Towards a high fidelity numerical algorithm for compressible multiphase flows

Keh-Ming Shyue

Institute of Applied Mathematical Sciences
National Taiwan University

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Outline

State-of-the-art relaxation models for compressible multiphase flow with cavitation including phase transition take the form:

$$\partial_t \boldsymbol{q} + \operatorname{div} \mathbf{F}(\boldsymbol{q}) + \Pi(\boldsymbol{q}, \nabla \boldsymbol{q}) = \psi_p(\boldsymbol{q}) + \psi_{\mathbf{u}}(\boldsymbol{q}) + \psi_T(\boldsymbol{q}) + \psi_{pTg}(\boldsymbol{q}) + \cdots$$

Model is approximated by fractional-step method:

1. Homogeneous hyperbolic step

$$\partial_t \boldsymbol{q} + \operatorname{div} \mathbf{F}(\boldsymbol{q}) + \Pi(\boldsymbol{q}, \nabla \boldsymbol{q}) = 0$$

2. Source-term relaxation step

$$\partial_t \boldsymbol{q} = \psi_p(\boldsymbol{q}) + \psi_{\mathbf{u}}(\boldsymbol{q}) + \psi_T(\boldsymbol{q}) + \psi_{pTg}(\boldsymbol{q}) + \cdots$$

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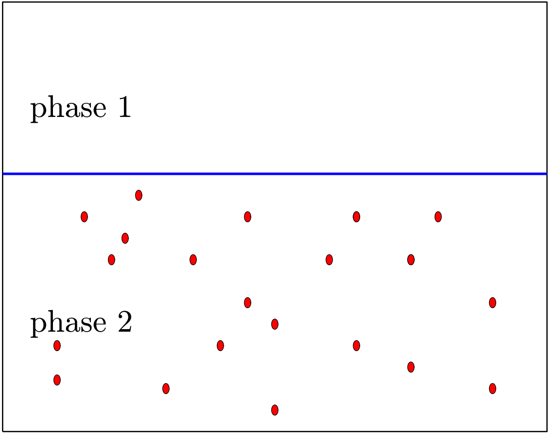
Aim: Discuss arbitrary-rate relaxation method for Step 2

Compressible barotropic 2-phase,2-component flow

Model problem: Bubbly liquid with interface



Compressible barotropic 2-phase,2-component flow

L.-R. Plumerault (2009) proposed

$$\partial_t (\alpha_1\rho_1) + \operatorname{div}(\alpha_1\rho_1\mathbf{u}) = 0 \tag{1a}$$

$$\partial_t (\alpha_2\rho_2) + \operatorname{div}(\alpha_2\rho_2\mathbf{u}) = 0 \tag{1b}$$

$$\partial_t (\alpha_2\rho_2 y_1) + \operatorname{div}(\alpha_2\rho_2 \mathrm{y}_1\mathbf{u}) = 0 \tag{1c}$$

$$\partial_t (\rho\mathbf{u}) + \operatorname{div}(\rho\mathbf{u}\otimes\mathbf{u}) + \nabla \mathrm{p} = 0 \tag{1d}$$

- Density-mixture conditions:

$$\rho = \alpha_1\rho_1 + \alpha_2\rho_2, \qquad \rho_2 = \beta_1\rho_{2,1} + \beta_2\rho_{2,2}$$

- Saturation conditions for phase α_j & component β_k:

$$\alpha_1 + \alpha_2 = 1, \quad \beta_1 + \beta_2 = 1$$

- Mass fraction for phase Y_j & component y_k:

$$Y_1 + Y_2 = 1, \quad y_1 + y_2 = 1, \quad Y_j = \frac{\alpha_j\rho_j}{\rho}, \quad y_j = \frac{\beta_j\rho_{2,j}}{\rho_2}$$

- Pressure-mixture condition:

$$p = \alpha_1 p_1 + \alpha_2 p_2, \qquad p_2 = \beta_1 p_{2,1} + \beta_2 p_{2,2}$$

- Model closure (pressure relaxation)

  1. Pressure equilibrium for multicomponent

  $$p_{2,1}\left(\rho_{2,1}\right) = p_{2,2}\left(\rho_{2,2}\right) = p_2$$

  2. Pressure equilibrium for multiphase

  $$p_1 = p_2$$

- Wood's sound speed for (phase 2) multicomponent mixture

$$\frac{1}{\rho_2 c_2^2} = \frac{\beta_1}{\rho_{2,1} c_{2,1}^2} + \frac{\beta_2}{\rho_{2,2} c_{2,2}^2}$$

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- Murnaghan isentropic EOS for p_k,

$$p_k(\rho_k) = \left(p_{0,k} + \frac{K_{0S,k}}{K'_{0S,k}}\right)\left(\frac{\rho_k}{\rho_{0,k}}\right)^{K'_{0S,k}} - \frac{K_{0S,k}}{K'_{0S,k}} \qquad (2)$$

Compressible barotropic 2-phase,2-component flow

Model equations in relaxation (pressure nonequilibrium) form are:

$$\partial_t (\alpha_1 \rho_1) + \operatorname{div} (\alpha_1 \rho_1 \mathbf{u}) = 0 \tag{3a}$$

$$\partial_t (\alpha_2 \rho_2) + \operatorname{div} (\alpha_2 \rho_2 \mathbf{u}) = 0 \tag{3b}$$

$$\partial_t (\alpha_2 \rho_2 y_1) + \operatorname{div} (\alpha_2 \rho_2 \mathrm{y}_1 \mathbf{u}) = 0 \tag{3c}$$

$$\partial_t (\rho \mathbf{u}) + \operatorname{div} (\rho \mathbf{u} \otimes \mathbf{u}) + \nabla (\alpha_1 \mathrm{p}_1 + \alpha_2 \mathrm{p}_2) = 0 \tag{3d}$$

$$\partial_t \alpha_1 + \mathbf{u} \cdot \nabla \alpha_1 = \mu (p_1 - p_2) \tag{3e}$$

$$\partial_t \alpha_2 + \mathbf{u} \cdot \nabla \alpha_2 = \mu (p_2 - p_1) \tag{3f}$$

Written (3) in compact form, we have

$$\partial_t \boldsymbol{q} + \operatorname{div} \mathbf{F}(\boldsymbol{q}) + \Pi(\boldsymbol{q}, \nabla \boldsymbol{q}) = \psi_{\mathrm{p}}(\boldsymbol{q}) \tag{4}$$

Assume relaxation constant μ is known a priori. In pressure (mechanical) relaxation step, from (3) we have

$$\partial_t \boldsymbol{q} = \psi_p(\boldsymbol{q}) \tag{5a}$$

$$\boldsymbol{q} = \left[\alpha_1\rho_1, \alpha_2\rho_2, \alpha_2\rho_2 y_1, \rho\mathbf{u}, \alpha_1, \alpha_2\right]^T \tag{5b}$$

$$\psi(\boldsymbol{q}) = \left[0, 0, 0, 0, \mu\left(p_1 - p_2\right), \mu\left(p_2 - p_1\right)\right]^T \tag{5c}$$

In exponential mechanical relaxation method, as in J.-M. Hérard & coworkers, in addition to (5), we introduce

$$\partial_t p_1 = -\frac{\rho_1 c_1^2}{\alpha_1}\,\partial_t \alpha_1 = -\mu\frac{\rho_1 c_1^2}{\alpha_1}\left(p_1 - p_2\right)$$

$$\partial_t p_2 = -\frac{\rho_2 c_2^2}{\alpha_2}\,\partial_t \alpha_2 = -\mu\frac{\rho_2 c_2^2}{\alpha_2}\left(p_2 - p_1\right)$$

Let $\Delta p = p_1 - p_2$. We have ODE for Δp:

$$\partial_t \Delta p = -\mu\left(\frac{\rho_1 c_1^2}{\alpha_1} + \frac{\rho_2 c_2^2}{\alpha_2}\right)\Delta p$$

With initial Δp^0, we find exact solution of Δp over Δt:

$$\Delta p^* = \Delta p^0 \exp\left\{-\mu\left(Z_1 + Z_2\right)\Delta t\right\}, \qquad Z_j = \rho_j c_j^2/\alpha_j$$

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- Update volume fractions using Δp^*, where $\alpha_1^* + \alpha_2^* = 1$:

$$\alpha_1^* = \alpha_1^0 - \left(Z_1 + Z_2\right)^{-1} \left(\Delta p^* - \Delta p^0\right)$$
$$\alpha_2^* = \alpha_2^0 + \left(Z_1 + Z_2\right)^{-1} \left(\Delta p^* - \Delta p^0\right)$$

If positivity condition $\alpha_k^* \in (0, 1)$, $k = 1, 2$ is satistied; we are done.

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$$\frac{\alpha_1 \rho_1}{\rho_1(p_1)} + \frac{\alpha_2 \rho_2}{\rho_2(p_1 - \Delta p^*)} = 1$$

for p_1^* & set $p_2^* = p_1^* - \Delta p^*$ with arbitrary rate constant μ

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If $\mu \to \infty$ (instantaneous relaxation), we have $\Delta p^* \to 0$, yielding equilibrium pressure $p_1^* = p_2^* = p^*$

Compressible barotropic 3-phase,2-component flow

Model equations in non-equilibrium form:

$$\partial_t(\alpha_1\rho_1) + \operatorname{div}(\alpha_1\rho_1\mathbf{u}) = 0 \tag{6a}$$

$$\partial_t(\alpha_2\rho_2) + \operatorname{div}(\alpha_2\rho_2\mathbf{u}) = 0 \tag{6b}$$

$$\partial_t(\alpha_3\rho_3) + \operatorname{div}(\alpha_3\rho_3\mathbf{u}) = 0 \tag{6c}$$

$$\partial_t(\alpha_3\rho_3 y_1) + \operatorname{div}(\alpha_3\rho_3\mathrm{y}_1\mathbf{u}) = 0 \tag{6d}$$

$$\partial_t(\rho\mathbf{u}) + \operatorname{div}(\rho\mathbf{u}\otimes\mathbf{u}) + \nabla(\alpha_1\mathrm{p}_1 + \alpha_2\mathrm{p}_2 + \alpha_3\mathrm{p}_3) = 0 \tag{6e}$$

$$\partial_t\alpha_1 + \mathbf{u}\cdot\nabla\alpha_1 = \mu_{12}(p_1 - p_2) + \mu_{13}(p_1 - p_3) \tag{6f}$$

$$\partial_t\alpha_2 + \mathbf{u}\cdot\nabla\alpha_2 = \mu_{21}(p_2 - p_1) + \mu_{23}(p_2 - p_3) \tag{6g}$$

$$\partial_t\alpha_3 + \mathbf{u}\cdot\nabla\alpha_3 = \mu_{31}(p_3 - p_1) + \mu_{32}(p_3 - p_2) \tag{6h}$$

- Density-mixture conditions:

$$\rho = \alpha_1\rho_1 + \alpha_2\rho_2 + \alpha_3\rho_3, \qquad \rho_3 = \beta_1\rho_{3,1} + \beta_2\rho_{3,2}$$

- Saturation conditions for phase α_j & component β_k:

$$\alpha_1 + \alpha_2 + \alpha_3 = 1, \quad \beta_1 + \beta_2 = 1$$

- Mass fraction for phase Y_j & component y_k:

$$Y_1+Y_2+Y_3 = 1, \quad y_1+y_2 = 1, \quad Y_j = \frac{\alpha_j\rho_j}{\rho}, \quad y_j = \frac{\beta_j\rho_{3,j}}{\rho_2}$$

Barotropic 3-phase model: pressure relaxation

Assume relaxation constant $\mu_{ij} = \mu_{ji}$, $\forall i, j$ is known a priori. In pressure relaxation step, from (6) we have

$$\begin{aligned}
&\partial_t (\alpha_k \rho_k) = 0, \quad k = 1, 2, 3 \\
&\partial_t (\alpha_3 \rho_3 y_1) = 0, \qquad \partial_t (\rho \mathbf{u}) = 0 \\
&\partial_t \alpha_1 = \mu_{12} (p_1 - p_2) + \mu_{13} (p_1 - p_3) \\
&\partial_t \alpha_2 = \mu_{12} (p_2 - p_1) + \mu_{23} (p_2 - p_3) \\
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&\partial_t \alpha_3 = \mu_{13} \left(p_3 - p_1\right) + \mu_{23} \left(p_3 - p_2\right)
\end{aligned}$$

In exponential relaxation method, if we use $\Delta p_{12} = p_1 - p_2$, $\Delta p_{13} = p_1 - p_3$, we obtain ODEs for Δp_{12}, Δp_{13}:

$$\partial_t \begin{bmatrix} \Delta p_{12} \\ \Delta p_{13} \end{bmatrix} = -\mathcal{A} \begin{bmatrix} \Delta p_{12} \\ \Delta p_{13} \end{bmatrix}$$

$$\mathcal{A} = \begin{bmatrix} \mu_{12} Z_1 + \left(\mu_{12} + \mu_{23}\right) Z_2 & \mu_{13} Z_1 - \mu_{23} Z_2 \\ \mu_{12} Z_1 - \mu_{23} Z_3 & \mu_{13} Z_1 + \left(\mu_{13} + \mu_{23}\right) Z_3 \end{bmatrix}$$

With initial $(\Delta p_{12}^0, \Delta p_{13}^0)$, exact solution of ODE over Δt is

$$\begin{bmatrix}\Delta p_{12} \\ \Delta p_{13}\end{bmatrix}^* = \exp\{-\mathcal{A}\Delta t\} \begin{bmatrix}\Delta p_{12} \\ \Delta p_{13}\end{bmatrix}^0$$

Eigenvalues of $\mathcal{A}$ are $\lambda_\pm = \frac{1}{2}\left(\mathrm{tr}(\mathcal{A}) \pm \sqrt{\mathrm{tr}(\mathcal{A})^2 - 4\det(\mathcal{A})}\right)$

- Stability condition of the method is $\mathrm{Re}(\lambda_\pm) \geq 0$; if not we set $\Delta p_{12}^* = 0$ & $\Delta p_{13}^* = 0$, for example

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- Update volume fractions using Δp_{12}^* & Δp_{13}^*,

$$\partial_t \begin{bmatrix} \alpha_1 \\ \alpha_2 \\ \alpha_3 \end{bmatrix} = \mathcal{B} \begin{bmatrix} \Delta p_{12} \\ \Delta p_{13} \end{bmatrix}, \quad \mathcal{B} = \begin{bmatrix} \mu_{12} & \mu_{13} \\ -\mu_{12} - \mu_{23} & \mu_{23} \\ \mu_{23} & -\mu_{13} - \mu_{23} \end{bmatrix},$$

we have

$$\begin{bmatrix} \alpha_1^* \\ \alpha_2^* \\ \alpha_3^* \end{bmatrix} = \begin{bmatrix} \alpha_1^0 \\ \alpha_2^0 \\ \alpha_3^0 \end{bmatrix} - \mathcal{B}\mathcal{A} \begin{bmatrix} \Delta p_{12}^* - \Delta p_{12}^0 \\ \Delta p_{13}^* - \Delta p_{13}^0 \end{bmatrix}$$

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for p_1^* & set

$$p_2^* = p_1^* - \Delta p_{12}^*, \qquad p_3^* = p_1^* - \Delta p_{13}^*$$

with arbitrary rate constant μ_{ij}, yielding phasic density ρ_1^*, ρ_2^*, ρ_3^* and volume fraction α_1^*, α_2^*, α_3^*

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If $\mu_{ij} \to \infty$ (instantaneous relaxation), we have $\Delta p_{12}^* \to 0$ & $\Delta p_{13}^* \to 0$, yielding equilibrium pressure $p_1^* = p_2^* = p_3^* = p^*$

Compressible barotropic multiphase flow: summary

If $\mu_{ij} = \mu$, ODE systems in exponential pressure relaxation method are

- 2-phase case

$$\partial_t \Delta p_{12} = -\mu \left[Z_1 + Z_2 \right] \Delta p_{12}$$

- 3-phase case

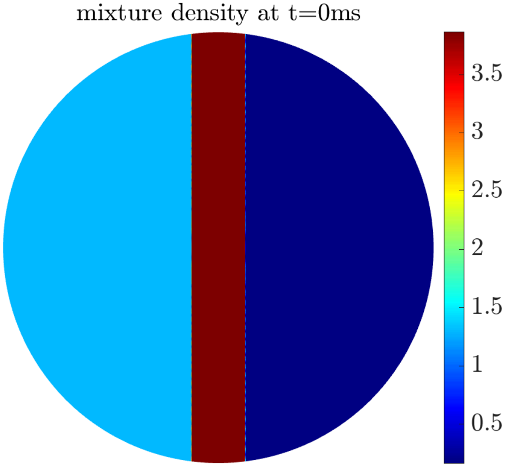
$$\partial_t \begin{bmatrix} \Delta p_{12} \\ \Delta p_{13} \end{bmatrix} = -\mu \begin{bmatrix} Z_1 + 2Z_2 & Z_1 - Z_2 \\ Z_1 - Z_3 & Z_1 + 2Z_3 \end{bmatrix} \begin{bmatrix} \Delta p_{12} \\ \Delta p_{13} \end{bmatrix}$$

- 4-phase case

$$\partial_t \begin{bmatrix} \Delta p_{12} \\ \Delta p_{13} \\ \Delta p_{14} \end{bmatrix} = -\mu \begin{bmatrix} Z_1 + 3Z_2 & Z_1 - Z_2 & Z_1 - Z_2 \\ Z_1 - Z_3 & Z_1 + 3Z_3 & Z_1 - Z_3 \\ Z_1 - Z_4 & Z_1 - Z_4 & Z_1 + 3Z_4 \end{bmatrix} \begin{bmatrix} \Delta p_{12} \\ \Delta p_{13} \\ \Delta p_{14} \end{bmatrix}$$

Moving vessel problem: all gas 3-phase case

Moving velocity $\mathbf{u} = (-100, 0)$
EOS: $p_k(\rho_k) = p_{0,k}\,(\rho_k/\rho_{k,0})^{\gamma_k}\ k = 1, 2, 3$



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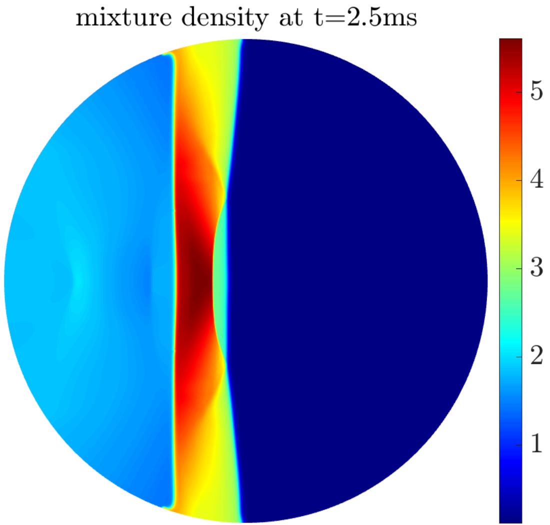

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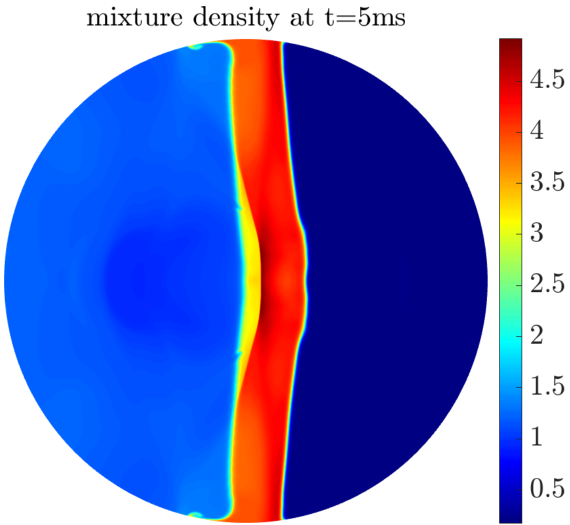

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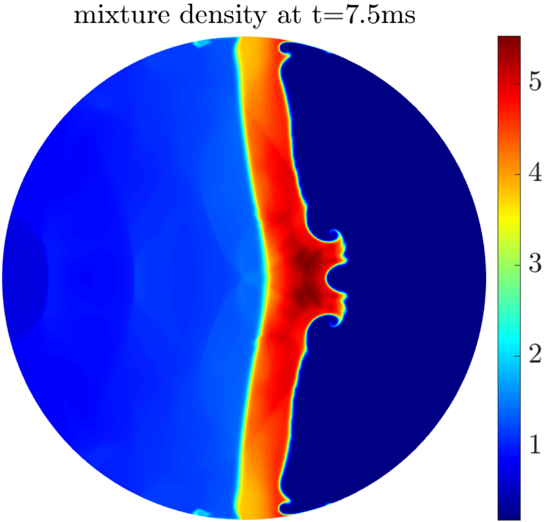

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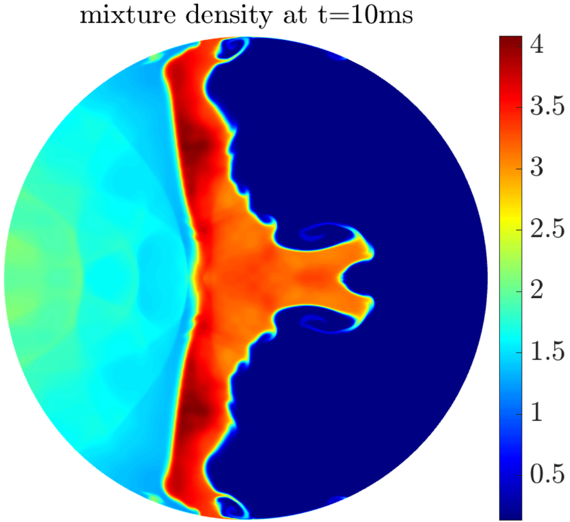

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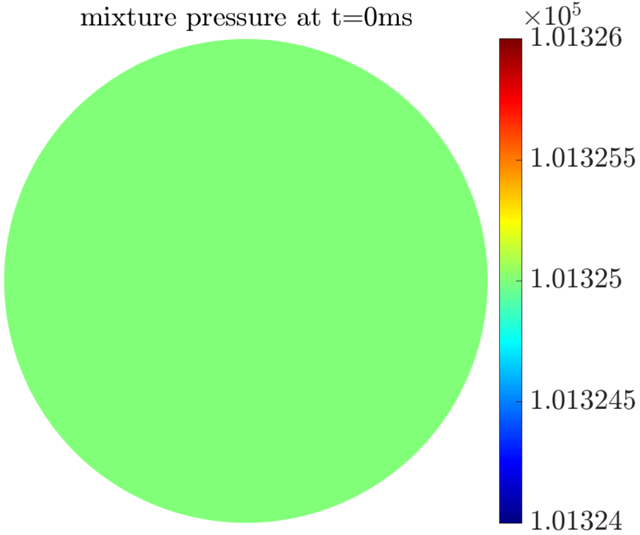

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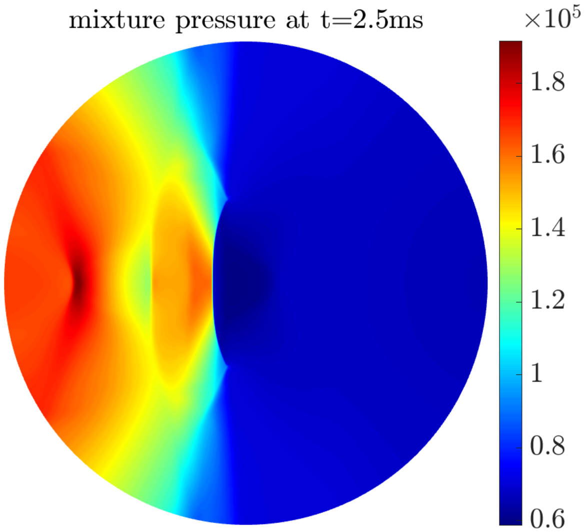

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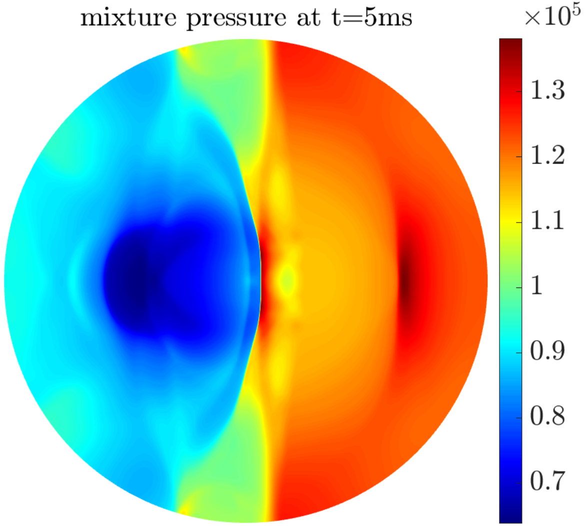

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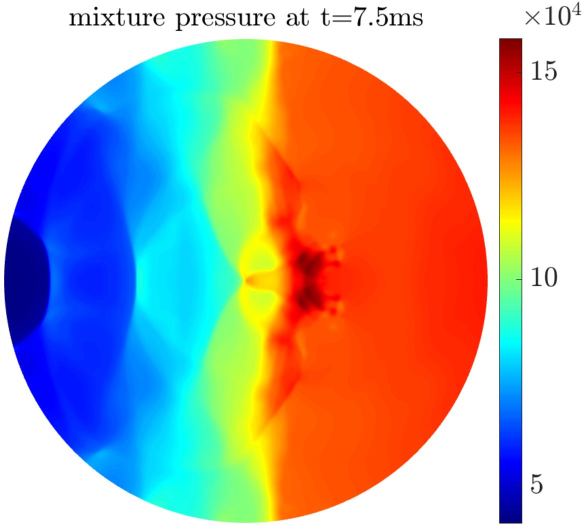

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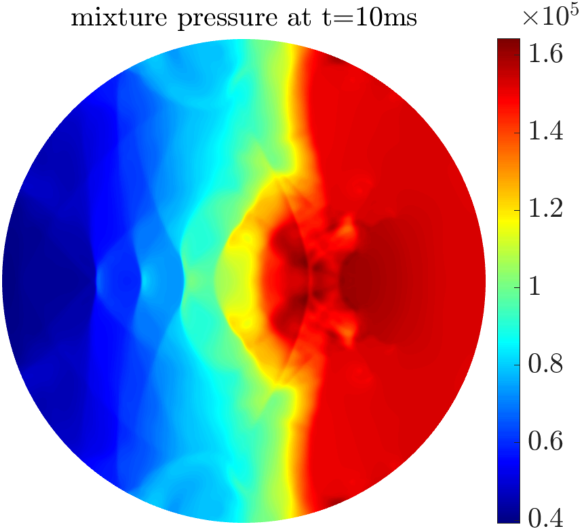
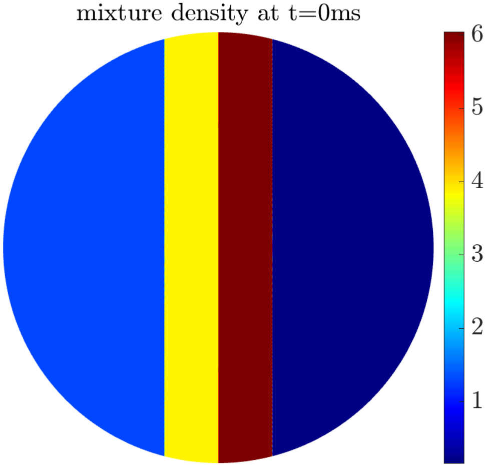


Moving vessel problem: all gas 4-phase case

Moving velocity $\mathbf{u} = (-100, 0)$
EOS: $p_k(\rho_k) = p_{0,k} \left(\rho_k / \rho_{k,0}\right)^{\gamma_k}$ $k = 1, 2, 3, 4$



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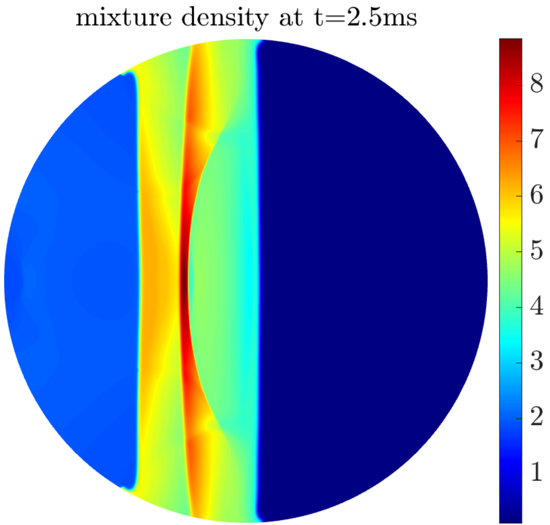
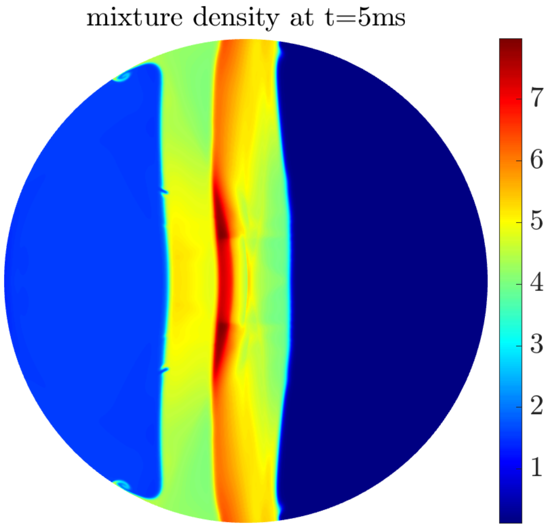
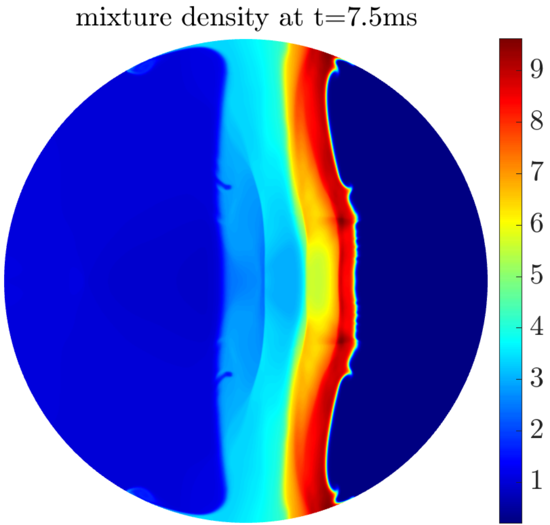


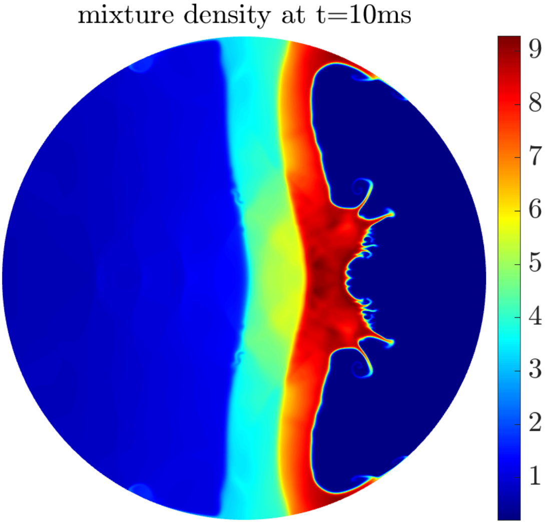
Moving vessel problem: all gas 4-phase case



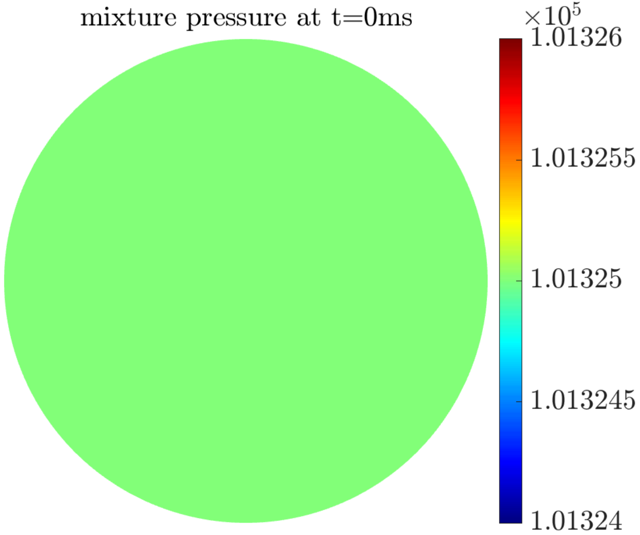
Moving vessel problem: all gas 4-phase case



Moving vessel problem: all gas 4-phase case



Moving vessel problem: all gas 4-phase case



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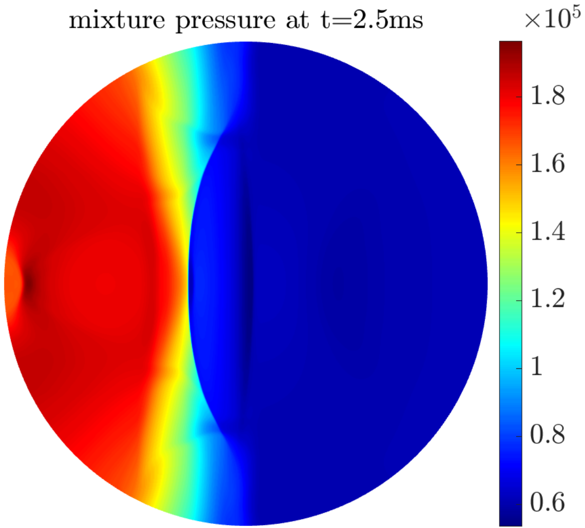

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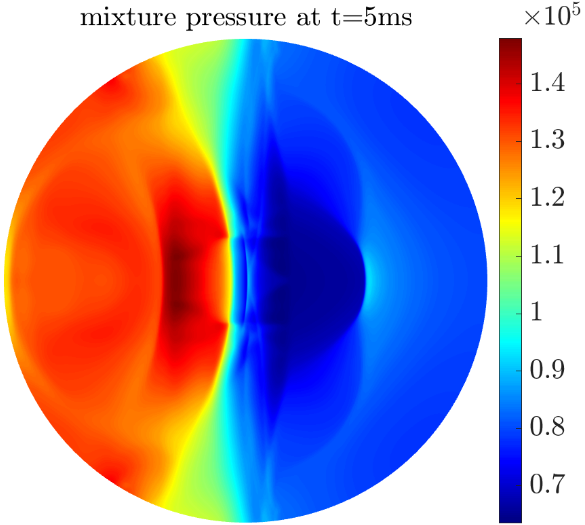
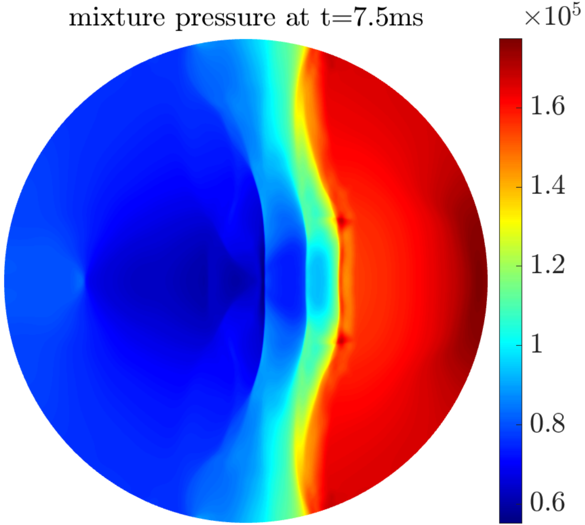
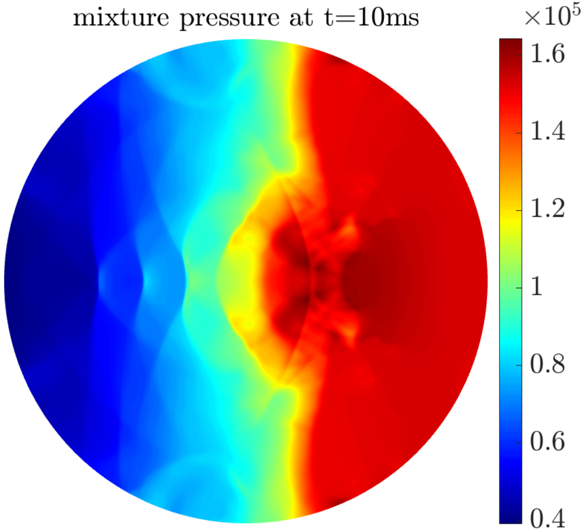


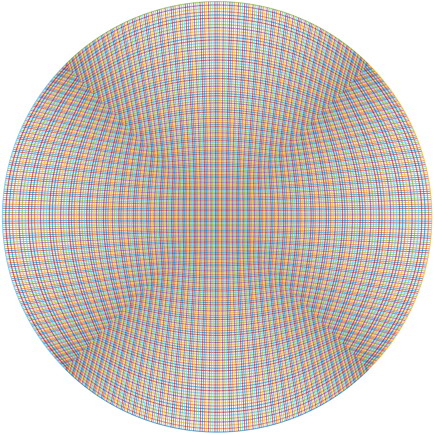
Moving vessel problem: all gas 4-phase case



Moving vessel problem: all gas 4-phase case

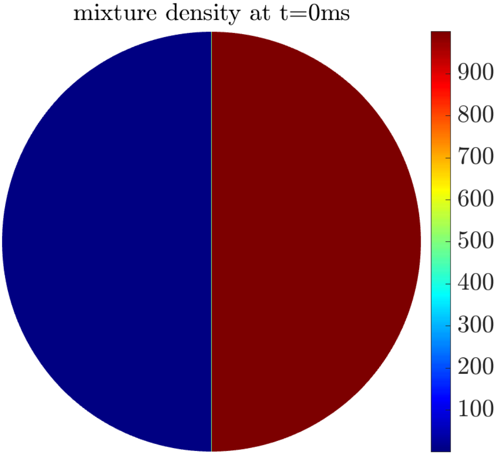


Moving vessel problem: mapped grid

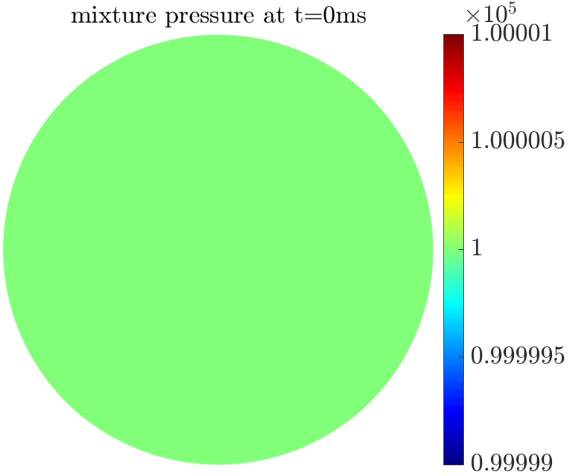


Moving vessel problem: gas-liquid case

Moving velocity $\mathbf{u} = (-100, 0)$
EOS for gas $p_1(\rho_1) = p_{0,1} \left(\rho_1/\rho_{1,0}\right)^{\gamma_1}$ &
for liquid $p_2(\rho_2) = \left(p_{0,2} + \varpi_2\right) \left(\rho_2/\rho_{2,0}\right)^{\gamma_2} + \varpi_2$

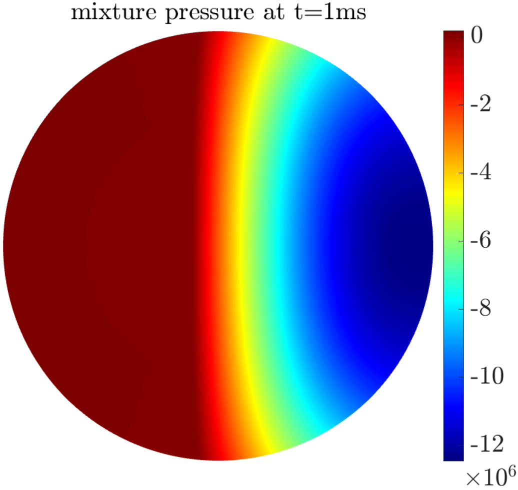


Moving vessel problem: gas-liquid case

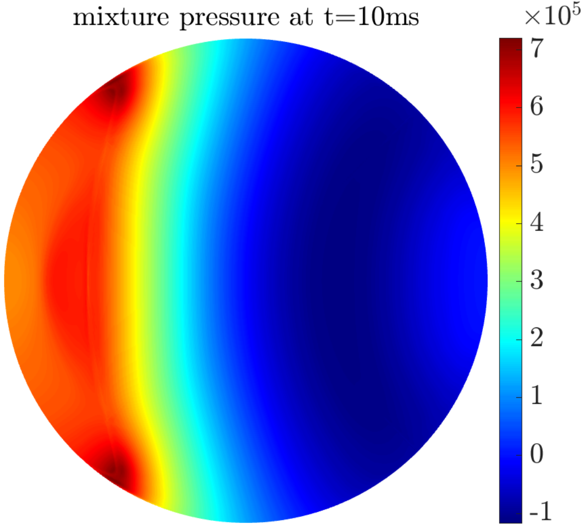


Moving vessel problem: gas-liquid case

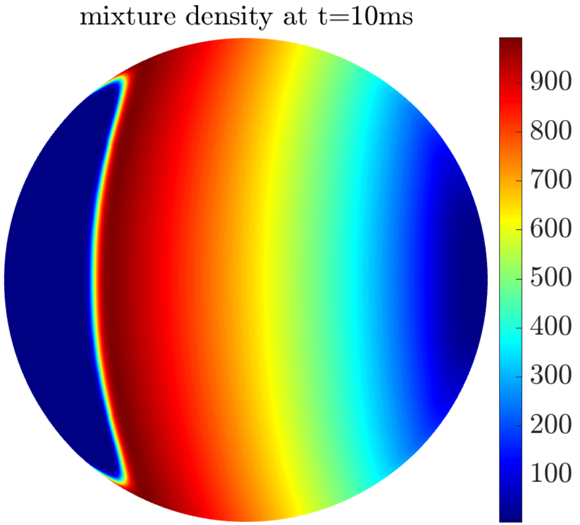
Formation of negative pressure



Moving vessel problem: gas-liquid case



Moving vessel problem: gas-liquid case



With hope to achieve fast convergence for feasible phasic pressure p_k, for 3-phase flow, for example, one may choose Δ_k for $k = 1, 2, 3$, and solve saturation equation

$$\frac{\alpha_1\rho_1}{\rho_1(\pi + \Delta_1)} + \frac{\alpha_2\rho_2}{\rho_2(\pi + \Delta_2)} + \frac{\alpha_3\rho_3}{\rho_3(\pi + \Delta_3)} = 1$$

for π. We then set

$$p_k = \pi + \Delta_k, \quad k = 1, 2, 3$$

Constraints for Δ_k are:

$$\Delta_1 - \Delta_2 = \Delta p_{12}, \quad \Delta_1 - \Delta_3 = \Delta p_{13}, \tag{7}$$

2 equations with 3 unknowns;

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2 equations with 3 unknowns; seek, for example, minimum-norm solution of (7)

$$\Delta_1 = \Delta p_{13}, \quad \Delta_2 = \Delta p_{13} - \Delta p_{12}, \quad \Delta_3 = 0$$

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$$\frac{\alpha_1\rho_1}{\rho_1(\pi + \Delta_1)} + \frac{\alpha_2\rho_2}{\rho_2(\pi + \Delta_2)} + \frac{\alpha_3\rho_3}{\rho_3(\pi + \Delta_3)} = 1$$

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2 equations with 3 unknowns; seek, for example, minimum-norm solution of (7)

$$\Delta_1 = \Delta p_{13}, \quad \Delta_2 = \Delta p_{13} - \Delta p_{12}, \quad \Delta_3 = 0$$

Relaxed solution depends strongly on initial condition from homogeneous hyperbolic step

Compressible non-barotropic 2-phase flow

Pelanti-Shyue (2014): 1-velocity phasic-total-energy model without phase transition

$$\partial_t (\alpha_1 \rho_1) + \mathrm{div}\,(\alpha_1 \rho_1 \mathbf{u}) = 0 \quad \text{(8a)}$$

$$\partial_t (\alpha_2 \rho_2) + \mathrm{div}\,(\alpha_2 \rho_2 \mathbf{u}) = 0 \quad \text{(8b)}$$

$$\partial_t(\rho \mathbf{u}) + \mathrm{div}\,(\rho \mathbf{u} \otimes \mathbf{u}) + \nabla (\alpha_1 \mathrm{p}_1 + \alpha_2 \mathrm{p}_2) = 0 \quad \text{(8c)}$$

$$\partial_t (\alpha_1 \rho_1 E_1) + \mathrm{div}\,(\alpha_1 \rho_1 \mathrm{H}_1 \mathbf{u}) + \Upsilon = -\mu \mathrm{p}_\mathrm{I} (\mathrm{p}_1 - \mathrm{p}_2) \quad \text{(8d)}$$

$$\partial_t (\alpha_2 \rho_2 E_2) + \mathrm{div}\,(\alpha_2 \rho_2 \mathrm{H}_2 \mathbf{u}) - \Upsilon = -\mu \mathrm{p}_\mathrm{I} (\mathrm{p}_2 - \mathrm{p}_1) \quad \text{(8e)}$$

$$\partial_t \alpha_1 + \mathbf{u} \cdot \nabla \alpha_1 = \mu (p_1 - p_2) \quad \text{(8f)}$$

$$\partial_t \alpha_2 + \mathbf{u} \cdot \nabla \alpha_2 = \mu (p_2 - p_1) \quad \text{(8g)}$$

$$\Upsilon = \mathbf{u} \cdot [Y_1 \nabla (\alpha_2 p_2) - Y_2 \nabla (\alpha_1 p_1)], \qquad H_k = E_k + \frac{p_k}{\rho_k}$$

Closure model: Mie-Grüneisen EOS for each p_k:

$$p_k(\rho_k, e_k) = p_{\mathrm{ref,k}}(\rho_k) + \frac{\Gamma_k}{\rho_k}(e_k - e_{\mathrm{ref,k}})$$

Non-barotropic 2-phase model: pressure relaxation

Assume relaxation constant μ is known a priori. In pressure relaxation step, from (8) we have

$$\begin{aligned}
\partial_t (\alpha_1\rho_1) &= 0 \\
\partial_t (\alpha_2\rho_2) &= 0 \\
\partial_t (\rho\mathbf{u}) &= 0 \\
\partial_t (\alpha_1\rho_1 E_1) &= -\mu p_I (p_1 - p_2) \\
\partial_t (\alpha_2\rho_2 E_2) &= -\mu p_I (p_2 - p_1) \\
\partial_t \alpha_1 &= \mu (p_1 - p_2) \\
\partial_t \alpha_2 &= \mu (p_2 - p_1)
\end{aligned}$$

Phasic total energy equations can be simplified as

$$\begin{aligned}
\partial_t (\alpha_1\rho_1 e_1) = (\alpha_1\rho_1)\,\partial_t e_1 = -\mu p_I (p_1 - p_2) \\
\partial_t (\alpha_2\rho_2 e_2) = (\alpha_2\rho_2)\,\partial_t e_2 = -\mu p_I (p_2 - p_1)
\end{aligned}$$

After simple algebraic manipulations, we have

$$\partial_t p_1 = -\mu \left(\frac{p_I - \rho_1^2 \partial_{\rho_1} e_1}{\alpha_1 \rho_1 \partial_{p_1} e_1} \right) (p_1 - p_2) = -\mu Z_1 (p_1 - p_2)$$

$$\partial_t p_2 = -\mu \left(\frac{p_I - \rho_2^2 \partial_{\rho_2} e_2 - p_I}{\alpha_2 \rho_2 \partial_{p_2} e_2} \right) (p_2 - p_1) = -\mu Z_2 (p_2 - p_1)$$

After simple algebraic manipulations, we have

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As before, in exponential relaxation method, we let $\Delta p = p_1 - p_2$, and obtain ODE for Δp:

$$\partial_t \Delta p = -\mu (Z_1 + Z_2) \Delta p$$

With initial condition Δp^0, exact solution of ODE over Δt is

$$\Delta p^* = \Delta p^0 \exp \{-\mu (Z_1 + Z_2) \Delta t\}$$

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$$\partial_t p_2 = -\mu \left(\frac{p_I - \rho_2^2 \partial_{\rho_2} e_2 - p_I}{\alpha_2 \rho_2 \partial_{p_2} e_2} \right) (p_2 - p_1) = -\mu Z_2 (p_2 - p_1)$$

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With initial condition Δp^0, exact solution of ODE over Δt is

$$\Delta p^* = \Delta p^0 \exp \{-\mu (Z_1 + Z_2) \Delta t\}$$

Stability condition of the method is $Z_1 + Z_2 \geq 0$; if not we set $\Delta p^* = 0$

- Use exponential solution for α_k^* & p_k^*, $k = 1{,}2$:

$$\alpha_1^* = \alpha_1^0 - (Z_1 + Z_2)^{-1} \left(\Delta p^* - \Delta p^0\right)$$
$$\alpha_2^* = \alpha_2^0 + (Z_1 + Z_2)^{-1} \left(\Delta p^* - \Delta p^0\right)$$
$$p_1^* = p_1^0 - Z_1 \left(\alpha_1^* - \alpha_1^0\right), \quad p_2^* = p_2^0 - Z_2 \left(\alpha_2^* - \alpha_2^0\right)$$

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If positivity condition $\alpha_k^* \in (0, 1)$, $k = 1, 2$ is satistied; we are done.

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$$\frac{\alpha_1 \rho_1}{\rho_1(p_1, e_1)} + \frac{\alpha_2 \rho_2}{\rho_2(p_1 - \Delta p^*, e_2)} = 1;$$

for p_1^* & set $p_2^* = p_1^* - \Delta p^*$ with arbitrary rate constant μ

- Use exponential solution for α_k^* & p_k^*, $k = 1{,}2$:

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for p_1^* & set $p_2^* = p_1^* - \Delta p^*$ with arbitrary rate constant μ

Pelanti (2022) considered $\mu \to \infty$, where equilibrium pressure p^* is updated from total internal energy

$$\sum_{k=1}^{2} \alpha_k\rho_k e_k(\rho_k, p^*) = \sum_{k=1}^{2} \alpha_k\rho_k E_k - \frac{1}{2}\rho\mathbf{u}\cdot\mathbf{u} = \text{constant}$$

Compressible non-barotropic multiphase flow

Pelanti-Shyue (2019): 1-velocity phasic-total-energy model
without phase transition

$$\partial_t(\alpha_k\rho_k) + \mathrm{div}(\alpha_\mathrm{k}\rho_\mathrm{k}\mathbf{u}) = 0\,, \quad \mathrm{k} = 1, 2, \ldots, \mathrm{N},$$
$$\partial_t(\rho\mathbf{u}) + \mathrm{div}\left(\rho\mathbf{u}\otimes\mathbf{u}\right) + \nabla\left(\sum_{\mathrm{k}=1}^{\mathrm{N}}\alpha_\mathrm{k}\mathrm{p}_\mathrm{k}\right) = 0$$
$$\partial_t(\alpha_1\rho_1 E_1) + \mathrm{div}(\alpha_1\rho_1\mathrm{H}_1\mathbf{u}) + \Upsilon_1 = -\sum_{\mathrm{j}=1}^{\mathrm{N}}\mathrm{p}_{\mathrm{I1j}}\mathcal{P}_{\mathrm{1j}}$$
$$\partial_t(\alpha_2\rho_2 E_2) + \mathrm{div}(\alpha_2\rho_2\mathrm{H}_2\mathbf{u}) + \Upsilon_2 = -\sum_{\mathrm{j}=1}^{\mathrm{N}}\mathrm{p}_{\mathrm{I2j}}\mathcal{P}_{\mathrm{2j}}$$
$$\partial_t(\alpha_k\rho_k E_k) + \mathrm{div}(\alpha_\mathrm{k}\rho_\mathrm{k}\mathrm{H}_\mathrm{k}\mathbf{u}) + \Upsilon_\mathrm{k} = -\sum_{\mathrm{j}=1}^{\mathrm{N}}\mathrm{p}_{\mathrm{Ikj}}\mathcal{P}_{\mathrm{kj}}$$
$$\partial_t\alpha_k + \mathbf{u}\cdot\nabla\alpha_k = \sum_{j=1}^{N}\mathcal{P}_{kj}\,, \quad k = 1, 2, \ldots, N$$

$$\Upsilon_k = \vec{u}\cdot\left(Y_k\nabla\left(\sum_{j=1}^{N}\alpha_j p_j\right) - \nabla(\alpha_k p_k)\right)\,, \quad k = 1, 2, \ldots, N$$

$$\mathcal{P}_{kj} = \mu_{kj}(p_k - p_j)$$

Non-barotropic multiphase flow: pressure relaxation

Assume $\mu_{kj} = \mu$, $p_{Ikj} = p_I$ for all k, j. ODE system for N-phase flow in exponential pressure relaxation method is

$$\partial_t \begin{bmatrix} \Delta p_{12} \\ \Delta p_{13} \\ \vdots \\ \Delta p_{1N} \end{bmatrix} = -\mu \mathcal{A} \begin{bmatrix} \Delta p_{12} \\ \Delta p_{13} \\ \vdots \\ \Delta p_{1N} \end{bmatrix}, \quad \text{with} \quad \mathrm{Z_k} = \frac{\mathrm{p_I} - \rho_\mathrm{k}^2 \partial_{\rho_\mathrm{k}} \mathrm{e_k}}{\alpha_\mathrm{k} \rho_\mathrm{k} \partial_{\mathrm{p_k}} \mathrm{e_k}},$$

$$\mathcal{A} = \begin{bmatrix} Z_1 + (N-1) Z_2 & Z_1 - Z_2 & \cdots & Z_1 - Z_2 \\ Z_1 - Z_3 & Z_1 + (N-1) Z_3 & \cdots & Z_1 - Z_3 \\ \vdots & \ddots & \ddots & \vdots \\ Z_1 - Z_N & Z_1 - Z_N & \cdots & Z_1 + (N-1) Z_N \end{bmatrix}$$

With initial condition Δp_{1k}^{0}, $k = 1, 2, \ldots, N$ & arbitrary rate μ, exact solution of ODEs over Δt is

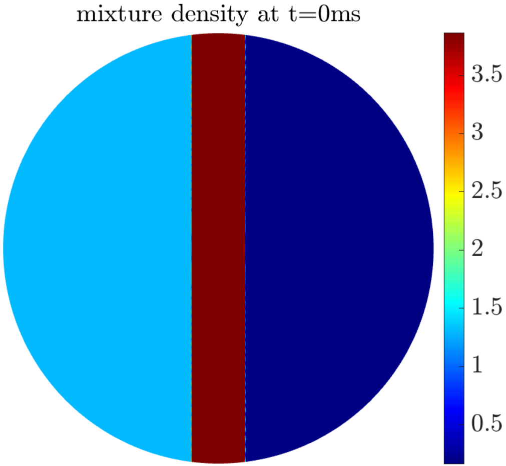
$$\begin{bmatrix} \Delta p_{12} \\ \Delta p_{13} \\ \vdots \\ \Delta p_{1N} \end{bmatrix}^{*} = \exp\left(-\mu\,\mathcal{A}\,\Delta t\right) \begin{bmatrix} \Delta p_{12} \\ \Delta p_{13} \\ \vdots \\ \Delta p_{1N} \end{bmatrix}^{0}$$

Stability condition for real part of eigenvalues of $\mathcal{A}$, $\mathrm{Re}(\lambda_{\mathrm{k}}(\mathcal{A})) \geq 0$ should be check first

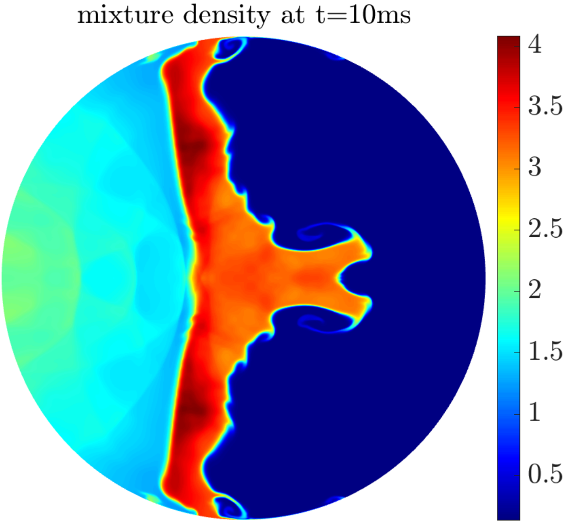
We then continue determining phasic pressure p_k for $k = 1, 2, \ldots, N$ using various techniques mentioned before

Moving vessel problem: all gas 3-phase case

Moving velocity $\mathbf{u} = (-100, 0)$
EOS: $p_k(\rho_k, e_k) = (\gamma_k - 1)\rho_k e_k$, $k = 1, 2, 3$

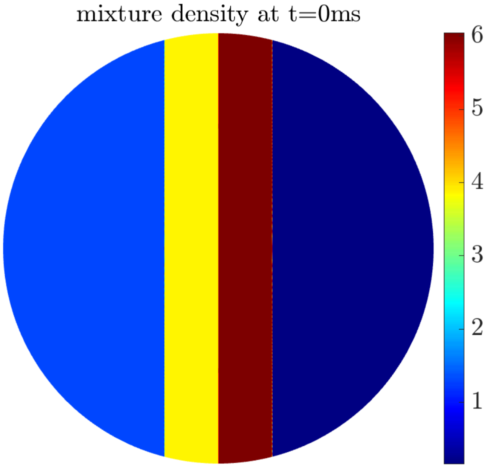


Moving vessel problem: all gas 3-phase case

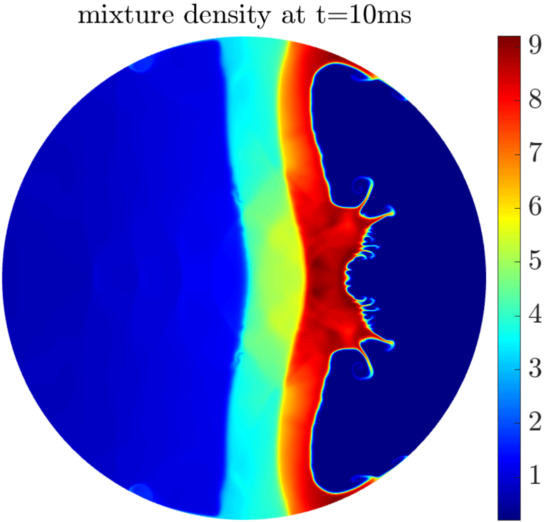


Moving vessel problem: all gas 4-phase case

Moving velocity $\mathbf{u} = (-100, 0)$
EOS: $p_k(\rho_k, e_k) = (\gamma_k - 1)\rho_k e_k$, $k = 1, 2, 3, 4$

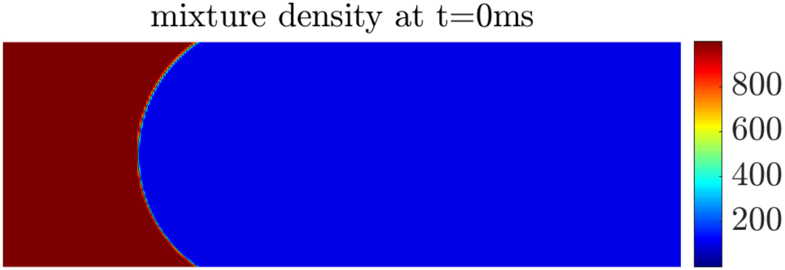


Moving vessel problem: all gas 4-phase case

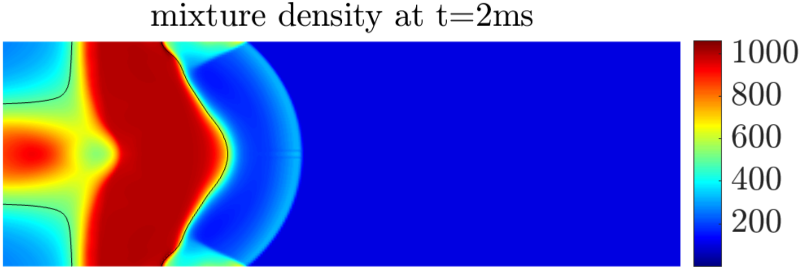


Cavitating Richtmyer-Meshkov: liquid-gas case

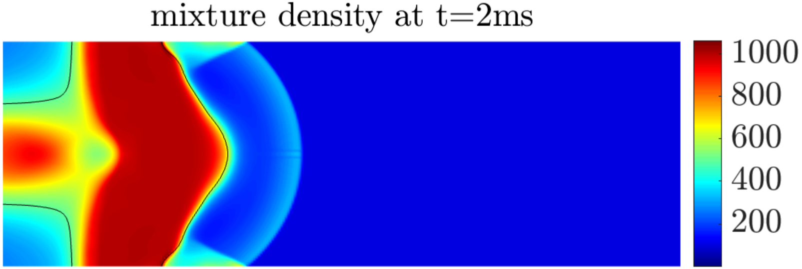
Moving velocity $\mathbf{u} = (-200, 0)$
EOS: stiffened gas for gas & liquid



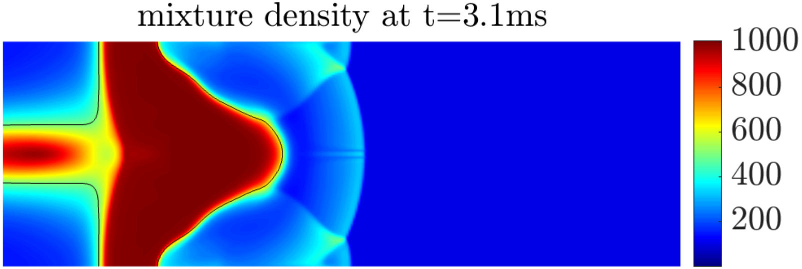
Cavitating Richtmyer-Meshkov: liquid-gas case



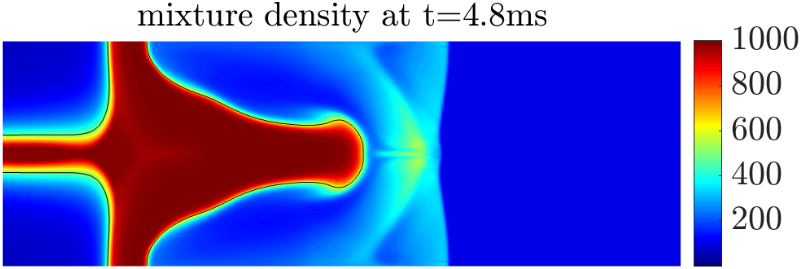
Cavitating Richtmyer-Meshkov: liquid-gas case



Cavitating Richtmyer-Meshkov: liquid-gas case

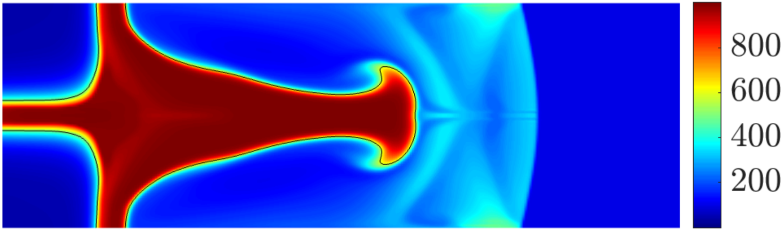


Cavitating Richtmyer-Meshkov: liquid-gas case

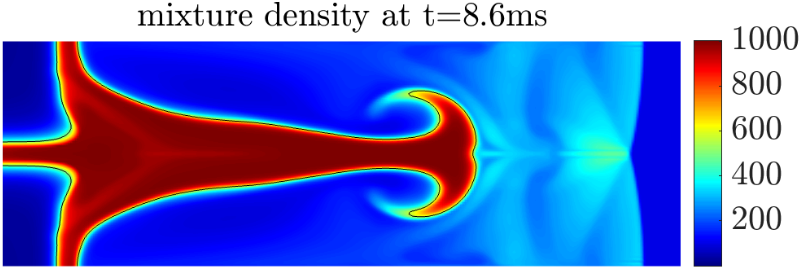


Cavitating Richtmyer-Meshkov: liquid-gas case

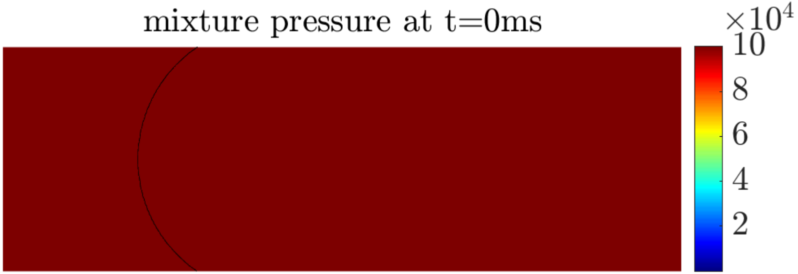
mixture density at t=6.4ms



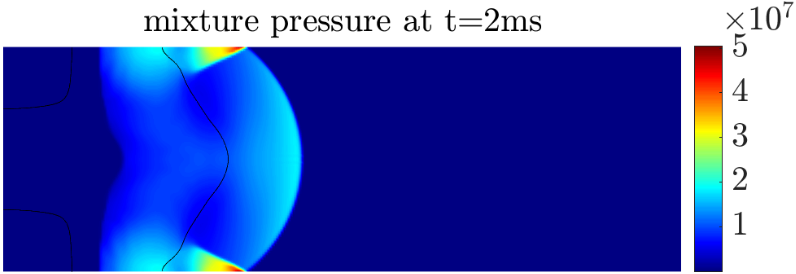
Cavitating Richtmyer-Meshkov: liquid-gas case



Cavitating Richtmyer-Meshkov: liquid-gas case



Cavitating Richtmyer-Meshkov: liquid-gas case



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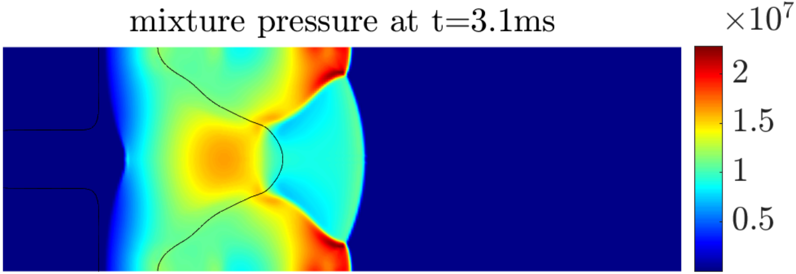

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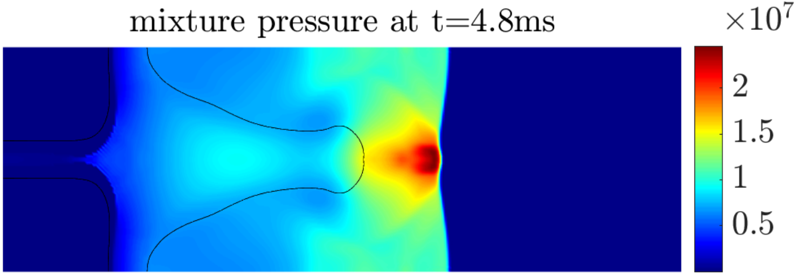

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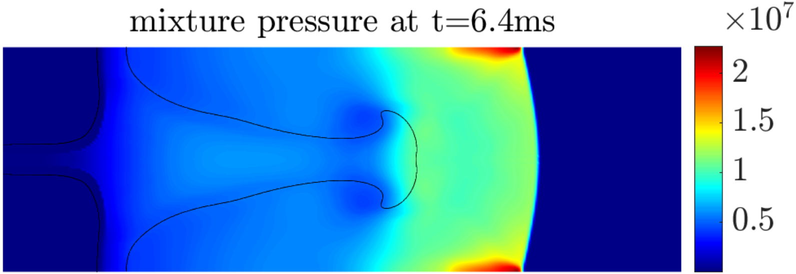

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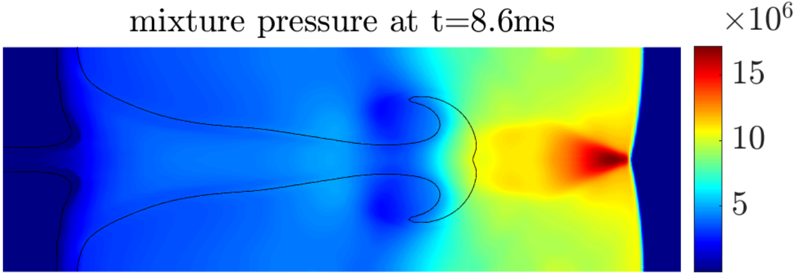

Hybrid barotropic & non-batropic 2-phase flow

Suppose we model liquid-gas 2-phase flow by hybrid barotropic & non-barotropic EOS, & use reduced model equations:

$$\partial_t (\alpha_1 \rho_1) + \mathrm{div}(\alpha_1 \rho_1 \mathbf{u}) = 0 \tag{9a}$$

$$\partial_t (\alpha_2 \rho_2) + \mathrm{div}(\alpha_2 \rho_2 \mathbf{u}) = 0 \tag{9b}$$

$$\partial_t (\rho \mathbf{u}) + \mathrm{div}(\rho \mathbf{u} \otimes \mathbf{u}) + \nabla (\alpha_1 \mathrm{p}_1 + \alpha_2 \mathrm{p}_2) = 0 \tag{9c}$$

$$\partial_t (\alpha_2 \rho_2 E_2) + \mathrm{div}(\alpha_2 \rho_2 \mathrm{H}_2 \mathbf{u}) - \Upsilon = -\mu \mathrm{p}_{\mathrm{I}} (\mathrm{p}_2 - \mathrm{p}_1) \tag{9d}$$

$$\partial_t \alpha_1 + \mathbf{u} \cdot \nabla \alpha_1 = \mu (p_1 - p_2) \tag{9e}$$

$$\partial_t \alpha_2 + \mathbf{u} \cdot \nabla \alpha_2 = \mu (p_2 - p_1) \tag{9f}$$

- Murnaghan isentropic EOS for phase 1

$$p_1(\rho_1) = \left(p_{0,1} + \frac{K_{0S,1}}{K'_{0S,1}} \right) \left(\frac{\rho_1}{\rho_{0,1}} \right)^{K'_{0S,1}} - \frac{K_{0S,1}}{K'_{0S,1}}$$

- Mie-Grüneisen EOS for phase 2

$$p_2(\rho_2, e_2) = p_{\mathrm{ref},2}(\rho_2) + \frac{\Gamma_2}{\rho_2}(e_2 - e_{\mathrm{ref},2})$$

As before, in exponential relaxation method, we let $\Delta p = p_1 - p_2$, and obtain ODE for Δp:

$$\partial_t \Delta p = -\mu \left(Z_1 + Z_2 \right) \Delta p$$

with

$$Z_1 = \frac{\rho_1 c_1^2}{\alpha_1}$$

$$Z_2 = \frac{p_I - \rho_2^2 \, \partial_{\rho_2} e_2}{\alpha_2 \rho_2 \, \partial_{p_2} e_2}$$

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With initial condition Δp^0, exact solution of ODE over Δt is

$$\Delta p^* = \Delta p^0 \exp \left\{ -\mu \left(Z_1 + Z_2 \right) \Delta t \right\}$$

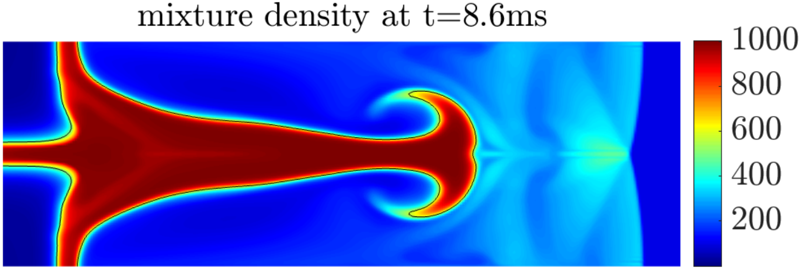
Model extension to multiphase flow can be formulated analogously

Cavitating Richtmyer-Meshkov: liquid-gas case

Moving velocity $\mathbf{u} = (-200, 0)$
EOS: Tait for liquid & ideal for gas

mixture density at t=0ms

Cavitating Richtmyer-Meshkov: liquid-gas case



Compressible multiphase flow with phase transition

Pelanti-Shyue (2019): 1-velocity model for compressible multiphase flow with liquid-vapor-gas phase transition is

$$\partial_t(\alpha_1\rho_1) + \mathrm{div}(\alpha_1\rho_1\mathbf{u}) = \mathcal{M}$$
$$\partial_t(\alpha_2\rho_2) + \mathrm{div}\cdot(\alpha_2\rho_2\mathbf{u}) = -\mathcal{M}$$
$$\partial_t(\alpha_k\rho_k) + \mathrm{div}(\alpha_\mathrm{k}\rho_\mathrm{k}\mathbf{u}) = 0\,, \quad \mathrm{k} = 3,\ldots,\mathrm{N}$$
$$\partial_t(\rho\mathbf{u}) + \mathrm{div}\,(\rho\mathbf{u}\otimes\mathbf{u}) + \nabla\left(\sum_{\mathrm{k}=1}^{\mathrm{N}}\alpha_\mathrm{k}\mathrm{p}_\mathrm{k}\right) = 0$$
$$\partial_t\alpha_k + \mathbf{u}\cdot\nabla\alpha_k = \sum_{j=1}^{N}\mathcal{P}_{kj}\,, \quad k = 1,2,\ldots,N$$

Here we have

$\mathcal{P}_{kj} = \mu_{kj}(p_k - p_j)$ (volume transfer)

$\mathcal{Q}_{kj} = \vartheta_{kj}(T_j - T_k)$ (heat transfer)

$\mathcal{M} = \nu(g_2 - g_1)$ (mass transfer between liquid & vapor phases)

$g_k = h_k - T_k s_k$ (Gibbs free energy), $h_k = e_k + p_k/\rho_k$

Equations for total energy of each phase k are:

$$\partial_t(\alpha_1\rho_1 E_1) + \mathrm{div}(\alpha_1\rho_1 \mathrm{H}_1 \mathbf{u}) + \Upsilon_1 = -\sum_{\mathrm{j}=1}^{\mathrm{N}} \mathrm{p}_{\mathrm{I1j}} \mathcal{P}_{\mathrm{1j}} + \sum_{j=1}^{N} \mathcal{Q}_{1j} + \left(g_{\mathrm{I}} + \frac{|\mathbf{u}|^2}{2}\right)\mathcal{M}$$

$$\partial_t(\alpha_2\rho_2 E_2) + \mathrm{div}(\alpha_2\rho_2 \mathrm{H}_2 \mathbf{u}) + \Upsilon_2 = -\sum_{\mathrm{j}=1}^{\mathrm{N}} \mathrm{p}_{\mathrm{I2j}} \mathcal{P}_{\mathrm{2j}} + \sum_{j=1}^{N} \mathcal{Q}_{2j} - \left(g_{\mathrm{I}} + \frac{|\mathbf{u}|^2}{2}\right)\mathcal{M}$$

$$\partial_t(\alpha_k\rho_k E_k) + \mathrm{div}(\alpha_{\mathrm{k}}\rho_{\mathrm{k}} \mathrm{H}_{\mathrm{k}} \mathbf{u}) + \Upsilon_{\mathrm{k}} = -\sum_{\mathrm{j}=1}^{\mathrm{N}} \mathrm{p}_{\mathrm{Ikj}} \mathcal{P}_{\mathrm{kj}} + \sum_{j=1}^{N} \mathcal{Q}_{kj}\,, \quad k = 3, \ldots, N$$

Closure model: Stiffened gas EOS (linear EOS)

Constitutive law: metastable fluid

Stiffened gas equation of state (SG EOS) with

- Pressure

$$p_k(e_k, \rho_k) = (\gamma_k - 1)e_k - \gamma_k \varpi_k - (\gamma_k - 1)\rho_k \eta_k$$

- Temperature

$$T_k(p_k, \rho_k) = \frac{p_k + \varpi_k}{(\gamma_k - 1)C_{Vk}\rho_k}$$

- Entropy

$$s_k(p_k, T_k) = C_{Vk} \log \frac{{T_k}^{\gamma_k}}{(p_k + \varpi_k)^{\gamma_k - 1}} + \eta'_k$$

- Helmholtz free energy $a_k = e_k - T_k s_k$
- Gibbs free energy $g_k = a_k + p_k V_k$

Metastable fluid: saturation curve

Assume two phases in chemical equilibrium with equal Gibbs free energies ($g_1 = g_2$), saturation curve is

$$\mathcal{G}(p,T) = A + \frac{B}{T} + C \log T + D \log(p + \varpi_1) - \log(p + \varpi_2) = 0$$

$$A = \frac{C_{p1} - C_{p2} + \eta_2' - \eta_1'}{C_{p2} - C_{v2}}, \qquad B = \frac{\eta_1 - \eta_2}{C_{p2} - C_{v2}}$$

$$C = \frac{C_{p2} - C_{p1}}{C_{p2} - C_{v2}}, \qquad D = \frac{C_{p1} - C_{v1}}{C_{p2} - C_{v2}}$$

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$$C = \frac{C_{p2} - C_{p1}}{C_{p2} - C_{v2}}, \qquad D = \frac{C_{p1} - C_{v1}}{C_{p2} - C_{v2}}$$

or, from $dg_1 = dg_2$, we get Clausius-Clapeyron equation

$$\frac{dp(T)}{dT} = \frac{L_h}{T(v_2 - v_1)}$$

$L_h = T(s_2 - s_1)$: latent heat of vaporization

Thermo-chemical relaxation: instantaneous rate

Look for solution of ODEs in limits $\mu,\ \theta,\ \&\ \nu \to \infty$

$$
\begin{aligned}
\partial_t (\alpha_1\rho_1) &= \mathcal{M} \\
\partial_t (\alpha_2\rho_2) &= -\mathcal{M} \\
\partial_t (\alpha_k\rho_k) &= 0, \quad k = 3, 4, \ldots, N \\
\partial_t (\rho\mathbf{u}) &= 0 \\
\partial_t (\alpha_1\rho_1 E_1) &= -\sum_{j=1}^{N} p_{\mathrm{I}1j}\mathcal{P}_{1j} + \sum_{j=1}^{N} \mathcal{Q}_{1j} + \left(g_{\mathrm{I}} + \frac{|\mathbf{u}|^2}{2}\right)\mathcal{M} \\
\partial_t (\alpha_2\rho_2 E_2) &= -\sum_{j=1}^{N} p_{\mathrm{I}2j}\mathcal{P}_{2j} + \sum_{j=1}^{N} \mathcal{Q}_{2j} - \left(g_{\mathrm{I}} + \frac{|\mathbf{u}|^2}{2}\right)\mathcal{M} \\
\partial_t (\alpha_k\rho_k E_k) &= -\sum_{j=1}^{N} p_{\mathrm{I}kj}\mathcal{P}_{kj} + \sum_{j=1}^{N} \mathcal{Q}_{kj}\,, \quad k = 3, \ldots, N \\
\partial_t \alpha_k &= \sum_{j=1}^{N} \mathcal{P}_{kj}\,, \quad k = 1, 2, \ldots, N
\end{aligned}
$$

under mechanical-thermal-chemical equilibrium conditons

$$
p_1 = p_2, \quad T_1 = T_2, \quad g_1 = g_2
$$

Infinite-rate pTg relaxation: algebraic apporach

In this case, states remain in equilibrium are

$$\rho = \rho_0, \quad \rho\mathbf{u} = \rho_0\mathbf{u}_0, \quad \rho E = (\rho E)_0, \quad e = e_0,$$

& $\alpha_k\rho_k = (\alpha_k\rho_k)_0$, but $\alpha_k\rho_k \neq \alpha_{k0}\rho_{k0}$ & $Y_k \neq Y_{k0}$, $k = 1, 2$

Impose mechanical-thermal-chemical equilibrium to

1. Saturation condition for temperature

$$\mathcal{G}(p, T) = 0$$

2. Saturation condition for volume fraction

$$\frac{Y_1}{\rho_1(p, T)} + \frac{Y_2}{\rho_2(p, T)} = \frac{1}{\rho_0}$$

3. Equilibrium of internal energy

$$Y_1\, e_1(p, T) + Y_2\, e_2(p, T) = e_0$$

From saturation condition for temperature

$$\mathcal{G}(p, T) = 0$$

we get T in terms of p, while from

$$\frac{Y_1}{\rho_1(p, T)} + \frac{Y_2}{\rho_2(p, T)} = \frac{1}{\rho_0}$$

&

$$Y_1 \, e_1(p, T) + Y_2 \, e_2(p, T) = e_0$$

we obtain algebraic equation for p

$$Y_1 = \frac{1/\rho_2(p) - 1/\rho_0}{1/\rho_2(p) - 1/\rho_1(p)} = \frac{e_0 - e_2(p)}{e_1(p) - e_2(p)}$$

which is solved by iterative method

Instantaneous-rate pTg relaxation: remarks

- Having known Y_k & p, T can be solved from, *e.g.*,

$$Y_1\, e_1(p,T) + Y_2\, e_2(p,T) = e_0$$

  yielding update ρ_k & α_k

- Feasibility of solutions, *i.e.*, positivity of physical quantities ρ_k, α_k, p, & T, for example
  - Employ hybrid method *i.e.*, combination of above method with differential-based approach (not discuss here), when it becomes necessary

Arbitrary-rate pTg relaxation: 2-phase flow case

Pelanti (2022): In exponential thermo-chemical relaxation method, we write ODEs governing chemical relaxation process as ODEs for $\Delta g = g_1 - g_2$:

$$\partial_t (\alpha_1 \rho_1) = -\nu (g_1 - g_2) \tag{10a}$$

$$\partial_t (\alpha_2 \rho_2) = -\nu (g_2 - g_1) \tag{10b}$$

$$\partial_t g_1 = -\nu \left(\frac{\mathcal{S}_p}{\rho_1} - s_1 \mathcal{S}_T \right) (g_1 - g_2) \tag{10c}$$

$$\partial_t g_2 = \nu \left(\frac{\mathcal{S}_p}{\rho_2} - s_2 \mathcal{S}_T \right) (g_2 - g_1) \tag{10d}$$

$$\partial_t \alpha_1 = -\nu \mathcal{S}_\alpha (g_1 - g_2) \tag{10e}$$

$$\partial_t \alpha_2 = -\nu \mathcal{S}_\alpha (g_2 - g_1) \tag{10f}$$

See Pelanti (IJMF 2022) for explicit expression of terms: $\mathcal{S}_\alpha$, $\mathcal{S}_p$, $\mathcal{S}_T$

With initial condition Δg^0, we find the exact solution of Δg over Δt:

$$\Delta g^* = \Delta g^0 \exp\left\{-\nu\left(K_1 - K_2\right)\Delta t\right\}, \quad K_j = \frac{\mathcal{S}_p}{\rho_j} - s_j \mathcal{S}_T$$

As before, we may use exponential solution Δg to compute $\alpha_k \rho_k$ & α_k, $k = 1, 2$ under stability condition $K_1 - K_2 \geq 0$

Choice of relaxation parameters ?

Homogeneous hyperbolic step: remark

To achieve high resolution in step 1, care must be taken

- Positivity preserving

  The larger phase N is, the more difficulty in obtaing positivity preserving is

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  - BVD (boundary variation diminishing); use 2 or more solution reconstruction techniques as basis, & take one by BVD criterion

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- Riemann solver in finite-volume Godunov method

  Solution differs not much by any state-of-the-art solver

Thank you