to obtain the missing "mixed" cell information
- Interpolate in the phase space by solving the corresponding Riemann problem using the data from both sides of the "mixed" cell

Interface tracking methods are very robust in the 1-D case, but their extensions to multi-D problems are rather cumbersome! The accuracy is restricted to the first order at the interface!

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<sup>13</sup>Chertock, Karni, and Kurganov, 2008.

## Hybrid Multifluid Algorithm – 1-D<sup>14</sup>

$$\begin{pmatrix} \rho \\ \rho u \\ E \\ \rho\phi \end{pmatrix}_t + \begin{pmatrix} \rho u \\ \rho u^2 + p \\ u(E + p) \\ \rho u\phi \end{pmatrix}_x = \mathbf{0} \quad \Leftrightarrow \quad \begin{aligned} \mathbf{U}_t + \mathbf{F}(\mathbf{U})_x &= \mathbf{0} \\ \text{EOS: } p &= (\gamma - 1) \left[ E - \frac{\rho}{2} u^2 \right] - \gamma p_\infty \end{aligned}$$

Assume:

- A multifluid problem with two components

$$\gamma = \gamma_I, \quad p_\infty = p_{\infty,I}$$

$$\gamma = \gamma_{II}, \quad p_\infty = p_{\infty,II}$$

- There is only one material interface and  $\phi$  is the level-set function used to determine its position. The case of a larger, but finite number of interfaces can be treated similarly.

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<sup>14</sup>Chertock, Chu, and Kurganov, 2021.

## Hybrid Multifluid Algorithm – 1-D

- We assume that at some time  $t \geq 0$  the cell averages of the **conservative variables** are available:

$$\bar{U}_j = (\bar{\rho}_j, \bar{\rho}u_j, \bar{E}_j, \bar{\rho}\phi_j)^\top$$

- We compute
  - values of **primitive variables**

$$\mathbf{V}_j = (\bar{\rho}_j, u_j, p_j, \phi_j)^\top$$

$$u_j = \frac{\bar{\rho}u_j}{\bar{\rho}_j}, \quad p_j = (\gamma_j - 1) \left[ \bar{E}_j - \frac{((\bar{\rho}u)_j)^2}{2\bar{\rho}_j} - \gamma_j (p_\infty)_j \right], \quad \phi_j = \frac{\bar{\rho}\phi_j}{\bar{\rho}_j}$$

- values of  $\gamma$  and  $p_\infty$

$$\gamma_j = \begin{cases} \gamma_I, & \text{if } \phi_j > 0, \\ \gamma_{II}, & \text{otherwise,} \end{cases} \quad (p_\infty)_j = \begin{cases} p_{\infty,I}, & \text{if } \phi_j > 0, \\ p_{\infty,II}, & \text{otherwise.} \end{cases}$$

- We say that cells  $C_J$  and  $C_{J+1}$  are the **interface cells** if

$$\phi_J(t) \cdot \phi_{J+1}(t) \leq 0$$



## Hybrid Multifluid Algorithm – Main Idea

- $j \notin \{J, J + 1\}$  – consider the original system

$$\begin{pmatrix} \rho \\ \rho u \\ E \\ \rho \phi \end{pmatrix}_t + \begin{pmatrix} \rho u \\ \rho u^2 + p \\ u(E + p) \\ \rho u \phi \end{pmatrix}_x = \mathbf{0} \quad \Leftrightarrow \quad \mathbf{U}_t + \mathbf{F}(\mathbf{U})_x = \mathbf{0}$$

- $j \in \{J, J + 1\}$  – replace the  $E$ -equation with the  $p$ -equation<sup>15</sup>

$$\begin{pmatrix} \rho \\ \rho u \\ p \\ \rho \phi \end{pmatrix}_t + \begin{pmatrix} \rho u \\ \rho u^2 + p \\ up \\ \rho u \phi \end{pmatrix}_x = \begin{pmatrix} 0 \\ 0 \\ -[(\gamma - 1)p + \gamma p_\infty] u_x \\ 0 \end{pmatrix} \quad \Leftrightarrow \quad \mathbf{u}_t + \mathcal{F}(\mathbf{u})_x = B(\mathbf{u})\mathbf{u}_x$$

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<sup>15</sup>Karni, 1996.

# Hybrid Multifluid Algorithm – Main Idea

$j \notin \{J, J + 1\}$	$j \in \{J, J + 1\}$
Solve the <i>conservative</i> system $\mathbf{U}_t + \mathbf{F}(\mathbf{U})_x = \mathbf{0}$	Solve the <i>nonconservative</i> system $\mathbf{u}_t + \mathcal{F}(\mathbf{u})_x = B(\mathbf{u})\mathbf{u}_x$
<b>Second-Order FV Method</b>	
Implement central-upwind (CU) scheme	Implement path-conservative central-upwind (PCCU) scheme
<b>Fifth-Order FD Method</b>	
Implement alternative WENO (A-WENO) scheme	Implement path-conservative A-WENO scheme

## Semi-Discrete CU scheme

$$U_t + F(U)_x = 0$$

$$\frac{d\bar{U}_j}{dt} = -\frac{H_{j+\frac{1}{2}} - H_{j-\frac{1}{2}}}{\Delta x}, \quad j \notin \{J, J+1\}$$

- $H_{j\pm\frac{1}{2}}$  are CU numerical fluxes<sup>16</sup>:

$$H_{j+\frac{1}{2}} = \frac{a_{j+\frac{1}{2}}^+ F(U_{j+\frac{1}{2}}^-) - a_{j+\frac{1}{2}}^- F(U_{j+\frac{1}{2}}^+)}{a_{j+\frac{1}{2}}^+ - a_{j+\frac{1}{2}}^-} + \frac{a_{j+\frac{1}{2}}^+ a_{j+\frac{1}{2}}^-}{a_{j+\frac{1}{2}}^+ - a_{j+\frac{1}{2}}^-} (U_{j+\frac{1}{2}}^+ - U_{j+\frac{1}{2}}^-)$$

- $a_{j+\frac{1}{2}}^\pm$  are the one-sided local speeds of propagation obtained from the largest and the smallest eigenvalues of the Jacobian  $\frac{\partial F}{\partial U}$ :

$$a_{j+\frac{1}{2}}^\pm = \max_{\min} \left\{ u_{j+\frac{1}{2}}^- \pm c_{j+\frac{1}{2}}^-, u_{j+\frac{1}{2}}^+ \pm c_{j+\frac{1}{2}}^+, 0 \right\}, \quad c := \sqrt{\gamma(p + p_\infty)/\rho}$$

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<sup>16</sup>Kurganov, 2016.

## Semi-Discrete CU scheme

$$\frac{d\bar{U}_j}{dt} = -\frac{H_{j+\frac{1}{2}} - H_{j-\frac{1}{2}}}{\Delta x}, \quad j \notin \{J, J+1\}$$

### Important!!!

- **Reconstruct primitive variables  $V$**  since both the pressure and velocity are continuous across the material interface

$$\tilde{V}_j(x, t) = \mathbf{V}_j(t) + (\mathbf{V}_x)_j(x - x_j), \quad x \in C_j \quad \Rightarrow \quad \mathbf{V}_{j+\frac{1}{2}}^\pm(t)$$

- **Use**

$$\tilde{\gamma}_j(x) = \begin{cases} \gamma_I, & \text{if } x < x_{J+\frac{1}{2}}, \\ \gamma_{II}, & \text{otherwise,} \end{cases} \quad (\tilde{p}_\infty)_j(x) = \begin{cases} p_{\infty, I}, & \text{if } x < x_{J+\frac{1}{2}}, \\ p_{\infty, II}, & \text{otherwise} \end{cases}$$

$$\gamma_{j+\frac{1}{2}}^\pm = \gamma_j = \gamma_{j+1},$$

$$(p_\infty)_{j+\frac{1}{2}}^\pm = (p_\infty)_j = (p_\infty)_{j+1}$$

$$\{\bar{U}_j(t)\} \rightarrow \{\mathbf{V}_j\} \rightarrow \left\{ \mathbf{V}_{j+\frac{1}{2}}^\pm \right\} \rightarrow \left\{ \mathbf{U}_{j+\frac{1}{2}}^\pm \right\} \rightarrow \left\{ \mathbf{H}_{j+\frac{1}{2}} \right\} \rightarrow \{\bar{U}_j(t + \Delta t)\}$$

## Reformulating CU scheme

$$U_t + F(U)_x = 0$$

 $\Rightarrow$ 

$$\frac{d\bar{U}_j}{dt} = -\frac{H_{j+\frac{1}{2}} - H_{j-\frac{1}{2}}}{\Delta x}$$

$$U_t + A(U)U_x = 0$$

$$A(U) = \frac{\partial F(U)}{\partial U}$$

 $\Rightarrow$ 

$$\frac{d\bar{U}_j}{dt} = ?$$

A straightforward discretization:

~~$$A_j = \frac{1}{\Delta x} \int_{C_j} A(U)U_x dx$$~~

Consistent only for smooth solution and doesn't account for the contribution of the nonconservative products at the cell interfaces.

## Reformulating CU scheme

$$\frac{d\bar{U}_j}{dt} = -\frac{H_{j+\frac{1}{2}} - H_{j-\frac{1}{2}}}{\Delta x}$$

$\Updownarrow$

$$\frac{d\bar{U}_j}{dt} = -\frac{1}{\Delta x} \left[ \underbrace{H_{j+\frac{1}{2}} - F(U_{j+\frac{1}{2}}^-)}_{D_{j+\frac{1}{2}}^-} + \underbrace{F(U_{j-\frac{1}{2}}^+) - H_{j-\frac{1}{2}}}_{D_{j-\frac{1}{2}}^+} + F(U_{j+\frac{1}{2}}^-) - F(U_{j-\frac{1}{2}}^+) \right]$$

$$\frac{d\bar{U}_j}{dt} = -\frac{1}{\Delta x} \left[ D_{j+\frac{1}{2}}^- + D_{j-\frac{1}{2}}^+ + F(U_{j+\frac{1}{2}}^-) - F(U_{j-\frac{1}{2}}^+) \right]$$

$$\frac{d\bar{U}_j}{dt} = -\frac{1}{\Delta x} \left[ \underbrace{D_{j+\frac{1}{2}}^- + D_{j-\frac{1}{2}}^+}_{?} + \underbrace{\int_{C_j} A(\tilde{U}_j(x)) (\tilde{U}_j(x))_x dx}_{A_j} \right]$$

**Recall:** A piecewise-linear reconstruction:

$$\tilde{U}_j(x) = \bar{U}_j + (U_x)_j(x - x_j), \quad x \in C_j$$

## Reformulating CU scheme

$$D_{j+\frac{1}{2}}^- = H_{j+\frac{1}{2}} - F(U_{j+\frac{1}{2}}^-), \quad D_{j-\frac{1}{2}}^+ = F(U_{j-\frac{1}{2}}^+) - H_{j-\frac{1}{2}}$$

CU fluxes:

$$H_{j+\frac{1}{2}} = \frac{a_{j+\frac{1}{2}}^+ F(U_{j+\frac{1}{2}}^-) - a_{j+\frac{1}{2}}^- F(U_{j+\frac{1}{2}}^+)}{a_{j+\frac{1}{2}}^+ - a_{j+\frac{1}{2}}^-} + \frac{a_{j+\frac{1}{2}}^+ a_{j+\frac{1}{2}}^-}{a_{j+\frac{1}{2}}^+ - a_{j+\frac{1}{2}}^-} (U_{j+\frac{1}{2}}^+ - U_{j+\frac{1}{2}}^-)$$

$\Downarrow$

$$D_{j+\frac{1}{2}}^- = \frac{1 - \alpha_{j+\frac{1}{2}}}{2} \left[ \underbrace{F(U_{j+\frac{1}{2}}^+) - F(U_{j+\frac{1}{2}}^-)}_{?} \right] - \frac{\beta_{j+\frac{1}{2}}}{2} (U_{j+\frac{1}{2}}^+ - U_{j+\frac{1}{2}}^-)$$

$$\alpha_{j+\frac{1}{2}} = \frac{a_{j+\frac{1}{2}}^+ + a_{j+\frac{1}{2}}^-}{a_{j+\frac{1}{2}}^+ - a_{j+\frac{1}{2}}^-}, \quad \beta_{j+\frac{1}{2}} = \frac{-2a_{j+\frac{1}{2}}^+ a_{j+\frac{1}{2}}^-}{a_{j+\frac{1}{2}}^+ - a_{j+\frac{1}{2}}^-}$$

## Reformulating CU scheme

$$D_{j+\frac{1}{2}}^- = \frac{1 - \alpha_{j+\frac{1}{2}}}{2} \underbrace{\left[ \mathbf{F}(U_{j+\frac{1}{2}}^+) - \mathbf{F}(U_{j+\frac{1}{2}}^-) \right]}_{?} - \frac{\beta_{j+\frac{1}{2}}}{2} (U_{j+\frac{1}{2}}^+ - U_{j+\frac{1}{2}}^-)$$

Consider a sufficiently smooth path  $\Psi_{j+\frac{1}{2}}(s) := \Psi_{j+\frac{1}{2}}(s; U_{j+\frac{1}{2}}^-, U_{j+\frac{1}{2}}^+)$ :

$$\Psi : [0, 1] \times \mathbb{R}^N \times \mathbb{R}^N \rightarrow \mathbb{R}^N,$$

$$\Psi_{j+\frac{1}{2}}\left(0; U_{j+\frac{1}{2}}^-, U_{j+\frac{1}{2}}^+\right) = U_{j+\frac{1}{2}}^-, \quad \Psi_{j+\frac{1}{2}}\left(1; U_{j+\frac{1}{2}}^-, U_{j+\frac{1}{2}}^+\right) = U_{j+\frac{1}{2}}^+$$

$\Downarrow$

$$D_{j+\frac{1}{2}}^- = \frac{1 - \alpha_{j+\frac{1}{2}}}{2} \underbrace{\int_0^1 A(\Psi_{j+\frac{1}{2}}(s)) (\Psi_{j+\frac{1}{2}}(s))_s ds}_{A_{\Psi, j+\frac{1}{2}}} - \frac{\beta_{j+\frac{1}{2}}}{2} (U_{j+\frac{1}{2}}^+ - U_{j+\frac{1}{2}}^-)$$



## Reformulating CU scheme

$$U_t + A(U)U_x = \mathbf{0} \quad \Rightarrow \quad \frac{d\bar{U}_j}{dt} = -\frac{1}{\Delta x} \left[ D_{j+\frac{1}{2}}^- + D_{j-\frac{1}{2}}^+ + A_j \right]$$

Here:

$$D_{j+\frac{1}{2}}^\pm = \frac{1 \pm \alpha_{j+\frac{1}{2}}}{2} A_{\Psi, j+\frac{1}{2}} \pm \frac{\beta_{j+\frac{1}{2}}}{2} \left( U_{j+\frac{1}{2}}^+ - U_{j+\frac{1}{2}}^- \right)$$

$$\alpha_{j+\frac{1}{2}} = \frac{a_{j+\frac{1}{2}}^+ + a_{j+\frac{1}{2}}^-}{a_{j+\frac{1}{2}}^+ - a_{j+\frac{1}{2}}^-}, \quad \beta_{j+\frac{1}{2}} = \frac{-2a_{j+\frac{1}{2}}^+ a_{j+\frac{1}{2}}^-}{a_{j+\frac{1}{2}}^+ - a_{j+\frac{1}{2}}^-}$$

$$A_{\Psi, j+\frac{1}{2}} := \int_0^1 A\left(\Psi_{j+\frac{1}{2}}(s)\right) \left(\Psi_{j+\frac{1}{2}}(s)\right)_s ds, \quad A_j := \int_{C_j} A(\tilde{U}_j(x)) \left(\tilde{U}_j(x)\right)_x dx$$

$$\Psi_{j+\frac{1}{2}}(s) := \Psi_{j+\frac{1}{2}}\left(s; U_{j+\frac{1}{2}}^-, U_{j+\frac{1}{2}}^+\right), \quad \tilde{U}_j(x) = \bar{U}_j + (U_x)_j(x-x_j), \quad x \in C_j$$

# Hybrid Multifluid Algorithm – Main Idea

$j \notin \{J, J + 1\}$	$j \in \{J, J + 1\}$
Solve the <i>conservative</i> system $\mathbf{U}_t + \mathbf{F}(\mathbf{U})_x = \mathbf{0}$	Solve the <i>nonconservative</i> system $\mathbf{u}_t + \mathcal{F}(\mathbf{u})_x = B(\mathbf{u})\mathbf{u}_x$
<b>Second-Order FV Method</b>	
Implement central-upwind (CU) scheme	Implement path-conservative central-upwind (PCCU) scheme
<b>Fifth-Order FD Method</b>	
Implement alternative WENO (A-WENO) scheme	Implement path-conservative A-WENO scheme

## Semi-Discrete PCCU scheme

$$\mathbf{u}_t + \mathcal{F}(\mathbf{u})_x = B(\mathbf{u})\mathbf{u}_x$$

$$\begin{pmatrix} \rho \\ \rho u \\ p \\ \rho\phi \end{pmatrix}_t + \begin{pmatrix} \rho u \\ \rho u^2 + p \\ up \\ \rho u\phi \end{pmatrix}_x = \begin{pmatrix} 0 \\ 0 \\ -[(\gamma - 1)p + \gamma p_\infty] u_x \\ 0 \end{pmatrix}$$

$$= \underbrace{\begin{pmatrix} 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \\ \frac{[(\gamma - 1)p + \gamma p_\infty] u}{\rho} & \frac{(1 - \gamma)p - \gamma p_\infty}{\rho} & 0 & 0 \\ 0 & 0 & 0 & 0 \end{pmatrix}}_{B(\mathbf{u})} \begin{pmatrix} \rho \\ \rho u \\ p \\ \rho\phi \end{pmatrix}_x$$

## Semi-Discrete PCCU Scheme

$$\mathbf{u}_t + \mathcal{F}(\mathbf{u})_x = B(\mathbf{u})\mathbf{u}_x$$

⇓

$$\mathbf{u}_t + \mathcal{A}(\mathbf{u})\mathbf{u}_x = \mathbf{0}, \quad \mathcal{A}(\mathbf{u}) := \frac{\partial \mathcal{F}(\mathbf{u})}{\partial \mathbf{u}} - B(\mathbf{u})$$

⇓

$$\frac{d\bar{U}_j}{dt} = -\frac{1}{\Delta x} \left[ \mathbf{D}_{j+\frac{1}{2}}^- + \mathbf{D}_{j-\frac{1}{2}}^+ + \mathbf{A}_j \right], \quad j \in \{J, J+1\}$$

⇓

$$\frac{d\mathbf{u}_j}{dt} = -\frac{1}{\Delta x} \left[ \underbrace{\mathcal{H}_{j+\frac{1}{2}} - \mathcal{H}_{j-\frac{1}{2}}}_{\text{CU fluxes}} - \underbrace{B_j - \frac{a_{j-\frac{1}{2}}^+}{a_{j-\frac{1}{2}}^+ - a_{j-\frac{1}{2}}^-} B_{\Psi, j-\frac{1}{2}} + \frac{a_{j+\frac{1}{2}}^-}{a_{j+\frac{1}{2}}^+ - a_{j+\frac{1}{2}}^-} B_{\Psi, j+\frac{1}{2}}}_{\text{discretization of the nonconservative terms}} \right]$$

## Semi-Discrete PCCU scheme

$$\mathbf{u}_t + \mathcal{F}(\mathbf{u})_x = B(\mathbf{u})\mathbf{u}_x$$

$$\frac{d\mathbf{u}_j}{dt} = -\frac{1}{\Delta x} \left[ \mathcal{H}_{j+\frac{1}{2}} - \mathcal{H}_{j-\frac{1}{2}} - B_j - \frac{a_{j-\frac{1}{2}}^+}{a_{j-\frac{1}{2}}^+ - a_{j-\frac{1}{2}}^-} B_{\Psi, j-\frac{1}{2}} + \frac{a_{j+\frac{1}{2}}^-}{a_{j+\frac{1}{2}}^+ - a_{j+\frac{1}{2}}^-} B_{\Psi, j+\frac{1}{2}} \right], \quad j \in \{J, J+1\}$$

We use a piecewise linear reconstruction and a linear path

$$\mathcal{H}_{j+\frac{1}{2}} = \frac{a_{j+\frac{1}{2}}^+ \mathcal{F}(\mathbf{u}_{j+\frac{1}{2}}^-) - a_{j+\frac{1}{2}}^- \mathcal{F}(\mathbf{u}_{j+\frac{1}{2}}^+)}{a_{j+\frac{1}{2}}^+ - a_{j+\frac{1}{2}}^-} + \frac{a_{j+\frac{1}{2}}^+ a_{j+\frac{1}{2}}^-}{a_{j+\frac{1}{2}}^+ - a_{j+\frac{1}{2}}^-} (\mathbf{u}_{j+\frac{1}{2}}^+ - \mathbf{u}_{j+\frac{1}{2}}^-)$$

$$B_j = \left( 0, 0, - \int_{C_j} [(\tilde{\gamma}_j(x) - 1)\tilde{p}_j(x) + \tilde{\gamma}_j(x)(\tilde{p}_\infty)_j(x)] (u_x)_j dx, 0 \right)^\top$$

$$B_{\Psi, j+\frac{1}{2}} = \left( 0, 0, \int_0^1 B(p_{j+\frac{1}{2}}(s))(u_{j+\frac{1}{2}})_s ds, 0 \right)^\top$$

# Hybrid Multifluid Algorithm – Main Idea

$j \notin \{J, J + 1\}$	$j \in \{J, J + 1\}$
Solve the <i>conservative</i> system $\mathbf{U}_t + \mathbf{F}(\mathbf{U})_x = \mathbf{0}$	Solve the <i>nonconservative</i> system $\mathbf{u}_t + \mathcal{F}(\mathbf{u})_x = B(\mathbf{u})\mathbf{u}_x$
<b>Second-Order FV Method</b>	
Implement central-upwind (CU) scheme	Implement path-conservative central-upwind (PCCU) scheme
<b>Fifth-Order FD Method</b>	
Implement alternative WENO (A-WENO) scheme	Implement path-conservative A-WENO scheme

## Fifth-Order A-WENO Scheme<sup>18</sup>

$$U_t + F(U)_x = 0 \quad \Rightarrow \quad \frac{dU_j}{dt} = -\frac{\mathfrak{H}_{j+\frac{1}{2}} - \mathfrak{H}_{j-\frac{1}{2}}}{\Delta x}, \quad j \neq \{J, J+1\}$$

- $U_j(t) \approx U(x_j, t)$
- $\mathfrak{H}_{j+\frac{1}{2}}$  is the fifth-order numerical flux:

$$\mathfrak{H}_{j+\frac{1}{2}} = H_{j+\frac{1}{2}} - \frac{1}{24}(\Delta x)^2 (F_{xx})_{j+\frac{1}{2}} + \frac{7}{5760}(\Delta x)^4 (F_{xxxx})_{j+\frac{1}{2}}$$

- $H_{j+\frac{1}{2}} = H(U_{j+\frac{1}{2}}^\pm)$  is the FV numerical flux with a **fifth-order accurate** (WENO-Z)<sup>17</sup> reconstruction applied, as before, to primitive variables  $V_j$
- $(F_{xx})_{j+\frac{1}{2}}$  and  $(F_{xxxx})_{j+\frac{1}{2}}$  are computed using the second- and fourth-order finite differences

---

<sup>17</sup>Wang, Li, Gao, and Don, 2018.

<sup>18</sup>Wang, Don, Garg, and Kurganov, 2020.

## Fifth-Order Path-Conservative A-WENO Scheme<sup>19</sup>

$$\mathbf{u}_t + \mathcal{F}(\mathbf{u})_x = B(\mathbf{u})\mathbf{u}_x, \quad j \in \{J, J+1\}$$

$$\begin{aligned} \frac{d\mathbf{u}_j}{dt} = & -\frac{1}{\Delta x} \left[ \mathcal{H}_{j+\frac{1}{2}} - \mathcal{H}_{j-\frac{1}{2}} \right. \\ & - B_j - \frac{a_{j-\frac{1}{2}}^+}{a_{j-\frac{1}{2}}^+ - a_{j-\frac{1}{2}}^-} B_{\Psi, j-\frac{1}{2}} + \frac{a_{j+\frac{1}{2}}^-}{a_{j+\frac{1}{2}}^+ - a_{j+\frac{1}{2}}^-} B_{\Psi, j+\frac{1}{2}} \\ & \left. + \frac{\Delta x}{24} \left[ (\mathbf{K}_{xx})_{j+\frac{1}{2}} - (\mathbf{K}_{xx})_{j-\frac{1}{2}} \right] - \frac{7}{5760} (\Delta x)^3 \left[ (\mathbf{K}_{xxxx})_{j+\frac{1}{2}} - (\mathbf{K}_{xxxx})_{j-\frac{1}{2}} \right] \right] \end{aligned}$$

where

$$\mathbf{K}(\mathbf{u}(\cdot, t)) = \mathcal{F}(\mathbf{u}(x, t)) - \int_{-\infty}^x B(\mathbf{u}(\xi, t))\mathbf{u}_x(\xi, t) d\xi$$

---

<sup>19</sup>Chu, Kurganov, and Na, 2021.



## Mixed-Order Approach

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### Algorithm

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**Reconstruct** all of the required point values using a WENO-Z interpolant

**Check** monotonicity for the following sequences:

$$\left(\rho_j, \rho_{j+\frac{1}{2}}^-, \rho_{j+\frac{1}{2}}^+, \rho_{j+1}\right), \left(u_j, u_{j+\frac{1}{2}}^-, u_{j+\frac{1}{2}}^+, u_{j+1}\right), \left(p_j, p_{j+\frac{1}{2}}^-, p_{j+\frac{1}{2}}^+, p_{j+1}\right)$$

**Check** if the pressure profile is locally smooth, namely,

$$\frac{|p_{j+\frac{1}{2}}^+ - p_{j+\frac{1}{2}}^-|}{\max\{p_{j+\frac{1}{2}}^+, p_{j+\frac{1}{2}}^-\}} < C(\Delta x)^2$$

**if** *the monotonicity and smoothness conditions are satisfied at  $x = x_{j+\frac{1}{2}}$*   
**then**

*use the fifth-order A-WENO fluxes*

**else**

*switch locally to the second-order CU fluxes*

---

# Numerical Examples

- 1-D examples
  - Shock-tube problem
  - Stiff shock-tube problem
  - Water-air model problem
- 2-D examples
  - Helium bubble problem
  - R22 bubble problem

$$\phi(x, 0) = \begin{cases} 1, & x \in \Omega_I, \\ -1, & x \in \Omega_{II} \end{cases}$$

$$\phi(x, y, 0) = \begin{cases} 1, & (x, y) \in \Omega_I, \\ -1, & (x, y) \in \Omega_{II} \end{cases}$$

**Time evolution:** three-stage third-order strong SSP Runge-Kutta method<sup>20</sup>; CFL=0.3

**smoothness constant:**  $C = 1$  (1-D) and  $C = 5$  (2-D)

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<sup>20</sup>Gottlieb, Shu, and Tadmor, 2001.

## Shock-Tube Problem

Consider

$$\rho_t + (\rho u)_x = 0$$

$$(\rho u)_t + (\rho u^2 + p)_x = 0$$

$$E_t + [u(E + p)]_x = 0$$

$$(\rho\phi)_t + (\rho u\phi)_x = 0$$

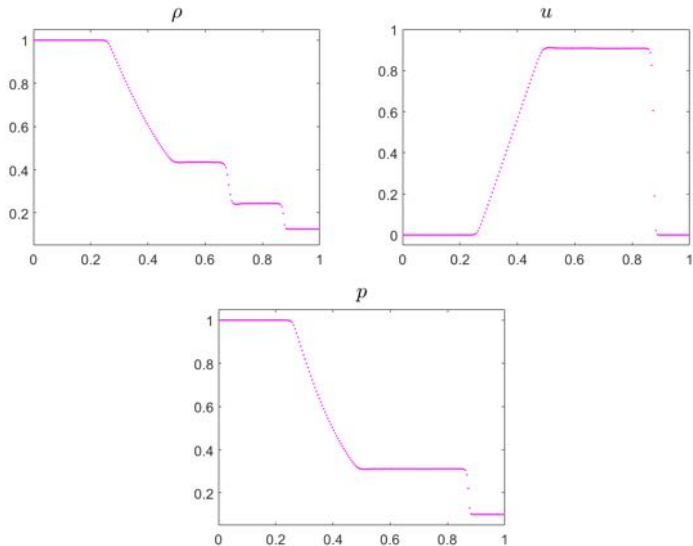
combined with the EOS

$$p = (\gamma - 1) \left[ E - \frac{1}{2} \rho u^2 \right] - \gamma p_\infty$$

Initial condition:

$$(\rho, u, p; \gamma, p_\infty) = \begin{cases} (1.000, 0, 1.0; \mathbf{1.4}, \mathbf{0}), & x < 0.5 \\ (0.125, 0, 0.1; \mathbf{1.6}, \mathbf{0}), & x > 0.5 \end{cases}$$

# Shock-Tube Problem



Mixed-order A-WENO scheme:  $\Delta x = 1/200, t = 0.2$

## Shock-Tube Problem

Relative conservation error in the computation of the total energy  $E$ :

$$\text{err} := \frac{\sum_j \bar{E}_j(t) - \sum_j \bar{E}_j(0)}{\sum_j \bar{E}_j(0)}$$

$\Delta x$	err	rate
1/200	8.35e-4	-
1/400	5.84e-4	0.52
1/800	4.58e-4	0.35
1/1600	2.70e-4	0.76
1/3200	1.62e-4	0.74

## Stiff Shock-Tube Problem

Consider

$$\rho_t + (\rho u)_x = 0$$

$$(\rho u)_t + (\rho u^2 + p)_x = 0$$

$$E_t + [u(E + p)]_x = 0$$

$$(\rho \phi)_t + (\rho u \phi)_x = 0$$

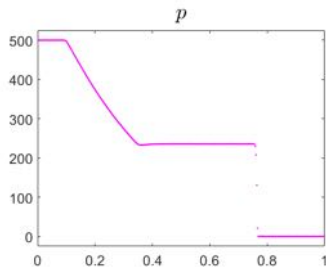
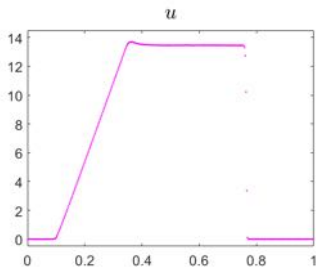
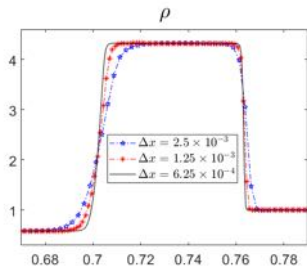
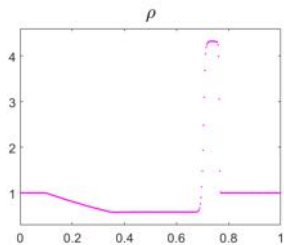
combined with the EOS

$$p = (\gamma - 1) \left[ E - \frac{1}{2} \rho u^2 \right] - \gamma p_\infty$$

Initial condition:

$$(\rho, u, p; \gamma, p_\infty) = \begin{cases} (1, 0, 500; 1.4, 0), & x < 0.5 \\ (1, 0, 0.2; 1.6, 0), & x > 0.5 \end{cases}$$

# Stiff Shock-Tube Problem



Mixed-order A-WENO scheme:  $\Delta x = 1/400, t = 0.015$

## Shock-Tube Problem

Relative conservation error in the computation of the total energy  $E$ :

$$\text{err} := \frac{\sum_j \bar{E}_j(t) - \sum_j \bar{E}_j(0)}{\sum_j \bar{E}_j(0)}$$

$\Delta x$	err	rate
1/400	1.82e-3	-
1/800	8.12e-4	1.16
1/1600	5.27e-4	0.62
1/3200	3.74e-4	0.49
1/6400	2.50e-4	0.58



## Water-Air Model with the Stiff Equation of State

Consider

$$\rho_t + (\rho u)_x = 0$$

$$(\rho u)_t + (\rho u^2 + p)_x = 0$$

$$E_t + [u(E + p)]_x = 0$$

$$(\rho \phi)_t + (\rho u \phi)_x = 0$$

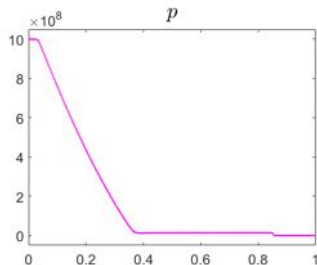
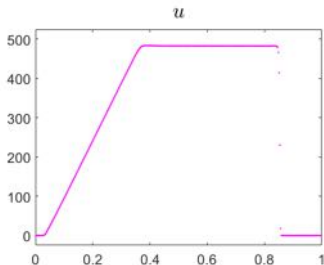
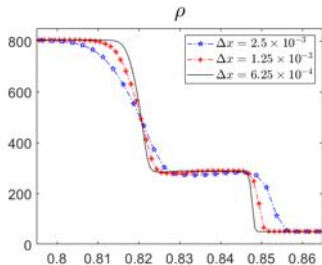
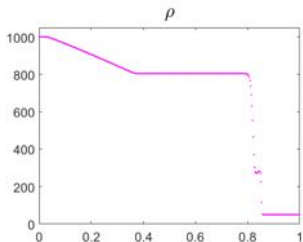
combined with the EOS

$$p = (\gamma - 1) \left[ E - \frac{1}{2} \rho u^2 \right] - \gamma p_\infty$$

Initial condition:

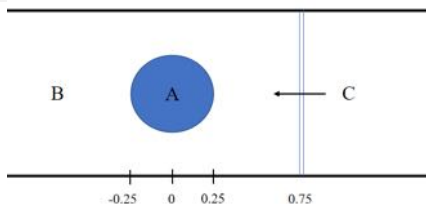
$$(\rho, u, p; \gamma, p_\infty) = \begin{cases} (1000, 0, 10^9; 4.4, 6 \cdot 10^8), & x < 0.7 \\ (50, 0, 10^5; 1.4, 0), & x > 0.7 \end{cases}$$

# Water-Air Model with the Stiff Equation of State



Mixed-order A-WENO scheme:  $\Delta x = 1/400, t = 0.00025$

## 2-D Examples



Consider

$$\rho_t + (\rho u)_x + (\rho v)_y = 0$$

$$(\rho u)_t + (\rho u^2 + p)_x + (\rho uv)_y = 0$$

$$(\rho v)_t + (\rho uv)_x + (\rho v^2 + p)_y = 0$$

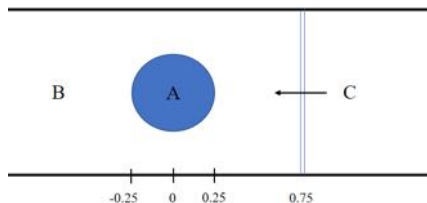
$$E_t + [u(E + p)]_x + [v(E + p)]_y = 0$$

$$(\rho\phi)_t + (\rho u\phi)_x + (\rho v\phi)_y = 0$$

combined with the EOS

$$p = (\gamma - 1) \left[ E - \frac{1}{2} \rho u^2 \right] - \gamma p_\infty$$

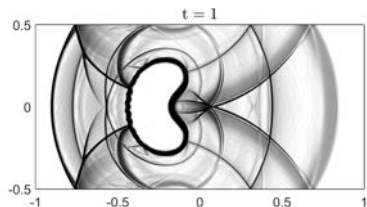
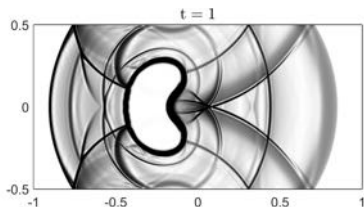
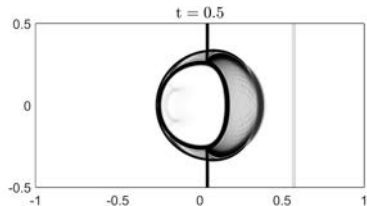
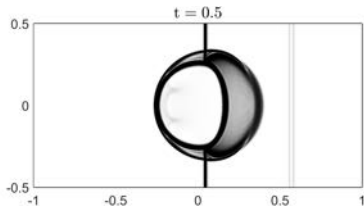
## Helium Bubble



$$(\rho, u, p; \gamma, p_\infty) = \begin{cases} (4/29, 0, 0, 1; 5/3, 0), & \text{in region A} \\ (1, 0, 0, 1; 1.4, 0), & \text{in region B} \\ (4/3, -0.3535, 0, 1.5; 1.4, 0), & \text{in region C} \end{cases}$$

The top and bottom boundaries are solid walls, while the left and right boundaries are open

# Helium Bubble

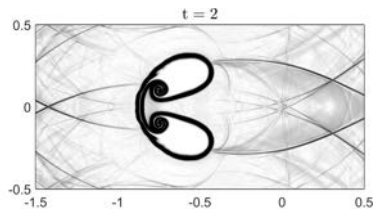
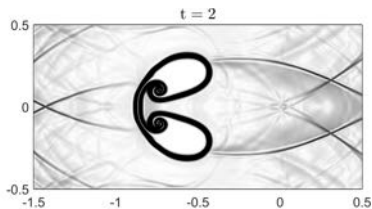
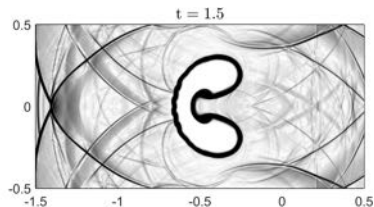
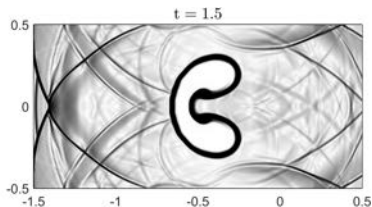


second-order CU scheme

mixed-order A-WENO scheme

$$\Delta x = \Delta y = 1/500$$

# Helium Bubble

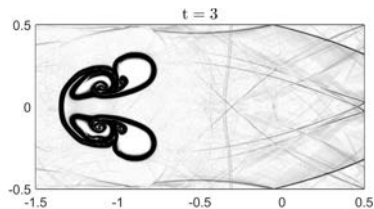
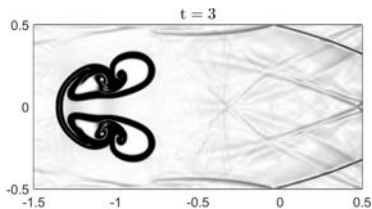
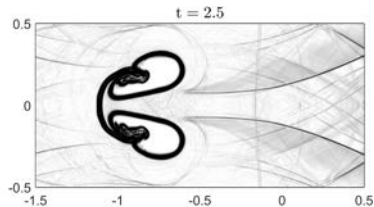
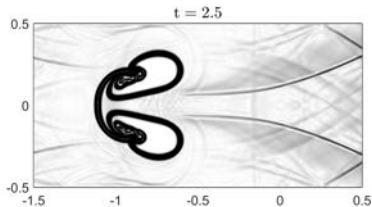


second-order CU scheme

mixed-order A-WENO scheme

$$\Delta x = \Delta y = 1/500$$

# Helium Bubble

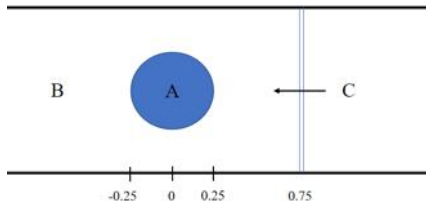


second-order CU scheme

mixed-order A-WENO scheme

$$\Delta x = \Delta y = 1/500$$

## R22 Bubble

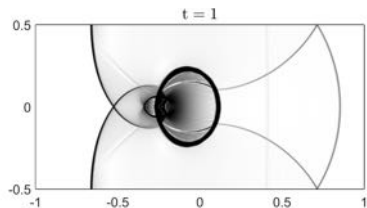
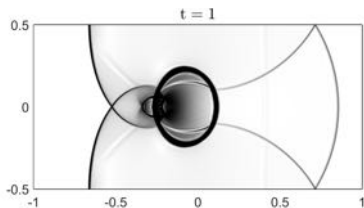
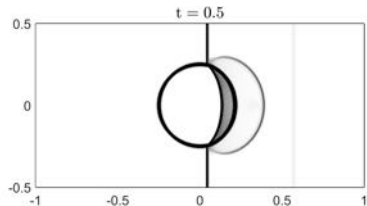
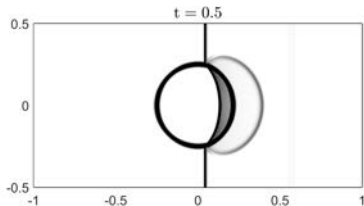


$$(\rho, u, p; \gamma, p_\infty) = \begin{cases} (3.1538, 0, 0, 1; 1.249, 0), & \text{in region A} \\ (1, 0, 0, 1; 1.4, 0), & \text{in region B} \\ (4/3, -0.3535, 0, 1.5; 1.4, 0), & \text{in region C} \end{cases}$$

The top and bottom boundaries are solid walls, while the left and right boundaries are open



# Helium Bubble

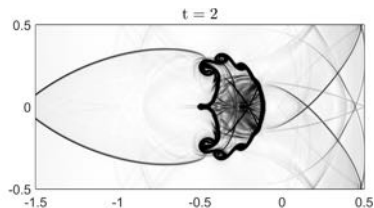
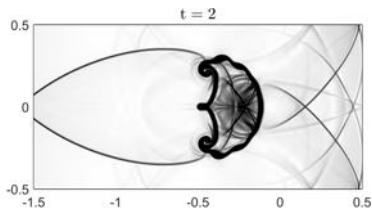
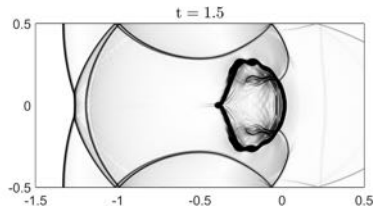
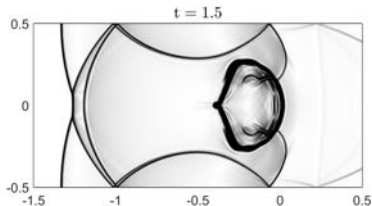


second-order CU scheme

mixed-order A-WENO scheme

$$\Delta x = \Delta y = 1/500$$

# Helium Bubble

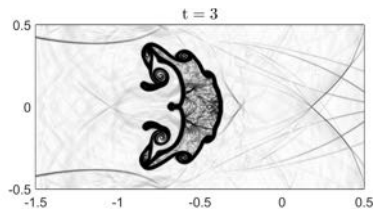
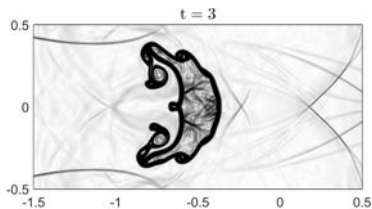
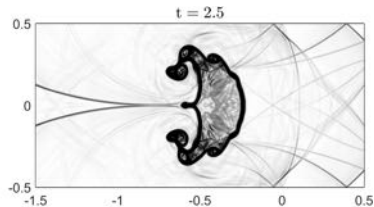
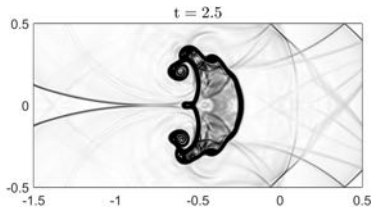


second-order CU scheme

mixed-order A-WENO scheme

$$\Delta x = \Delta y = 1/500$$

# Helium Bubble



second-order CU scheme

mixed-order A-WENO scheme

$$\Delta x = \Delta y = 1/500$$

**Thank you!**

# References

- Abgrall, R. (1996). "How to prevent pressure oscillations in multicomponent flow calculations: a quasi-conservative approach". In: *J. Comput. Phys.* 125.1, pp. 150–160.
- (1998). "Generalization of the ROE scheme for the computation of mixture of perfect gases". In: *Rech. Aéropat.* 6, pp. 31–43.
- Abgrall, R. and S. Karni (2001). "Ghost-fluids for the poor: a single fluid algorithm for multifluids". In: *Hyperbolic problems: theory, numerics, applications, Vol. I, II (Magdeburg, 2000)*. Vol. 141. Internat. Ser. Numer. Math., 140. Basel: Birkhäuser, pp. 1–10.
- Abgrall, R. and R. Saurel (2003). "Discrete equations for physical and numerical compressible multiphase flow mixtures". In: *J. Comput. Phys.* 186.2, pp. 361–396.
- Allaire, G., S. Clerc, and S. Kokh (2002). "A five-equation model for the simulation of interfaces between compressible fluids". In: *J. Comput. Phys.* 181.2, pp. 577–616.
- Cheng, J., F. Zhang, and T. G. Liu (2020). "A quasi-conservative discontinuous Galerkin method for solving five equation model of compressible two-medium flows". In: *J. Sci. Comput.* 85, pp. 12–35.
- Chertock, A., S. Chu, and A. Kurganov (2021). "Hybrid multifluid algorithms based on the path-conservative central-upwind scheme". In: *J. Sci. Comput.* 89.2, Paper No. 48, 24.
- Chertock, A., S. Karni, and A. Kurganov (2008). "Interface tracking method for compressible multifluids". In: *M2AN Math. Model. Numer. Anal.* 42, pp. 991–1019.
- Chertock, A. and A. Kurganov (2005). "Conservative locally moving mesh method for multifluid flows". In: *Finite Volumes for Complex Applications IV*. Ed. by F. Benkhaldoun, D. Ouazar, and S. Raghay. Hermes Science, pp. 273–284.
- Chu, S., A. Kurganov, and M. Na (2021). "Fifth-order A-WENO schemes based on the path-conservative central-upwind method". In: submitted.
- Davis, S. F. (1992). "An interface tracking method for hyperbolic systems of conservation laws". In: *Appl. Numer. Math.* 10, pp. 447–472.
- Fedkiw, R. P., T. Aslam, B. Merriman, and S. Osher (1999). "A non-oscillatory Eulerian approach to interfaces in multimaterial flows (the ghost fluid method)". In: *J. Comput. Phys.* 152.2, pp. 457–492.
- Gottlieb, S., C.-W. Shu, and E. Tadmor (2001). "Strong stability-preserving high-order time discretization methods". In: *SIAM Rev.* 43.1, pp. 89–112.
- Harten, A. and J. M. Hyman (1983). "Self-adjusting grid methods for one-dimensional hyperbolic conservation laws". In: *J. Comput. Phys.* 50.2, pp. 235–269.
- Karni, S. (1994). "Multicomponent flow calculations by a consistent primitive algorithm". In: *J. Comput. Phys.* 112.1, pp. 31–43.
- (1996). "Hybrid multifluid algorithms". In: *SIAM J. Sci. Comput.* 17.5, pp. 1019–1039.
- Kurganov, A. (2016). "Central schemes: A powerful black-box solver for nonlinear hyperbolic PDEs". In: *Handbook of numerical methods for hyperbolic problems*. Ed. by R. Abgrall and C.-W. Shu. Vol. 17. Handb. Numer. Anal. Amsterdam: Elsevier/North-Holland, pp. 525–548.
- Larroutourou, B. (1991). "How to preserve the mass fractions positivity when computing compressible multi-component flows". In: *J. Comput. Phys.* 95.1, pp. 59–84.
- Mulder, W., S. Osher, and J. A. Sethian (1992). "Computing interface motion in compressible gas dynamics". In: *J. Comput. Phys.* 100.2, pp. 209–228.
- Roe, P. L. (1982). "Fluctuations and signals — A framework for numerical evolution problems". In: *Numerical Methods for Fluid Dynamics*. Ed. by K. Morton and M. Baines. Academic Press, New York, pp. 219–257.
- Saurel, R. and R. Abgrall (1999a). "A multiphase Godunov method for compressible multifluid and multiphase flows". In: *J. Comput. Phys.* 150.2, pp. 425–467.
- (1999b). "A simple method for compressible multifluid flows". In: *SIAM J. Sci. Comput.* 21.3, pp. 1115–1145.
- Shyue, K. M. (1998). "An efficient shock-capturing algorithm for compressible multicomponent problems". In: *J. Comput. Phys.* 142.1, pp. 208–242.
- Wang, B.-S., W. S. Don, N. K. Garg, and A. Kurganov (2020). "Fifth-order A-WENO finite-difference schemes based on a new adaptive diffusion central numerical flux". In: *SIAM J. Sci. Comput.* 42.6, A3932–A3956.
- Wang, B.-S., P. Li, Z. Gao, and W. S. Don (2018). "An improved fifth order alternative WENO-Z finite difference scheme for hyperbolic conservation laws". In: *J. Comput. Phys.* 374.1, pp. 469–477.
- Wang, C. and C.-W. Shu (2010). "An interface treating technique for compressible multi-medium flow with Runge-Kutta discontinuous Galerkin method". In: *J. Comput. Phys.* 229.23, pp. 8823–8843.