Multiphysics Modelling for Four States of Matter

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Contents

1 2018-19 (MOCK)

1.1 Q1

1. (a)

$$\text{Eikonal equation: } |\boldsymbol{\nabla}\phi| = 1$$

(b) Reinitialisation: returning a function to a signed distance function, whilst maintaining the location of the interface (zero-contour). It involves solving the Eikonal equation.

Why perform reinitialisation?

- A level set function ϕ that describes the location of an interface is advected using interface material velocity.
- However, this velocity is not constant in space and can generate non-linear behaviour.
- This causes ϕ to become too smeared or too steep.
- If ϕ becomes too steep and resemble a discontinuity, the non-conservative method use for evolving ϕ fails, resulting in the interface being in the wrong position.
- If ϕ becomes too smeared, it is easy to introduce errors into the interface with any small errors in the update such as round-off error.
- Returning ϕ to a signed distance function prevents all these from happening.

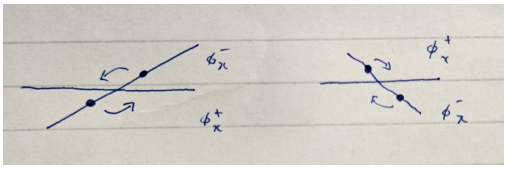
(c) **Iterative reinitialisation**:

- Idea is to consider the solution process to the Eikonal equation as evolving the following PDE to steady state:

$$\frac{\partial \phi}{\partial \tau} + \text{sgn}(\phi) \underbrace{(|\boldsymbol{\nabla}\phi| - 1)}_{\substack{\text{signed-distance} \\ \text{function}}} = 0$$

  where τ is a fictitious time variable.
- The PDE will evolve to steady state provided the slopes of ϕ are calculated in the upwind direction (outwards from the interface).
- We can approximate $|\boldsymbol{\nabla}\phi|$ with first order derivatives and the sign of $\text{sgn}(\phi)\frac{\partial \phi}{\partial x}$ tells us which is the upwind direction.

$$\phi_x = \begin{cases} \phi^-_{x,i} = \frac{\phi_{i,j,k} - \phi_{i-1,j,k}}{\Delta x} & \text{, if } \text{sgn}(\phi)\frac{\partial \phi}{\partial x} \geq 0 \\ \phi^+_{x,i} = \frac{\phi_{i+1,j,k} - \phi_{i,j,k}}{\Delta x} & \text{, otherwise} \end{cases}$$



- Information is propagated outwards from the interface, so we can get an accurate level set function close to the interface relatively quickly (Fedkiw say ~ 10 iterations). We just need to ensure ϕ looks good close to the interface.

Fast Marching Method:

- Says that there is a correct order in which we consider the cells during reinitialisation.
- Start with the closest cell to the interface and reinitialise (i.e. solve the Eikonal equation) all its possible neighbours. Insert the neighbours into an ordered list of cells sorted by distance to interface.
- Now, there is no more information we can get out of this cell, so we can mark it as known, removing it from further reinitialisation.
- We move on to the next closest cell and repeat until we go through every cell in the domain.
- Uses multimap as data structure. It has time complexity $\mathcal{O}(N \log N)$.

Fast Sweeping Method:

- Treats the reinitialisation procedure as a series of 1D reinitialisation steps, $(\mathcal{O}(N))$.
- Start by setting values not adjacent to the interface to a sufficiently large value, effectively "removing them". This way, if any newly-calculated ϕ is smaller than the current value, we know it is a better approximation, and we keep it.
- Algorithm:
  i. Start with the first cell in the sweep and check if we are close to the interface i.e. $\phi_i \phi_{i+1} < 0$. Repeat until we are adjacent to the interface, and then keep going until we are no longer adjacent to the interface, but the previous cell in the sweep was adjacent.
  ii. Compute the neighbours with minimum magnitude $(\phi_x,\, \phi_y,\, \phi_z)$. For positive ϕ, $\phi_x = \min(\phi_{i+1,j,k}, \phi_{i-1,j,k})$. For negative ϕ, $\phi_x = \max(\phi_{i+1,j,k}, \phi_{i-1,j,k})$.
  iii. Plug these values into our squared Eikonal equation, giving a quadratic in $\hat{\phi}_{i,j,k}$:

$$\left(\frac{\hat{\phi}_{i,j,k} - \phi_x}{\Delta x}\right)^2 + \left(\frac{\hat{\phi}_{i,j,k} - \phi_y}{\Delta y}\right)^2 + \left(\frac{\hat{\phi}_{i,j,k} - \phi_z}{\Delta z}\right)^2 = 1$$

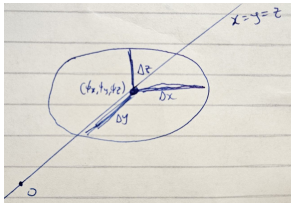


Figure 1: Geometrically, it is the intersection of an ellipsoid centred at (ϕ_x, ϕ_y, ϕ_z) with line $x = y = z$.

  iv. Keep $\hat{\phi}_{i,j,k}$ if it is smaller in magnitude than the current guess for this cell. Take positive root for $+\phi$ and negative root for $-\phi$. If the solution is ill-defined, remove the largest of ϕ_x, ϕ_y, ϕ_z and try again.
  v. If we reach another cell interface, we do not do anything until we got to a non-adjacent cell whose previous cell was adjacent.
  vi. Once we reached the edge of the domain, move on to the next 1D sweep in the same direction.
  vii. Once we complete the sweep for every cell in the domain, we switch directions.
  viii. We continue the sweep algorithm until we cover all dimensions and all directions.

(d) Mesh in cut cell method is generated by 'cutting out' the geometry of the rigid body from a background grid. It suffers from the small cell problem, where the maximum stable timestep is restricted by the size of the smallest cell in the domain.

A level set approach implicitly defines the boundary of the rigid body, using a level set function. It uses the ghost fluid method to maintain the sharp interface, with reflective boundary conditions applied.

(e) Flux stabilisation and cell linking.

1.2 Q2

2. (a) Sharp and diffuse interface methods.

(b) Ghost fluid method with reflective boundary condition applied, or cut-cell method.

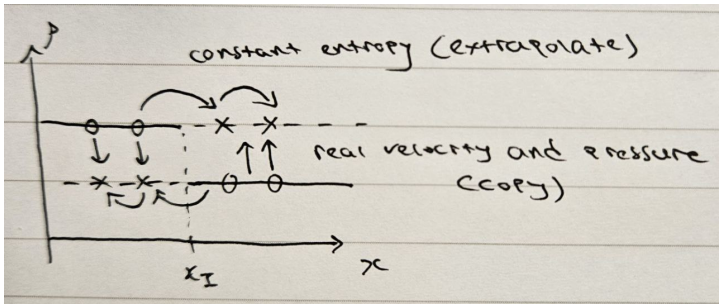
(c) i. Small air bubble in water hit by shock wave: sharp or diffuse interface method. High pressure of shock wave cause the bubble to rapidly compress, leading to forceful collapse and jet formation.
Sharp: capture fine features such as small bubbles
Diffuse: capture mixing behaviour

ii. Explosion within steel box containing mixture of fuel and air: diffuse interface method. Natural approach to dealing with chemical reaction and mixing, using a single system of equations and mixture rules. It allows all materials to exist at every point in the domain, with their own ρ, v, p. The amount of material in each computational cell is tracked by evolving a volume/mass fraction.

iii. Air flow over a commercial airliner travelling at a constant speed (rigid body modelling): cut-cell method, evolution to steady state.

(d) **Original ghost fluid method**:

- Ghost fluid methods is a numerical technique that provides dynamic boundary conditions for sharp and implicitly represented interface between materials.
- A level set function ϕ is used to define the interface. Its evolution follows an advection equation:
$$\frac{\partial \phi}{\partial t} + \boldsymbol{v} \cdot \boldsymbol{\nabla} \phi = 0$$
- The numerical update for ϕ is:
$$\phi_i^{n+1} = \phi_i^n - v_{x,i}^n \left(\frac{\partial \phi}{\partial x} \right)_i^n \Delta t$$
where an upwind approach can be used to compute the derivative of ϕ:
$$\left(\frac{\partial \phi}{\partial x} \right)_i^n = \begin{cases} \phi_{x,i}^- = \frac{\phi_{i,j,k} - \phi_{i-1,j,k}}{\Delta x} & , \text{if } v_{x,i} > 0 \\ \phi_{x,i}^+ = \frac{\phi_{i+1,j,k} - \phi_{i,j,k}}{\Delta x} & , \text{if } v_{x,i} < 0 \end{cases}$$
- A good choice for ϕ is the signed distance function, $|\boldsymbol{\nabla} \phi| = 1$, where its magnitude gives the shortest distance to the interface. However, the evolution of the level set function does not necessarily maintain the SDF nature. Here, reinitialisation is required to return ϕ to an SDF, whilst maintaining the location of the zero-contour. Otherwise, ϕ might become too steep or too smeared.
- The conditions for thermodynamically consistent boundary conditions are constant entropy across the interface, and velocity and pressure copied from the real material to the ghost fluid to ensure velocity and pressure equilibrium.



- We can enforce constant entropy using:

$$\frac{p}{\rho^\gamma} = \text{const}$$

such that:

$$\frac{p_I}{\rho_I^{\gamma_I}} = \frac{p_G}{\rho_G^{\gamma_I}} \quad \Rightarrow \quad \rho_G = \rho_I \left(\frac{p_G}{p_I}\right)^{1/\gamma_I}$$

We can compute the corresponding density in the ghost region as we know its pressure.

- The original GFM performs an isobaric fix by extending the extrapolation of entropy, taking the value from one cell further from the interface in the real material. As a result, this also changes the density in the real cell adjacent to the interface.
- Isobaric fix helps fix issues caused by shock wave ("overheating"), but it can add additional conservation errors.

1.3 Q3

3. (a) Consider,

$$\frac{\partial v}{\partial t} + v\frac{\partial v}{\partial x} + \frac{1}{\rho}\frac{\partial p}{\partial x} = \frac{Dv}{Dt} + \frac{1}{\rho}\frac{\partial p}{\partial x} = 0$$

$$\cancel{\left[\frac{Dv}{Dt}\right]} + \left[\frac{1}{\rho}\frac{\partial p}{\partial x}\right] = 0$$

$$\left[\frac{1}{\rho}\frac{\partial p}{\partial x}\right] = 0$$

Consider,

$$\frac{\partial p}{\partial t} + \rho c_s^2\frac{\partial v}{\partial x} + v\frac{\partial p}{\partial x} = 0$$

$$\cancel{\left[\frac{Dp}{Dt}\right]} + \left[\gamma p\frac{\partial v}{\partial x}\right] = 0$$

$$\left[\gamma\frac{\partial v}{\partial x}\right] = 0 \quad \text{, since } [p] = 0$$

(b) To the left,

$$\rho_x^L = \frac{\rho_i - \rho_{i-1}}{\Delta x}$$

$$\begin{aligned}\rho_L &= \rho_x^L(x_\phi - x_i) + \rho_i \\ &= \rho_i\left(\frac{x_\phi - x_i}{\Delta x} + 1\right) - \rho_{i-1}\left(\frac{x_\phi - x_i}{\Delta x}\right) \\ &= -\theta\rho_{i-1} + (1+\theta)\rho_i\end{aligned}$$

(c) To the right,

$$\rho_x^R = \frac{\rho_{i+2} - \rho_{i+1}}{\Delta x}$$

$$\begin{aligned}\rho_R &= \rho_{i+1} - \rho_x^R(x_{i+1} - x_\phi) \\ &= \rho_{i+1}\left(1 + \frac{x_{i+1} - x_\phi}{\Delta x}\right) - \rho_{i+2}\left(\frac{x_{i+1} - x_\phi}{\Delta x}\right) \\ &= \rho_{i+1}\left(1 + \frac{x_i + \Delta x - x_\phi}{\Delta x}\right) - \rho_{i+2}\left(\frac{x_i + \Delta x - x_\phi}{\Delta x}\right) \\ &= \rho_{i+1}\left(2 - \frac{x_\phi - x_i}{\Delta x}\right) - \rho_{i+2}\left(-\frac{x_\phi - x_i}{\Delta x} + 1\right) \\ &= (2-\theta)\rho_{i+1} - (1+\theta)\rho_{i+2}\end{aligned}$$

(d) At x_i,

$$p_i = p^L + (x_i - x_\phi)p_x^L$$

At x_{i+1},

$$p_{i+1} = p^R + (x_{i+1} - x_\phi)p_x^R$$

There is no jump in p and $\frac{1}{\rho}\frac{\partial p}{\partial x}$ across the interface, so:

$$p^L = p^R \quad \text{and} \quad \frac{1}{\rho^L}p_x^L = \frac{1}{\rho^R}p_x^R \Rightarrow p_x^R = \frac{\rho^R}{\rho^L}p_x^L$$

$$\begin{cases} p_i & = p^L + (x_i - x_\phi)p_x^L \\ p_{i+1} & = p^L + (x_i + \Delta x - x_\phi)\frac{\rho^R}{\rho^L}p_x^L \end{cases}$$

$$\begin{pmatrix} p_i \\ p_{i+1} \end{pmatrix} = \begin{pmatrix} 1 & -\theta\Delta x \\ 1 & (1-\theta)\Delta x\frac{\rho^R}{\rho^L} \end{pmatrix} \begin{pmatrix} p^L \\ p_x^L \end{pmatrix}$$

(e)

$$\frac{p_{i+1} - p_i}{\Delta x} = \left((1-\theta)\frac{\rho^R}{\rho^L} + \theta\right) p_x^L$$

$$p_x^L = \frac{p_{i+1} - p_i}{\Delta x}\frac{\rho^L}{(1-\theta)\rho^R + \theta\rho^L}$$

Substitute expression for p_x^L into equation (1),

$$p_i = p^L - \theta\frac{(p_{i+1} - p_i)\rho^L}{(1-\theta)\rho^R + \theta\rho^L}$$

$$p^L = p_i + \theta\frac{(p_{i+1} - p_i)\rho^L}{(1-\theta)\rho^R + \theta\rho^L}$$

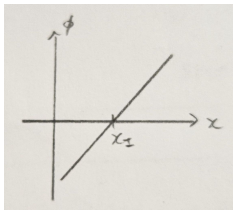
$$p^L = \frac{p_i(1-\theta)\rho^R + p_{i+1}\theta\rho^L}{(1-\theta)\rho^R + \theta\rho^L}$$

2 2019-20 (MOCK)

2.1 Q1

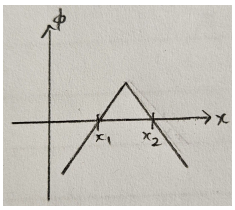
1. (a) i. A line:

$$x = x_I$$
$$\Rightarrow \phi = x - x_I$$



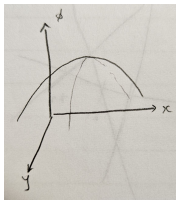
ii. A sawtooth:

$$\{x = x_1 \ , \ x = x_2\}$$
$$\{\phi_1 = x - x_1 \ , \ \phi_2 = x_2 - x\}$$
$$\phi = \min(\phi_1, \phi_2)$$

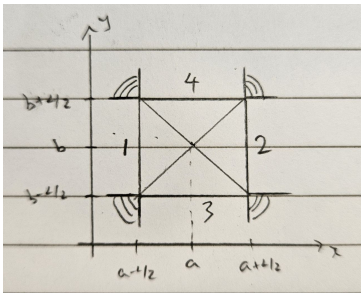


iii. A cone:

$$(x-a)^2 + (y-b)^2 = r_0^2$$
$$\phi = r_0 - \sqrt{(x-a)^2 + (x-b)^2}$$



iv. A pyramid:



$$\{x = a - L/2 \ , \ x = a + L/2 \ , \ y = b + L/2 \ , \ y = b - L/2\}$$
$$\{\phi_1 = x - (a - L/2) \ , \ \phi_2 = (a + L/2) - x \ , \ \phi_3 = y - (b - L/2) \ , \ \phi_4 = (b + L/2) - y\}$$

$$\phi = \begin{cases} \min(\phi_1, \phi_2, \phi_3, \phi_4) & , \text{ if } \phi_1 > 0 \ , \ \phi_2 > 0 \ , \ \phi_3 > 0 \ , \ \phi_4 > 0 \\ \sqrt{(x - (a - L/2))^2 + (y - (b - L/2))^2} & , \text{ if } \phi_1 < 0 \ , \ y < b - L/2 \\ \phi_1 & , \text{ if } \phi_1 < 0 \ , \ b - L/2 < y < b + L/2 \\ \sqrt{(x - (a - L/2))^2 + (y - (b + L/2))^2} & , \text{ if } \phi_1 < 0 \ , \ y > b + L/2 \\ \\ \sqrt{(x - (a + L/2))^2 + (y - (b - L/2))^2} & , \text{ if } \phi_2 < 0 \ , \ y < b - L/2 \\ \phi_2 & , \text{ if } \phi_2 < 0 \ , \ b - L/2 < y < b + L/2 \\ \sqrt{(x - (a + L/2))^2 + (y - (b + L/2))^2} & , \text{ if } \phi_2 < 0 \ , \ y > b + L/2 \\ \phi_3 & , \text{ if } \phi_3 < 0 \\ \phi_4 & , \text{ if } \phi_4 < 0 \end{cases}$$

(b) First order upwinded Hamilton-Jacobi scheme:

- Level set equation can be written in the form of Hamilton-Jacobi equation:

$$\frac{\partial \phi}{\partial t} + H(\boldsymbol{\nabla}\phi) = 0$$

where in this case,

$$H(\boldsymbol{\nabla}\phi) = v_x \frac{\partial \phi}{\partial x} + v_y \frac{\partial \phi}{\partial y} + v_z \frac{\partial \phi}{\partial z}$$

- In discretised form:

$$\frac{\phi^{n+1}_{i,j,k} - \phi^{n}_{i,j,k}}{\Delta t} + v^n_{x,i,j,k} \left(\frac{\partial \phi}{\partial x}\right)^n_{i,j,k} + v^n_{y,i,j,k} \left(\frac{\partial \phi}{\partial y}\right)^n_{i,j,k} + v^n_{z,i,j,k} \left(\frac{\partial \phi}{\partial z}\right)^n_{i,j,k} = 0$$

where i, j, k are the positions in the x, y and z direction. Δx and Δt is the discretised space and time.

- Upwinded first-order approximation to the spatial derivative:

$$\left(\frac{\partial \phi}{\partial x}\right)^n_{i,j,k} = \begin{cases} \phi^-_{x,i,j,k} = \frac{\phi_{i,j,k} - \phi_{i-1,j,k}}{\Delta x} & \text{, if } v_{x,i,j,k} > 0 \\ \phi^+_{x,i,j,k} = \frac{\phi_{i+1,j,k} - \phi_{i,j,k}}{\Delta x} & \text{, if } v_{x,i,j,k} < 0 \end{cases}$$

- Similarly for the y- and z-derivatives.

(c) No, it would not work, as:

- The velocity is dependent on the shape of the interface.
- An upwinded difference would lose information from the interface, leading to instabilities.

(d)

$$\frac{\partial \phi}{\partial t} + \underbrace{A \frac{\boldsymbol{\nabla}\phi}{|\boldsymbol{\nabla}\phi|}}_{\boldsymbol{v} = A\hat{\boldsymbol{n}}} \cdot \boldsymbol{\nabla}\phi = 0$$

$$\frac{\partial \phi}{\partial t} + A|\boldsymbol{\nabla}\phi| = 0$$

2.2 Q2

2. (a) Spurious oscillations originating at the discontinuity. Instability.

(b) **Why standard FVM fail for multiphysics problems?**

- As the system evolves, γ smears, according to the average of the individual $\gamma\rho$:

$$\gamma\rho = \frac{1}{2}(\gamma_1\rho_1 + \gamma_2\rho_2)$$

- and it assumes this represents the physical mixing of the gases.
- But, this is wrong, as we need to know the volume fraction of the gases. This model leads to an underdetermined system.
- We have 6 independent variables $\{\rho_1, \rho_2, v, p, e, \gamma\}$, but only 4 evolution equations and 1 EoS.

(c) Mathematically, the solution is a moving contact discontinuity at constant speed v with no evolution of γ. Numerically, there is no guarantee that the smearing of conserved variable $\gamma\rho$ and ρ is consistent. Any error will lead to a mixture region, which is not supported by this formulation. Spurious oscillations may result.

(d) **Describe interface methods and their advantages/disadvantages.**

Diffuse interface modelling:

Description

- Can use for both sharp (!!) and diffuse transition.
- Model the multiphysics problem using a single system of equations.
- Each computational cell can contain more than one material.
- Supplement the individual $\{\rho\,,\ \rho v, E\}$ conservation/balance laws with a transport equation for the volume fraction. Physics is captured in the balance terms.
- Ensure stability of method in mixture regions using thermodynamic mixture rules.

Advantages

- The formulation handles both material interaction and interface, and allows for a physical representation of mixtures.
- No need to track the interface, it is interface capturing.
- Simple to incorporate surface forces e.g. surface tension as source terms.
- Natural formulation for phase change and chemical reactions.

Disadvantages

- May require non-conservative formulation.
- Each combination of materials requires its own formulation, difficult to deal very difference systems of equations e.g. solids.

- Diffuse treatment of sharp interface: interface smearing from numerical evolution introduces considerable error. Can be reduced by sharpening and anti-diffusion techniques.
- For multi-fluid systems: relaxation is effectively converting pressure or velocity from one material to another in a thermodynamically consistent manner and this often requires complex root finding using the EoS + temperature closure condition may be unphysical.

Extension beyond two materials

- Trivially extended by including additional equations for volume fractions and densities.
- But, mixture rules become trickier, and primitive variables are harder to find which may require iterative root finding.

Sharp interface modelling:
Description

- Can only handle sharp transition.
- Model each material within the multiphysics problem with its own system of equations.
- An additional equation is required to track the position of the interface i.e. level set equation.
- Dynamic boundary conditions are applied at the interface location to ensure thermodynamically reasonable behaviour e.g. ghost fluid method.

Advantages

- Each material can have its own formulation and/or its own numerical method.
- Sharp interface can capture fine features, especially where you don't expect mixing to occur.

Disadvantages

- With only one material in a computational cell, there could be non-conservative errors from mass gain and losses as the interface move.
- Stepped interface due to cells being either in or out could generate additional waves/errors.
- Hard to model phase change/chemical change due to need to reassign mass.

Extension beyond two materials

- Simply add an extra level set equation and material system of equations for each material.
- But, need to use level set fix-up algorithms to ensure each computational cell belongs to a unique material.

Advantages of Level Set Methods

- Models material interface with high accuracy.
- They evolve a smooth function, rather than a discontinuous jump.
- Easy to compute normal direction and curvature of the level set function:

$$\hat{\boldsymbol{n}} = \frac{\nabla\phi}{|\nabla\phi|} \quad \text{and} \quad \kappa = \boldsymbol{\nabla}\cdot\hat{\boldsymbol{n}} = \boldsymbol{\nabla}\cdot\left(\frac{\nabla\phi}{|\nabla\phi|}\right)$$

  although these are generally computed at the cell centres, the smooth nature of ϕ means they are accurate enough close to the interface.
- Signed distance function ($|\boldsymbol{\nabla}\phi| = 1$), where the magnitude of ϕ gives the shortest distance to the interface in the normal direction.

2.3 Q3

3. (a) Consider the characteristic equation:

$$\begin{vmatrix} v-\lambda & \rho & 0 \\ 0 & v-\lambda & 1/\rho \\ 0 & \rho c_s^2 & v-\lambda \end{vmatrix} = 0$$

$$(v-\lambda)[(v-\lambda)^2 - c_s^2] = 0$$

$$\lambda_1 = v\,,\ \lambda_{2,3} = v \pm c_s$$

(b)

$$\begin{pmatrix} -c_s^2 & 0 & 1 \end{pmatrix} \begin{pmatrix} v & \rho & 0 \\ 0 & v & 1/\rho \\ 0 & \rho c_s^2 & v \end{pmatrix} = \begin{pmatrix} -vc_s^2 & 0 & v \end{pmatrix} = v \begin{pmatrix} -c_s^2 & 0 & 1 \end{pmatrix}$$

$$\begin{pmatrix} 0 & -\rho c_s & 1 \end{pmatrix} \begin{pmatrix} v & \rho & 0 \\ 0 & v & 1/\rho \\ 0 & \rho c_s^2 & v \end{pmatrix} = \begin{pmatrix} 0 & -\rho c_s(v-c_s) & v-c_s \end{pmatrix} = (v-c_s) \begin{pmatrix} 0 & -\rho c_s & 1 \end{pmatrix}$$

$$\begin{pmatrix} 0 & \rho c_s & 1 \end{pmatrix} \begin{pmatrix} v & \rho & 0 \\ 0 & v & 1/\rho \\ 0 & \rho c_s^2 & v \end{pmatrix} = \begin{pmatrix} 0 & \rho c_s(v+c_s) & v+c_s \end{pmatrix} = (v+c_s) \begin{pmatrix} 0 & \rho c_s(v+c_s) & v+c_s \end{pmatrix}$$

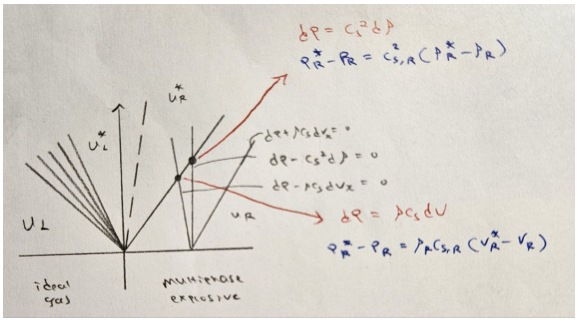
$\lambda_1 = v$ corresponds to $\boldsymbol{l}_1$, $\lambda_2 = v - c_s$ corresponds to $\boldsymbol{l}_2$ and $\lambda_3 = v + c_s$ corresponds to $\boldsymbol{l}_3$.

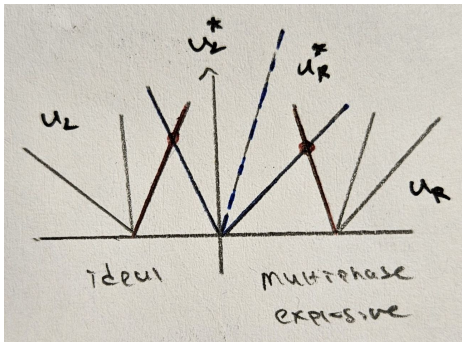
(c)

$$-c_s^2 d\rho + dp = 0 \quad \text{along } \lambda = v$$

$$-\rho c_s dv + dp = 0 \quad \text{along } \lambda = v - c_s$$

$$\rho c_s dv + dp = 0 \quad \text{along } \lambda = v + c_s$$





(d) For left-moving wave, use: $dp + \rho c_s dv = 0$,

$$p_L^* - p_L = -\rho_L c_{s,L}(v_L^* - v_L)$$

(e) For right-moving wave, use: $dp - \rho c_s dv = 0$,

$$p_R^* - p_R = \rho_R c_{s,R}(v_R^* - v_R)$$

(f) Across contact discontinuity, $p_L^* = p_R^* = p^*$ and $v_L^* = v_R^* = v^*$.

$$\begin{cases} p^* - p_L = -\rho_L c_{s,L}(v^* - v_L) \\ p^* - p_R = \rho_R c_{s,R}(v^* - v_R) \end{cases}$$

Subtracting,

$$-p_R + p_L = \rho_R c_{s,R}(v^* - v_R) + \rho_L c_{s,L}(v^* - v_L)$$
$$p_L - p_R = (\rho_R c_{s,R} + \rho_L c_{s,L})v^* - \rho_R v_R c_{s,R} - v_L \rho_L c_{s,L}$$
$$v^* = \frac{p_L - p_R + \rho_R v_R c_{s,R} + v_L \rho_L c_{s,L}}{\rho_R c_{s,R} + \rho_L c_{s,L}}$$

Also,

$$\begin{aligned} p^* &= p_R + \rho_R c_{s,R}\left(\frac{p_L - p_R + \rho_R v_R c_{s,R} + v_L \rho_L c_{s,L}}{\rho_R c_{s,R} + \rho_L c_{s,L}} - v_R\right) \\ &= p_R + \rho_R c_{s,R}\left(\frac{p_L - p_R + \cancel{\rho_R v_R c_{s,R}} + v_L \rho_L c_{s,L} - \cancel{\rho_R v_R c_{s,R}} - \rho_L v_R c_{s,L}}{\rho_R c_{s,R} + \rho_L c_{s,L}}\right) \\ &= p_R + \frac{\rho_R c_{s,R}(p_L - p_R) + \rho_R \rho_L c_{s,R} c_{s,L}(v_L - v_R)}{\rho_R c_{s,R} + \rho_L c_{s,L}} \\ &= \frac{\cancel{\rho_R c_{s,R} p_R} + \rho_L c_{s,L} p_R + \rho_R c_{s,R}(p_L \cancel{- p_R}) + \rho_R \rho_L c_{s,R} c_{s,L}(v_L - v_R)}{\rho_R c_{s,R} + \rho_L c_{s,L}} \\ &= \frac{\rho_L c_{s,L} p_R + \rho_R c_{s,R} p_L + \rho_R \rho_L c_{s,R} c_{s,L}(v_L - v_R)}{\rho_R c_{s,R} + \rho_L c_{s,L}} \end{aligned}$$

(g) For left-moving wave, use $dp - c_s^2 d\rho = 0$

$$p^* - p_L = c_{s,L}^2(\rho_L^* - \rho_L)$$
$$\rho_L^* = \rho_L + \frac{p^* - p_L}{c_{s,L}^2}$$

(h) **Assumption**: $A(\boldsymbol{w})$ is constant.
Advantage: Allow us to derive b.c. for arbitrary interfaces between two very different systems of equations.
Disadvantage: The assumption of a constant primitive matrix is not physical, and may fail under extreme conditions, leading to spurious oscillations.

(i) Slightly relax the assumption that $A(\boldsymbol{w}) = \text{const}$. Instead, we get an averaged state for $A(\bar{\boldsymbol{w}})$ using the intermediate state obtained from the method and the initial state:

$$p_R^* - p_R = \overline{\rho_R c_{s,R}}(v_x^* - v_R) \quad \text{, where} \quad \overline{\rho_R c_{s,R}} = \frac{1}{2}(\rho_R c_{s,R} + \rho_R^* c_{s,R}^*)$$

$$p_R^* - p_R = \overline{c_{s,R}^2}(\rho_R^* - \rho_R) \quad \text{, where} \quad \overline{c_{s,R}^2} = \frac{1}{2}(c_{s,R}^2 + c_{s,R}^{*2})$$

Since we no longer have a closed expression, the process of obtaining intermediate states via the jump conditions can be continued iteratively, until a steady state is reached.

Alternatively, an exact, or more accurate approximate Riemann solver may exist.

3 2019-20 (EXAM)

3.1 Q1

1. (a) To get thermodynamically consistent boundary conditions, the ghost fluid method assumes constant entropy across the interface and copies pressure and velocity from the real material to the ghost fluid.

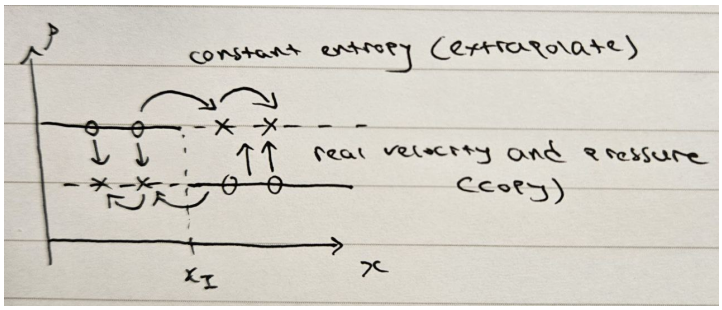
$$s = c_v \ln p - \gamma c_v \ln \rho + \text{const} = c_v \ln\left(\frac{p}{\rho^\gamma}\right) + \text{const} \quad \text{, where} \quad \gamma = \frac{c_p}{c_v} = \frac{c_v + R}{c_v}$$

$$\frac{s - \text{const}}{c_v} = \ln\left(\frac{p}{\rho^\gamma}\right)$$

We can enforce constant entropy using:

$$\frac{p}{\rho^\gamma} = \text{const}$$

Consider two cells, x_I is a real cell adjacent to the interface, and x_G is a cell within the ghost fluid region.



such that:

$$\frac{p_I}{\rho_I^{\gamma_I}} = \frac{p_G}{\rho_G^{\gamma_I}} \quad \Rightarrow \quad \rho_G = \rho_I \left(\frac{p_G}{p_I}\right)^{1/\gamma_I}$$

We can compute the density in the ghost region ρ_G as we know its pressure p_G (copied). The adiabatic index γ_I is that of the real material at the cell x_I.

(b) No.

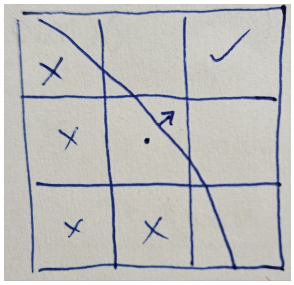
- The assumption of constant entropy across the interface is not true for shock waves.
- For a strong shock wave, it can predict a reflected rarefaction when there is actually a reflected shock wave.
- If there is a temperature gradient across the interface, the constant entropy assumption would not hold.

(c) **2D multiphysics system which contains an interface between an elastoplastic solid material and a liquid**:

- Requires Riemann-problem based ghost fluid methods. Either the real GFM or the Riemann GFM.

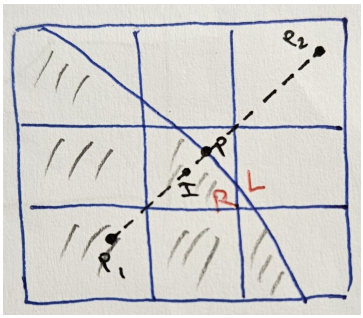
  How to setup and apply dynamic boundary conditions for cells adjacent to the interface?

- Firstly, on a discrete grid, a computational cell x_I next to the interface is identified through a change in sign of the level set function.
- **For real GFM**:



  - A mixed-material Riemann problem is then set up between x_I and one of the eight cells surrounding it.
  - The choice of cell is that it must align most closely with the normal vector and is in the other material.
  - Issue: two states for the Riemann problem are a different distance from the interface.

  For Riemann GFM:



  - Instead: aim to find two interpolated states, equidistant from the interface.
  - The value of ϕ at x_I tells you its distance from the interface, with the position given by $\boldsymbol{x}_P = \boldsymbol{x}_i - \boldsymbol{n}\phi$, assuming normal vector point into the shaded region.
  - Two points equidistant from the interface are constructed $\boldsymbol{x}_{P1,2} = \boldsymbol{x}_P \pm (1.5\Delta x)\hat{\boldsymbol{n}}$.
  - These two points are then used to interpolate two states for the mixed-material RP.
- Once we have these states, the normal vector can be used to rotate them normal to the interface. E.g.

$$(v_x, v_y, v_z)_L, (v_x, v_y, v_z)_L \rightarrow (v_n, (\boldsymbol{v} - v_n\boldsymbol{n}))_L, (v_n, (\boldsymbol{v} - v_n\boldsymbol{n}))_R$$

$$\Rightarrow (v^*, (\boldsymbol{v} - v_n\boldsymbol{n})_L), (v^*, (\boldsymbol{v} - v_n\boldsymbol{n})_R)$$

- The mixed-material RP between two neighbouring states, $\boldsymbol{q}_L$ and $\boldsymbol{q}_R$ is then solved to obtain two intermediate state, $\boldsymbol{q}_L^*$ and $\boldsymbol{q}_R^*$.
- Due to the complex nature of the evolution equations for a solid, a linearised solver will be required to obtain the intermediate states. It assumes the primitive variable matrix is constant.
- The value of cell $\boldsymbol{q}_I$ is then replaced with one of the left intermediate star states from the Riemann problem.
  - If x_I contains the real material, it is replaced by its own intermediate state.
  - If x_I contains the ghost material, it is replaced by the left intermediate state of the material the other side of the interface.

How to propagate information into ghost fluid regions?

- Once all cells adjacent to the interface have had their value set, these state need to be propagated (further) into the ghost fluid region, through constant extrapolation.
- This is done by the solution of a boundary-value problem: $\hat{\boldsymbol{n}} \cdot \boldsymbol{\nabla} Q = 0$.
- Appropriate methods for doing this are iterative pseudo-time evolution of the Eikonal equation, a fast marching method or a fast sweeping method.
- **For iterative**:
  - Solve:
$$\frac{\partial Q}{\partial \tau} + \text{sgn}(\phi)\hat{\boldsymbol{n}} \cdot \boldsymbol{\nabla} Q = 0$$
    for some fictitious time τ and all derivatives are first order upwind (based on ϕ).

  For Fast sweeping:
  - Solve:
$$\hat{\boldsymbol{n}} \cdot \boldsymbol{\nabla} Q = 0$$
$$n_x \left(\frac{Q_{i,j,k} - Q_x}{\Delta x} \right) + n_y \left(\frac{Q_{i,j,k} - Q_y}{\Delta y} \right) + n_z \left(\frac{Q_{i,j,k} - Q_z}{\Delta z} \right) = 0$$
  - where the direction of the normal vector determines the winding direction
  - Consider four sweeps of the domain, and compute the updated values.

  For Fast marching:
  - All points (further) in the ghost fluid region are ordered by the magnitude of the value of the level set function. In this order, the Eikonal equation with first order derivatives (again winded based on the normal direction) is solved.

(d)
- **Length scale**: if the scale of the simulation is sufficiently large that small-scale features due to wave interactions between the solid and the liquid are negligible.
- **Time scale**: if the timescale of the behaviour of interest is significantly larger than the timescale of waves propagating in the solid.

(e) Treat the solid as a rigid body, either as a reflective boundary condition applied with a ghost fluid method, or through cut cell methods.

3.2 Q2

2. (a) 5 equation:

$$\frac{\partial \alpha_1}{\partial t} + \boldsymbol{u} \cdot \boldsymbol{\nabla} \alpha_1 = 0$$
$$\frac{\partial \alpha_1 \rho_1}{\partial t} + \boldsymbol{\nabla} \cdot (\alpha_1 \rho_1 v) = 0$$
$$\frac{\partial \alpha_2 \rho_2}{\partial t} + \boldsymbol{\nabla} \cdot (\alpha_2 \rho_2 v) = 0$$
$$\frac{\partial \rho \boldsymbol{v}}{\partial t} + \boldsymbol{\nabla} \cdot (\rho \boldsymbol{v} \otimes \boldsymbol{v} + p \boldsymbol{I}) = 0$$
$$\frac{\partial \rho E}{\partial t} + \boldsymbol{\nabla} \cdot [(\rho E + p) \boldsymbol{v}] = 0$$

6 equation:

$$\frac{\partial \alpha_1}{\partial t} + \boldsymbol{u} \cdot \boldsymbol{\nabla} \alpha_1 = 0$$
$$\frac{\partial \alpha_1 \rho_1}{\partial t} + \boldsymbol{\nabla} \cdot (\alpha_1 \rho_1 v) = 0$$
$$\frac{\partial \alpha_2 \rho_2}{\partial t} + \boldsymbol{\nabla} \cdot (\alpha_2 \rho_2 v) = 0$$
$$\frac{\partial \rho \boldsymbol{v}}{\partial t} + \boldsymbol{\nabla} \cdot (\rho \boldsymbol{v} \otimes \boldsymbol{v} + p \boldsymbol{I}) = 0$$
$$\frac{\partial \alpha_1 \rho_1 e_1}{\partial t} + \boldsymbol{\nabla} \cdot [\alpha_1 (\rho_1 e_1 + p_1) \boldsymbol{v}] = 0$$
$$\frac{\partial \alpha_2 \rho_2 e_2}{\partial t} + \boldsymbol{\nabla} \cdot [\alpha_2 (\rho_2 e_2 + p_2) \boldsymbol{v}] = 0$$

Source terms: can add compaction terms for 5-equation formulation and cavitation terms for 6-equation formulation.

(b) Use:

$$\frac{\partial \alpha_a}{\partial t} = \mu (p_a - p_w) \quad \text{and} \quad \frac{\partial \alpha_a \rho_a e_a}{\partial t} = -p_I \mu (p_a - p_w)$$

Equate expressions for $\mu(p_a - p_w)$:

$$\frac{\partial \alpha_a}{\partial t} = -\frac{1}{p_I} \frac{\partial \alpha_a \rho_a e_a}{\partial t}$$
$$\alpha_a \rho_a \frac{\partial e_a}{\partial t} + \cancel{e_a \frac{\partial \alpha_a \rho_a}{\partial t}} = -p_I \frac{\partial \alpha_a}{\partial t}$$
$$\frac{\partial e_a}{\partial t} = -\frac{p_I}{\alpha_a \rho_a} \frac{\partial}{\partial t} \left(\frac{\alpha_a \rho_a}{\rho_a} \right)$$

(c)

$$\frac{\partial e_a}{\partial t} = -\frac{p_I}{\alpha_a \rho_a} \left(\alpha_a \rho_a \frac{\partial V_a}{\partial t} + V_a \cancel{\frac{\partial \alpha_a \rho_a}{\partial t}} \right)$$
$$\frac{\partial e_a}{\partial t} = -p_I \frac{\partial V_a}{\partial t}$$

where $B = -p_I$.

(d)

$$\frac{\partial \alpha_w}{\partial t} = \frac{\partial (1-\alpha_a)}{\partial t} = -\frac{\partial \alpha_a}{\partial t}$$

Will still get same form:

$$\frac{\partial e_w}{\partial t} = -p_I \frac{\partial V_w}{\partial t}$$

(e) Closure is provided by volume fraction:

$$\alpha_a + \alpha_w = 1$$

(f)

$$\alpha_a \rho_a V_a + \alpha_w \rho_w V_w = 1$$

(g) Stiffened gas EoS:

$$p = (\gamma - 1)\rho\varepsilon - \gamma p_\infty \quad \Rightarrow \quad e_w = \frac{p_w + \gamma_w p_{\infty,w}}{\gamma_w - 1} V_w$$

$$e_w(p, V_w) = e_w^0(p_w^0, V_w^0) - p(V_w - V_w^0)$$

$$\frac{p + \gamma_w p_{\infty,w}}{\gamma_w - 1} V_w = \frac{p_w^0 + \gamma_w p_{\infty,w}}{\gamma_w - 1} V_w^0 - p(V_w - V_w^0)$$

$$\frac{\cancel{p} + \gamma_w p_{\infty,w} + (\gamma_w \cancel{-1}) p}{\gamma_w - 1} V_w = \frac{p_w^0 + \gamma_w p_{\infty,w} + (\gamma_w - 1)p}{\gamma_w - 1} V_w^0$$

$$V_w = \frac{p_w^0 + \gamma_w p_{\infty,w} + (\gamma_w - 1)p}{\gamma_w p_{\infty,w} + \gamma_w p} V_w^0$$

(h) p is the relaxed pressure - the equilibrium state of the two initial pressures p_1 and p_2.

How does it model cavitation? This process assumes that the two pressures obtained from the evolution step of the compressible equations then instantaneously relax, $p_w = p_a$. Then, solve for the necessary cavitation behaviour that allows for this redistribution of mass from one phase to the other.

3.3 Q3

3. Same question as 2018-19 (MOCK) Q3. Link

4 2020-21 (EXAM)

4.1 Q1

1. (a) In sharp interface methods, one needs a technique to identify the location of a material interface, and use this to split the computational domain into two or more regions.

Explicit representation: one explicitly writes down the points that belong to the interface.

$$(x - x_0)^2 + (y - y_0)^2 + (z - z_0)^2 = r^2$$

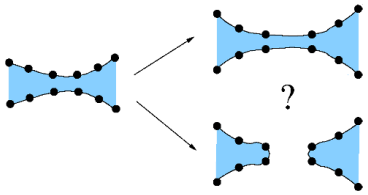
Implicit representation: defines the interface as the isocontour of some function ϕ.

$$\phi = (x - x_0)^2 + (y - y_0)^2 + (z - z_0)^2 - r^2$$

- Sometimes, knowing what side of the interface you are and how far from it is good enough.
- Merging and splitting happens trivially, without worrying about sub-cell scale behaviour.

(b) **Challenges with explicit boundaries**:

- Challenging to map a function to an arbitrary surface.
- If an interface becomes stretched, very difficult to work out if it is very thin, or broken.



(c) SDF: a function where the slope in the normal direction is unity.

$$|\nabla\phi| = 1$$

The absolute value of the function $|\phi|$ gives you the shortest distance to the zero-contour.

(d)
- ϕ is advected using interface material velocity.
- However, this velocity is not constant in space and can generate non-linear behaviour.
- This causes ϕ to become too smeared or too steep.
- If ϕ becomes too steep and resemble a discontinuity, the non-conservative method use for evolving ϕ fails, resulting in the interface being in the wrong position.
- If ϕ becomes too smeared, it is easy to introduce errors into the interface with any small errors in the update such as round-off error.
- Returning ϕ to a signed distance function prevents all these from happening.

(e) Expand and square $|\nabla\phi| = 1$ to give $(\partial_x\phi)^2 + (\partial_y\phi)^2 + (\partial_z\phi)^2 = 1$. Approximate the derivative using first-order difference. We try to get the approximated $\hat{\phi}_{i,j,k}$ for the current cell. $\phi_x = \min(\phi_{i+1,j,k}, \phi_{i-1,j,k})$ for positive level set and $\phi_x = \max(\phi_{i+1,j,k}, \phi_{i-1,j,k})$ for negative level set.

(f) The equation is an intersection between an ellipse at (ϕ_x, ϕ_y, ϕ_z) with semi-axis of lengths Δx, Δy, Δz with a line $x = y = z$. If the ellipse is too displaced from the origin, the line might not intersect the ellipse, and we fail to get a solution. Thus, we can try to remove the largest of ϕ_x, ϕ_y, ϕ_z values to bring the ellipse closer to the origin and reduce the dimension by one. Repeat one more time if still no real root.

(g) For fast sweeping, we know there are only 2*dimension sweeps to take. However, the iterative method involves solving an equation in fictitious time for 'enough' time steps. It is unclear what enough is, but will always be more than is needed for fast sweeping.

Also, iterative method requires storing a gradient of the level set for the update, whereas fast sweeping is a single operation.

(h) Constant extrapolation (in the normal direction) is the solution to a boundary-value problem:

$$\hat{\boldsymbol{n}} \cdot \boldsymbol{\nabla} u = 0$$

Can also be written as:

$$\frac{\boldsymbol{\nabla}\phi}{|\boldsymbol{\nabla}\phi|} \cdot \boldsymbol{\nabla} u = 0$$

(i)

$$\left(\frac{\Delta\phi_x}{\Delta x} \quad \frac{\Delta\phi_y}{\Delta y} \quad \frac{\Delta\phi_z}{\Delta z}\right) \cdot \left(\frac{\hat{u}_{i,j,k} - u_x}{\Delta x} \quad \frac{\hat{u}_{i,j,k} - u_y}{\Delta y} \quad \frac{\hat{u}_{i,j,k} - u_z}{\Delta z}\right) = 0$$

$$\hat{u}_{i,j,k}\left(\frac{\Delta\phi_x}{\Delta x^2} + \frac{\Delta\phi_y}{\Delta y^2} + \frac{\Delta\phi_z}{\Delta z^2}\right) = \frac{u_x\Delta\phi_x}{\Delta x^2} + \frac{u_y\Delta\phi_y}{\Delta y^2} + \frac{u_z\Delta\phi_z}{\Delta z^2}$$

$$\hat{u}_{i,j,k} = \frac{u_x\frac{\Delta\phi_x}{\Delta x^2} + u_y\frac{\Delta\phi_y}{\Delta y^2} + u_z\frac{\Delta\phi_z}{\Delta z^2}}{\frac{\Delta\phi_x}{\Delta x^2} + \frac{\Delta\phi_y}{\Delta y^2} + \frac{\Delta\phi_z}{\Delta z^2}}$$

$u_{x,y,z}$ are values of u from the appropriate cells chosen for $\phi_{x,y,z}$.

4.2 Q2

2. (a) Mixture rules:

$$\rho = \alpha_1\rho_1 + \alpha_2\rho_2$$
$$\rho v = \alpha_1\rho_1 v_1 + \alpha_2\rho_2 v_2$$
$$E = \alpha_1 E_1 + \alpha_2 E_2$$

(b) $E = \rho\varepsilon + \frac{1}{2}\rho v^2$.

$$E = \alpha_1\rho_1\varepsilon_1 + \alpha_2\rho_2\varepsilon_2 + \underbrace{\frac{1}{2}(\alpha_1\rho_1 v_1^2 + \alpha_2\rho_2 v_2^2)}_{KE_{\text{mix}}}$$

$$\varepsilon = \frac{E - KE_{\text{mix}}}{\rho} = \frac{\alpha_1\rho_1\varepsilon_1 + \alpha_2\rho_2\varepsilon_2}{\rho} \neq \alpha_1\varepsilon_1 + \alpha_2\varepsilon_2$$

(c) Instantaneous pressure relaxation: $\mu \to \infty$ and $p_1 = p_2 = p$. Instantaneous velocity relaxation: $\lambda \to \infty$ and $v_1 = v_2 = v$. We now only have a single pressure and velocity for the system.

Consider the momentum equation:

$$\frac{\partial \alpha_1\rho_1 v}{\partial t} + \frac{\partial \alpha_1(\rho_1 v^2 + p)}{\partial x} = p_I\frac{\partial \alpha_1}{\partial x} \quad \text{and} \quad \frac{\partial \alpha_2\rho_2 v}{\partial t} + \frac{\partial \alpha_2(\rho_2 v^2 + p)}{\partial x} = p_I\frac{\alpha_2}{x}$$

Combine them:

$$\frac{\partial}{\partial t}[(\underbrace{\alpha_1\rho_1 + \alpha_2\rho_2}_{\rho})v] + \frac{\partial}{\partial x}[(\underbrace{\alpha_1\rho_1 + \alpha_2\rho_2}_{\rho})v^2 + (\underbrace{\alpha_1 + \alpha_2}_{1})p] = p_I\frac{\partial}{\partial x}(\underbrace{\alpha_1 + \alpha_2}_{1})$$

$$\frac{\partial \rho v}{\partial t} + \frac{\partial(\rho v^2 + p)}{\partial x} = 0$$

Consider the energy equation:

$$\frac{\partial \alpha_1 E_1}{\partial t} + \frac{\partial \alpha_1(E_1 + p)v}{\partial x} = p_I v_I\frac{\partial \alpha_1}{\partial x} \quad \text{and} \quad \frac{\partial \alpha_2 E_2}{\partial t} + \frac{\partial \alpha_2(E_2 + p)v}{\partial x} = p_I v_I\frac{\partial \alpha_2}{\partial x}$$

Combine them:

$$\frac{\partial}{\partial t}[(\underbrace{\alpha_1 E_1 + \alpha_2 E_2}_{E})v] + \frac{\partial}{\partial x}[(\underbrace{\alpha_1 E_1 + \alpha_2 E_2}_{E})v^2 + (\underbrace{\alpha_1 + \alpha_2}_{1})pv] = p_I v_I\frac{\partial}{\partial x}(\underbrace{\alpha_1 + \alpha_2}_{1})$$

$$\frac{\partial E}{\partial t} + \frac{\partial(E + pv)}{\partial x} = 0$$

(d) For ideal gas:

$$p = (\gamma - 1)\rho\varepsilon$$

So,

$$\xi_K = \frac{\partial \rho_K\varepsilon_K}{\partial p}\Big|_{\rho_L} = \frac{1}{\gamma_K - 1}$$

(e)

$$\rho\varepsilon + \frac{1}{2}\rho v^2 = \alpha_1\rho_1\varepsilon_1 + \alpha_2\rho_2\varepsilon_2 + \frac{1}{2}(\alpha_1\rho_1 v_1^2 + \alpha_2\rho_2 v_2^2)$$
$$\Rightarrow \rho\varepsilon = \alpha_1\rho_1\varepsilon_1 + \alpha_2\rho_2\varepsilon_2$$

$$\begin{aligned} d(\rho\varepsilon) &= d(\alpha_1\rho_1\varepsilon_1 + \alpha_2\rho_2\varepsilon_2) \\ &= \rho_1\varepsilon_1 d\alpha_1 + \rho_2\varepsilon_2 d\alpha_2 + \alpha_1 d(\rho_1\varepsilon_1) + \alpha_2 d(\rho_2\varepsilon_2) \\ &= \rho_1\varepsilon_1 d\alpha_1 + \rho_2\varepsilon_2 d\alpha_2 + \alpha_1 \cancel{\frac{\partial\rho_1\varepsilon_1}{\partial\rho_1} d\rho_1} + \alpha_1\frac{\partial\rho_1\varepsilon_1}{\partial p}dp + \alpha_2 \cancel{\frac{\partial\rho_2\varepsilon_2}{\partial\rho_2} d\rho_2} + \alpha_2\frac{\partial\rho_2\varepsilon_2}{\partial p}dp \\ &= \rho_1\varepsilon_1 d\alpha_1 + \rho_2\varepsilon_2 d\alpha_2 + \frac{\alpha_1}{\gamma_1 - 1}dp + \frac{\alpha_2}{\gamma_2 - 1}dp \end{aligned}$$

(f)

$$\left(\frac{\alpha_1}{\gamma_1 - 1} + \frac{\alpha_2}{\gamma_2 - 1}\right) dp = d(\rho\varepsilon) - \rho_1\varepsilon_1 d\alpha_1 - \rho_2\varepsilon_2 d\alpha_2$$
$$(\alpha_1\xi_1 + \alpha_2\xi_2)dp = d(\rho\varepsilon) - \rho_1\varepsilon_1 d\alpha_1 + \rho_2\varepsilon_2 d\alpha_1$$
$$\xi dp = d(\rho\varepsilon) - (\rho_1\varepsilon_1 - \rho_2\varepsilon_2)d\alpha_1$$
$$dp = \frac{1}{\xi}d(\rho\varepsilon) - \frac{1}{\xi}(\rho_1\varepsilon_1 - \rho_2\varepsilon_2)d\alpha_1$$

(g) Identify terms:

$$\frac{\partial p}{\partial\rho\varepsilon} = \frac{1}{\xi}$$

$$\frac{\partial p}{\partial\rho_1\alpha_1} = \frac{\partial p}{\partial\rho_2\alpha_2} = 0$$
$$c_s^2 = \frac{1}{\xi}h = \frac{1}{\xi}\left(\frac{\alpha_1\rho_1}{\rho}h_1 + \frac{\alpha_2\rho_2}{\rho}h_2\right)$$
$$\therefore\ c_s^2 = \frac{1}{\xi}(Y_1 h_1 + Y_2 h_2)$$

(h)

$$p = (\gamma_K - 1)\rho_K\varepsilon_K \quad \text{and} \quad \varepsilon_K = \frac{p}{\rho_K(\gamma_K - 1)}$$

$$\begin{aligned} h_K &= \varepsilon_K + (\gamma_K - 1)\varepsilon_K \\ &= \gamma_K\varepsilon_K \\ &= \frac{\gamma_K p}{\rho_K(\gamma_K - 1)} \\ &= \frac{c_{s,K}^2}{\gamma_K - 1} \\ &= \xi_K c_{s,K}^2 \end{aligned}$$

$$c_s^2 = \frac{1}{\xi}\left(Y_1\xi_1 c_{s,1}^2 + Y_2\xi_2 c_{s,2}^2\right)$$

4.3 Q3

3. (a)

$$\boldsymbol{S}(\boldsymbol{u})_E = \delta(\boldsymbol{x} - \boldsymbol{x}_S)\boldsymbol{v} \cdot \boldsymbol{f}_S$$

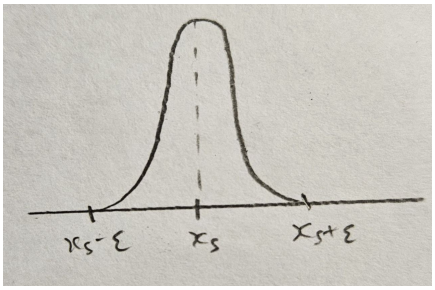
(b) Replace the delta function with a smeared delta function of finite width. The interface now occupies a finite volume, hence is a volume integral. It is necessary because it is hard to evaluate a true delta function on a discretised domain. We probably do not directly know x_S, and we need to employ interpolation to find it which can be expensive.

"Since $\delta(x) = 0$ almost everywhere, it seems unlikely that any standard numerical approximation based on sampling will give a good approximation to this integral. This is why we turned to a first-order smeared out approximation of $\delta(x)$."

Approximation: assumes the interface itself is modelled as smeared as well.

(c) Properties of smeared delta function:

- Integral under smeared delta function is 1.
- Centred at $x = x_S$.
- Appropriate choice of ϵ means delta function can cover more than one grid cell. Typically, $\epsilon = 1.5\Delta x$.
- The value and derivative of the function becomes zero at the edges, $|x - x_s| = \epsilon$. Similar to the original Dirac-delta function.



Idea: Surface tension forces acting on the interface are transformed to volume forces in regions near the interface via smeared delta functions, leading to ideally discontinuous interfacial jump conditions being modelled as smooth.

Effect: the numerical solution becomes continuous at the interface even if the jump conditions imply that the solution should be discontinuous. For example, surface tension forces induce a discontinuous pressure across a fluid-fluid interface, this method would smear the pressure profile into a numerically continuous function.

(d) σ is the surface tension with units of force per unit length. κ is the curvature. $\boldsymbol{n}$ is the normal vector to the surface.

(e) Start with momentum equation,

$$\frac{\partial \rho v}{\partial t} + \frac{\partial}{\partial x}(\rho v^2 + p) = \delta(\boldsymbol{x} - \boldsymbol{x}_S)\sigma\kappa\boldsymbol{n}$$

Since $v = 0$,

$$\frac{\partial p}{\partial x} = \delta(\boldsymbol{x} - \boldsymbol{x}_S)\sigma\kappa$$

Integrating w.r.t. x,

$$\Delta p = \sigma\kappa$$

(f) Curvature of the interface must be constant.

(g) Difficulties of diffuse interface approach:

- Diffuse interface method do not have distance information, it is more difficult to obtain the location of the interface x_S, and its normal and curvature from just the volume fraction.
- Diffuse interface may not be the same width as the smeared delta function.

(h)

$$\hat{\boldsymbol{n}} = \frac{\boldsymbol{\nabla}\phi}{|\boldsymbol{\nabla}\phi|} \quad \text{and} \quad \kappa = \boldsymbol{\nabla} \cdot \hat{\boldsymbol{n}}$$

(i) **Modelling surface tension effects using level set function**:

- Interface is now sharp, cannot use smeared delta function any more.
- To deal with a sharp interface, use the ghost fluid method (GFM), specifically a Riemann-problem based GFM, where the intermediate pressure is no longer continuous across the interface. Instead, there is a pressure jump of:

$$\Delta p = \sigma\kappa \quad , \quad p_R^* = p_L^* + \Delta p$$

- We incorporate the pressure jump into an exact Riemann solver. We then solve the following Riemann problem:

$$f_L(p_L^*, \boldsymbol{u}_L) + f_R(p_L^* + \sigma\kappa, \boldsymbol{u}_R) + \Delta v = 0$$

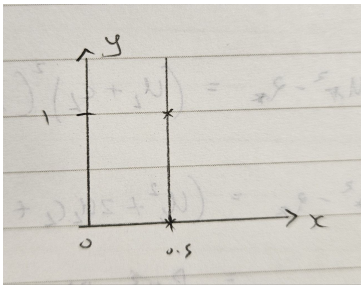
- After finding p_L^*, we can find p_R^*.
- The velocity is still continuous.
- Also works with linearised Riemann solvers for complex material interfaces.

5 2021-22 (EXAM)

5.1 Q1

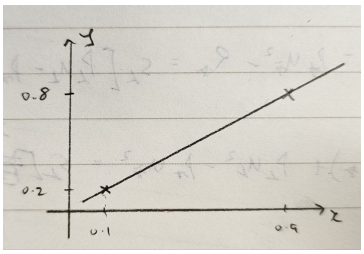
1. (a)
   - The exact location of the boundary is not known on a discretised mesh, but we do know which side we are on.
   - Instead it is considered as the zero-contour of a scalar field that exists across the entire physical domain.

   (b) Interface is a vertical line,



$$x = 0.5$$
$$\Rightarrow \phi(x, y) = x - 0.5$$

Interface is a sloped line:

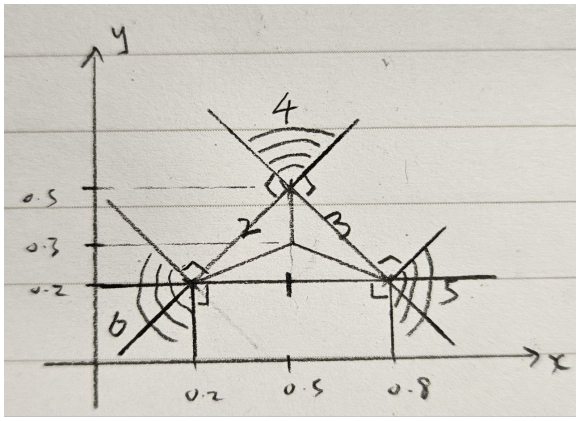


$$y = \frac{3}{4}x - \frac{1}{8}$$
$$\Rightarrow \phi(x, y) = y - \frac{3}{4}x - \frac{1}{8}$$

Powerful geometrical tools for level set method (implicit):

- The sign of ϕ tells us which side of the interface we are at.
- If ϕ_1 and ϕ_2 are two different implicit functions and they are convex, then $\phi(x) = \min(\phi_1, \phi_2)$ represents the union of the interior regions of ϕ_1 and ϕ_2. $\phi(x) = \max(\phi_1, \phi_2)$ represents the intersection of the interior regions of ϕ_1 and ϕ_2. $\phi(x) = \max(\phi_1, -\phi_2)$ represents the region obtained by subtracting the interior of ϕ_2 from the interior of ϕ_1.
- If ϕ is concave function. min represents intersect and max represents union.

Interface is a triangle in (x, y) space. In (x, y, ϕ) space, it is formed by the intersection of three planes, making a pyramid:



Geometry:

$$\text{lines: } \{y = 0.2 \quad , \quad y = x \quad , \quad y = -x + 1\}$$

Level set function is found by minimising the distance to the interface *e.g. triangular in this case. The lecture notes gave an example for a square.*

We separate the interface into 7 regions (1 interior, 3 edge and 3 corner) by drawing perpendicular lines to the edges at the corners.

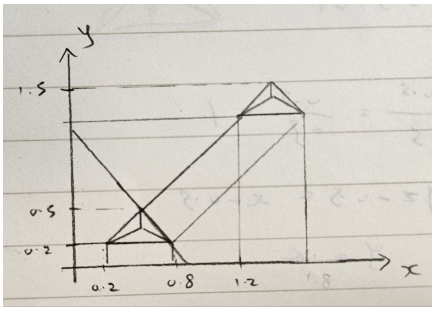
$$\text{Edges: } \{\phi_1 = y - 0.2 \quad , \quad \phi_2 = x - y \quad , \quad \phi_3 = 1 - x - y\}$$

$$\text{Corners: } \Big\{\phi_4 = \sqrt{(x-0.5)^2 + (y-0.5)^2} \quad , \quad \phi_5 = \sqrt{(x-0.8)^2 + (y-0.2)^2},$$
$$\phi_6 = \sqrt{(x-0.2)^2 + (y-0.2)^2} \Big\}$$

After defining all the corners and edges, we piece together the ϕ function by regions:

$$\phi_7 = \begin{cases} \min(\phi_1, \phi_2, \phi_3) & , \text{ if } \phi_1 > 0 \ , \ \phi_2 > 0 \ , \ \phi_3 > 0 \\ \\ \phi_4 & , \text{ if } \phi_2 < 0 \ , \ \phi_3 < 0 \\ \phi_2 & , \text{ if } \phi_2 < 0 \ , \ 0 < \phi_3 < \sqrt{0.3^2 + 0.3^2} \\ \phi_6 & , \text{ if } \phi_2 < 0 \ , \ \phi_3 > \sqrt{0.3^2 + 0.3^2} \\ \\ \phi_3 & , \text{ if } \phi_3 < 0 \ , \ 0 < \phi_2 < \sqrt{0.3^2 + 0.3^2} \\ \phi_5 & , \text{ if } \phi_3 < 0 \ , \ \phi_2 > \sqrt{0.3^2 + 0.3^2} \\ \\ \phi_1 & , \text{ if } \phi_1 < 0 \ , \ 0.2 < x < 0.8 \\ \phi_6 & , \text{ if } \phi_1 < 0 \ , \ x < 0.2 \\ \phi_5 & , \text{ if } \phi_1 < 0 \ , \ x > 0.8 \end{cases}$$

Interface is 2 identical triangles:



$$\text{lines: } \{y = 0.2 \quad , \quad y = x \quad , \quad y = -x + 1\}$$

Translate in positive x and y-direction by 1 unit, so $y \to y - 1$ and $x \to x - 1$

$$\text{lines: } \{y = 1.2 \quad , \quad y = x \quad , \quad y = -x + 3\}$$

The level set for a single pyramid is given in part (iii), ϕ_7. After replacing $y \to y - 1$ and $x \to x - 1$, we get a new level set function for the other pyramid, ϕ_8. Since they are concave functions, the max of them gives the union of their interior regions.

$$\phi = \max(\phi_7, \phi_8)$$

(c)

$$\hat{\boldsymbol{n}} = \frac{\boldsymbol{\nabla}\phi}{|\boldsymbol{\nabla}\phi|} \quad \text{and} \quad \kappa = \boldsymbol{\nabla} \cdot \hat{\boldsymbol{n}}$$

(d) General form of Hamilton-Jacobi equation:

$$\frac{\partial \phi}{\partial t} + H(\boldsymbol{\nabla}\phi) = 0$$

(e) Normal vector driven-velocity ($\boldsymbol{v} = V_n \hat{\boldsymbol{n}}$) is fine, curvature driven ($\boldsymbol{v} = \kappa \hat{\boldsymbol{n}}$) is not.

$$\frac{\partial \phi}{\partial t} + V_n |\boldsymbol{\nabla}\phi| = 0 \quad \text{and} \quad \frac{\partial \phi}{\partial t} + \left[\boldsymbol{\nabla} \cdot \left(\frac{\boldsymbol{\nabla}\phi}{|\boldsymbol{\nabla}\phi|}\right)\right] |\boldsymbol{\nabla}\phi| = 0$$

The curvature depends on the second derivative of ϕ, so it is not in the form of a HJ equation. On the other hand, normal-vector driven-velocity depends only on first derivative.

(f) **Why can upwinded methods be used for evolving the level set function describing an interface between two materials, but not for general Hamilton-Jacobi equations?**

The idea is that for upwind methods to make sense, you need an idea of "direction" of information travel.

- Level set equation is:
$$\frac{\partial \phi}{\partial t} + \boldsymbol{v} \cdot \boldsymbol{\nabla}\phi = 0$$
where $\boldsymbol{v}$ is the material velocity which determines the direction of flow.
- This means we always know which direction information travels in for a given cell. Hence, we can use upwinded schemes.
- For HJ equation, $H(\boldsymbol{\nabla}\phi)$ is a general function of the gradient of ϕ, there is no concept of a 'direction of flow'.

5.2 Q2

2. (a) **Assumptions across interface**:
   - Velocity equilibrium i.e. velocity is continuous.
   - Pressure equilibrium i.e. pressure is continuous.
   - Constant entropy for each material individually.

   (b) **Method**:
   - Pressure and velocity are copied from the real material to the ghost fluid cell.
   - $$s = c_v \ln p + c_p \ln v + \text{const} \quad \text{(note the symmetry)}$$
     where $\gamma = \frac{c_p}{c_v}$
   - Constant entropy means:
     $$pv^\gamma = \frac{p}{\rho^\gamma} = \text{const}$$
   - For real material cell adjacent to interface x_I and ghost material x_G:
     $$\frac{p_I}{\rho_I^{\gamma_I}} = \frac{p_G}{\rho_G^{\gamma_I}} \quad \Rightarrow \quad \rho_G = \rho_I \left(\frac{p_G}{p_I}\right)^{1/\gamma_I}$$
     Both the real and ghost cell are part of the same material so they have the same γ_I. p_G is copied from the real cell.

   (c) **In 2D/3D**:
   - The copying of pressure is unchanged.
   - Now, only the normal velocity is continuous across the interface, which needs to be computed and copied into the ghost cell.
     $$v_n = \hat{\boldsymbol{n}} \cdot \boldsymbol{v} = \frac{\boldsymbol{\nabla}\phi}{|\boldsymbol{\nabla}\phi|} \cdot \boldsymbol{v}$$
   - The tangential velocity jump across the interface.
     $$\boldsymbol{v}_t = \boldsymbol{v} - v_n \hat{\boldsymbol{n}}$$
   - An extrapolation technique needs to be used for entropy and the tangential velocity vector.
   - Finally, the density can be found, and the total velocity obtained from combining the normal velocity and the extrapolated tangential velocity.

   (d) **How many ghost cells need setting?** (1 more than the numerical stencil).
   - At least 3.
   - 2 ghost cell for MUSCL-Hancock scheme.
   - But over the course of a time step, the motion of the interface can cause a ghost cell to become a real cell.
   - To ensure this cell has been updated using reasonable values, we need to provide a good state for the third cell deep.

(e) **GFM dynamic boundary condition for contact discontinuity, rarefaction and shock**:

- Contact discontinuities - the ghost fluid method specifies the exact behaviour.
- Rarefaction - within a rarefaction, (normal) velocity and pressure are continuous, and entropy is constant - GFM gives suitable conditions.
- Shock waves - entropy, pressure and velocity all jump across a shock, GFM fails.

(f) Strong shock wave, large density gradients, very different material, incomplete EoS (entropy not available).

In practice, shock waves are often numerically smeared, hence there will be a continuous change in entropy which is captured reasonably well.

(g) Modified ghost fluid method:

- Sometimes the original GFM predicts a reflected rarefaction when there should be a reflected shock wave.
- Looking at Riemann problem solution can give information about when this would happen.
- It uses characteristic equations to approximate RP solution.

Explicit simplified interface method:

- Original GFM cannot handle entropy gradients across the interface.
- Physically, ESIM allows GFM to deal with temperature gradients.
- ESIM uses jump conditions of derivatives to allow linear extrapolation of entropy.

Real ghost fluid method:

- Similar to modified GFM, solves a Riemann problem to obtain the solution.
- In this case, the entire intermediate state of the mixed-material RP is computed.
- This ensures that we have a thermodynamically reasonable state within the ghost cell.

(h) **Should a GFM be applied before or after the time step is computed?**
Before. Since we might need to make a ghost fluid cell a real cell due to interface moving, we need to ensure the time step allows for suitable evolution of this cell.

(i) **Should a GFM be applied before or after the domain B.C. are computed?**
Either. At material boundaries, there will always be loss of information as to the shape of the interface. This means that conditions will always be a bit inaccurate.

How do you validate a Ghost Fluid Method? Shock tube test
If a shock wave hits a material interface, we expect:

(a) Transmitted shock wave

(b) Reflected rarefaction

(c) Advection of interface

5.3 Q3

3. (a) **Conservation errors**:

Sharp interface methods

- The level set equation is not in C. form, but it is a HJ equation, so no C. errors.
- Error comes from having only one material in a computational cell.
- When the interface moves, a cell can change from one material to another.
- As these cells do not have the same mass, there is mass loss or gain every time this happens.
- As a result, this slightly change the state near the interface and introduce error.
- But it does not result in incorrect shock wave placement, as each material is still evolved with a conservative equation.
- The errors can be reduced with resolution too.

- Also, as each computational cell is only made of a single material, thin regions can disappear entirely. This will completely change behaviour as wave interactions are altered.

Diffuse interface methods

- The volume fraction equation is not written in C. form, and other equations might not be written in C. form, such as the energy equation in the cavitation model.
- This means that there might be small conservation errors as a shock wave passes over the interface.
- If the interface is sharp (i.e. α is only slightly smeared), error only affects a very small region of the domain. If volume fraction is flat, there is no practical effect.
- Increasing resolution reduces smearing, as well as error.
- Sharpening techniques like THINC, exists to further minimise these errors.
- True mixture interface might suffer worse errors.

(b) Can combine with conservation of mass to give:

$$\frac{\partial \rho\phi}{\partial t} + \boldsymbol{\nabla} \cdot (\rho\phi v) = 0$$

and treated as an advected scalar. But this requires a discontinuity at $\phi = 0$. As a result, it introduces additional error at the only part of the domain we want accurate information from the level set function.

(c)

$$\frac{\partial \phi}{\partial t} + v_x \frac{\partial \phi}{\partial x} = 0$$

Differentiate both sides w.r.t to x and let $u = \frac{\partial \phi}{\partial x}$,

$$\frac{\partial}{\partial t}\left(\frac{\partial \phi}{\partial x}\right) + \frac{\partial}{\partial x}\left(v_x \frac{\partial \phi}{\partial x}\right) = 0 \quad \Rightarrow \quad \frac{\partial u}{\partial t} + \frac{\partial (v_x u)}{\partial x} = 0$$

It is in conservative form, where $f(u) = v_x u$.

(d) The level set equation is the integral solution to a conservation law. This means ϕ cannot generally develop a discontinuity unless the corresponding conservation law develops a delta function, which is physically unlikely. Thus, solution ϕ are typically smooth.

(e)
- l refers to liquid phase, g refers to gaseous phase.
- α is volume fraction.
- ρ, p, ε are density, pressure and specific internal energy for each phase.
- v_x is the single v-x velocity for the mixture.
- p_I is the interfacial pressure.
- μ is the pressure relaxation constant.

(f) Add another correction evolution equation to the cavitation model:

$$\frac{\partial E}{\partial t} + \frac{\partial (E+p)v_x}{\partial x} = 0$$

where E is total energy and p is the mixture pressure. This allows conservation errors in specific internal energy to be "corrected".

(g) The conservatively evolved total energy and the stiffened gas mixture rule is used to compute a mixture pressure using the equation given. Then, for each phase, the specific internal energy is computed using this mixture pressure:

$$\varepsilon_i = \varepsilon_i \left(p_{\text{mix}}, \frac{(\alpha\rho)_i}{\alpha_i} \right)$$

This term then replaces the specific internal energies in the two energy evolution equations (correction applied).

(h)

$$\sum_i \frac{\alpha_i}{\gamma_i - 1}$$

Volume weighted average of $\frac{1}{\gamma - 1}$.

$$\sum_i = \frac{\alpha_i \gamma_i p_{\infty,i}}{\gamma_i - 1}$$

Weighted average of γp_∞.

It comes from rearranging stiffened gas to obtain $\rho\varepsilon$, and determining suitable mixture rules for the various quantities. It has some similarity to the weighting in the mixture sound speed in Allaire model.

Allaire model sound speed weighting:

$$c_s^2 = \sum_i \frac{Y_i \xi_i c_{s,i}^2}{\xi}$$

6 2023-24 (EXAM)

6.1 Q1

1. Same question as 2024-25 (Mock) Q1. Link

6.2 Q2

2. (a) ρ and E are conserved quantities, their mixture rule is volume-weighted average:

$$\rho = \alpha_1\rho_1 + \alpha_2\rho_2$$

$$E = \alpha_1 E_1 + \alpha_2 E_2$$

(b) No, not required, they can be derived from mixture rules of conserved quantities.

$$v = \frac{\rho v}{\rho} = \frac{\alpha_1(\rho_1 v_1) + \alpha_2(\rho_2 v_2)}{\rho} = \frac{\alpha_1\rho_1}{\rho}v_1 + \frac{\alpha_2\rho_2}{\rho}v_2 = Y_1 v_1 + Y_2 v_2$$

$$p = (\gamma - 1)\left(E - \frac{1}{2}\frac{(\rho v)^2}{\rho}\right)$$

(c) For α_1:

$$\frac{\partial \alpha_1}{\partial t} + v\frac{\partial \alpha_1}{\partial x} = 0$$

For ρ_1:

$$\frac{\partial \alpha_1\rho_1}{\partial t} + \frac{\partial \alpha_1\rho_1 v}{\partial dx} = 0$$

$$\alpha_1\frac{\partial \rho_1}{\partial t} + \rho_1\cancel{\frac{\partial \alpha_1}{\partial t}} + \alpha_1\frac{\partial \rho_1 v}{\partial x} + \rho_1 v\cancel{\frac{\partial \alpha_1}{\partial x}} = 0$$

$$\frac{\partial \rho_1}{\partial t} + \frac{\partial \rho_1 v}{\partial x} = 0$$

$$\frac{\partial \rho_1}{\partial t} + \rho_1\frac{\partial v}{\partial x} + v\frac{\partial \rho_1}{\partial x} = 0$$

Similar for ρ_2,

$$\frac{\partial \rho_2}{\partial t} + \frac{\partial \rho_2 v}{\partial x} = 0$$

$$\frac{\partial \rho_2}{\partial t} + \rho_2\frac{\partial v}{\partial x} + v\frac{\partial \rho_2}{\partial x} = 0$$

For v:

$$\frac{\partial \rho v}{\partial t} + \frac{\partial(\rho v^2 + p)}{\partial x} = 0$$

$$\rho\frac{\partial v}{\partial t} + v\frac{\partial \rho}{\partial t} + \rho v\frac{\partial v}{\partial x} + v\frac{\partial \rho v}{\partial x} + \frac{\partial p}{\partial x} = 0$$

$$v\left(\frac{\partial \rho}{\partial t} + \frac{\partial \rho v}{\partial x}\right) + \rho\frac{\partial v}{\partial t} + \rho v\frac{\partial v}{\partial x} + \frac{\partial p}{\partial x} = 0$$

$$v\cancel{\left(\frac{\partial \alpha_i \rho_i}{\partial t} + \frac{\partial \alpha_i \rho_i v}{\partial x}\right)} + \rho \frac{\partial v}{\partial t} + \rho v \frac{\partial v}{\partial x} + \frac{\partial p}{\partial x} = 0$$

$$\frac{\partial v}{\partial t} + v \frac{\partial v}{\partial x} + \frac{1}{\rho} \frac{\partial p}{\partial x} = 0$$

(d)

$$\frac{\partial E}{\partial t} + \frac{\partial (E+p)v}{\partial x} = 0$$

$$\frac{\partial}{\partial t}\left(\rho\varepsilon + \frac{1}{2}\rho v^2\right) + \frac{\partial}{\partial x}\left(\rho\varepsilon v + \frac{1}{2}\rho v^3 + pv\right) = 0$$

$$\cancel{\varepsilon \frac{\partial \rho}{\partial t}} + \rho \frac{\partial \varepsilon}{\partial t} + \cancel{\frac{1}{2}\rho v \frac{\partial v}{\partial t}} + \cancel{\frac{1}{2} v \frac{\partial \rho v}{\partial t}} + \rho v \frac{\partial \varepsilon}{\partial x} + \cancel{\varepsilon \frac{\partial \rho v}{\partial x}} + \cancel{\frac{1}{2} v \frac{\partial \rho v^2}{\partial x}} + \cancel{\frac{1}{2}\rho v^2 \frac{\partial v}{\partial x}} + p \frac{\partial v}{\partial x} + \cancel{v \frac{\partial p}{\partial x}} = 0$$

$$\cancel{\frac{1}{2} v \left[\frac{\partial \rho v}{\partial t} + \frac{\partial \rho v^2}{\partial x} + \frac{\partial p}{\partial x}\right]} + \cancel{\varepsilon \left[\frac{\partial \rho}{\partial t} + \frac{\partial \rho v}{\partial x}\right]} + \cancel{\frac{1}{2}\rho v \left[\frac{\partial v}{\partial t} + v \frac{\partial v}{\partial x} + \frac{1}{\rho}\frac{\partial p}{\partial x}\right]} + \rho \frac{\partial \varepsilon}{\partial t} + \rho v \frac{\partial \varepsilon}{\partial x} + p \frac{\partial v}{\partial x} = 0$$

$$\rho \frac{\partial \varepsilon}{\partial t} + \rho v \frac{\partial \varepsilon}{\partial x} + p \frac{\partial v}{\partial x} = 0$$

Consider $p = p(\alpha_1, \alpha_1\rho_1, \alpha_2\rho_2, \rho\varepsilon)$,

Taking derivative w.r.t. t:

$$\frac{\partial p}{\partial t} = \frac{\partial p}{\partial \alpha_1}\frac{\partial \alpha_1}{\partial t} + \frac{\partial p}{\partial \alpha_1\rho_1}\frac{\partial \alpha_1\rho_1}{\partial t} + \frac{\partial p}{\partial \alpha_2\rho_2}\frac{\partial \alpha_2\rho_2}{\partial t} + \frac{\partial p}{\partial \rho\varepsilon}\frac{\partial \rho\varepsilon}{\partial t}$$

Taking derivative w.r.t. x:

$$\frac{\partial p}{\partial x} = \frac{\partial p}{\partial \alpha_1}\frac{\partial \alpha_1}{\partial x} + \frac{\partial p}{\partial \alpha_1\rho_1}\frac{\partial \alpha_1\rho_1}{\partial x} + \frac{\partial p}{\partial \alpha_2\rho_2}\frac{\partial \alpha_2\rho_2}{\partial x} + \frac{\partial p}{\partial \rho\varepsilon}\frac{\partial \rho\varepsilon}{\partial x}$$

$$\begin{aligned}\frac{\partial p}{\partial t} + v\frac{\partial p}{\partial x} = {} & \frac{\partial p}{\partial \alpha_1}\cancel{\left(\frac{\partial \alpha_1}{\partial t} + v\frac{\partial \alpha_1}{\partial x}\right)} + \frac{\partial p}{\partial \alpha_1\rho_1}\left(\frac{\partial \alpha_1\rho_1}{\partial t} + v\frac{\partial \alpha_1\rho_1}{\partial x}\right) \\ & + \frac{\partial p}{\partial \alpha_2\rho_2}\left(\frac{\partial \alpha_2\rho_2}{\partial t} + v\frac{\partial \alpha_2\rho_2}{\partial x}\right) + \frac{\partial p}{\partial \rho\varepsilon}\left(\frac{\partial \rho\varepsilon}{\partial t} + v\frac{\partial \rho\varepsilon}{\partial x}\right)\end{aligned}$$

$$\begin{aligned} = {} & \frac{\partial p}{\partial \alpha_1\rho_1}\left(\cancel{\frac{\partial \alpha_1\rho_1}{\partial t}} + \cancel{\frac{\partial \alpha_1\rho_1 v}{\partial x}} - \alpha_1\rho_1\frac{\partial v}{\partial x}\right) \\ & + \frac{\partial p}{\partial \alpha_2\rho_2}\left(\cancel{\frac{\partial \alpha_2\rho_2}{\partial t}} + \cancel{\frac{\partial \alpha_2\rho_2 v}{\partial x}} - \alpha_2\rho_2\frac{\partial v}{\partial x}\right) \\ & + \frac{\partial p}{\partial \rho\varepsilon}\left(\rho\frac{\partial \varepsilon}{\partial t} + \varepsilon\frac{\partial \rho}{\partial t} + \rho v\frac{\partial \varepsilon}{\partial x} + v\varepsilon\frac{\partial \rho}{\partial x}\right)\end{aligned}$$

$$\begin{aligned} = {} & \frac{\partial p}{\partial \alpha_1\rho_1}\left(-\alpha_1\rho_1\frac{\partial v}{\partial x}\right) + \frac{\partial p}{\partial \alpha_2\rho_2}\left(-\alpha_2\rho_2\frac{\partial v}{\partial x}\right) + \frac{\partial p}{\partial \rho\varepsilon}\left(\varepsilon\frac{\partial \rho}{\partial t} + v\varepsilon\frac{\partial \rho}{\partial x} - p\frac{\partial v}{\partial x}\right) \\ = {} & \frac{\partial p}{\partial \alpha_1\rho_1}\left(-\alpha_1\rho_1\frac{\partial v}{\partial x}\right) + \frac{\partial p}{\partial \alpha_2\rho_2}\left(-\alpha_2\rho_2\frac{\partial v}{\partial x}\right) + \frac{\partial p}{\partial \rho\varepsilon}\left(\cancel{\varepsilon\frac{\partial \rho}{\partial t}} + \cancel{\varepsilon\frac{\partial \rho v}{\partial x}} - \rho\varepsilon\frac{\partial v}{\partial x} - p\frac{\partial v}{\partial x}\right) \\ = {} & \frac{\partial p}{\partial \alpha_1\rho_1}\left(-\alpha_1\rho_1\frac{\partial v}{\partial x}\right) + \frac{\partial p}{\partial \alpha_2\rho_2}\left(-\alpha_2\rho_2\frac{\partial v}{\partial x}\right) + \frac{\partial p}{\partial \rho\varepsilon}\left(-\rho h\frac{\partial v}{\partial x}\right)\end{aligned}$$

Hence,

$$\frac{\partial p}{\partial t} + v\frac{\partial p}{\partial x} + \left(\rho h \frac{\partial p}{\partial \rho\varepsilon} + \alpha_1\rho_1 \frac{\partial p}{\partial \alpha_1\rho_1} + \alpha_2\rho_2 \frac{\partial p}{\partial \alpha_2\rho_2}\right)\frac{\partial v}{\partial x} = 0$$

(e) h is the enthalpy. From thermodynamics, $h = u + pv$.

(f) It can be interpreted as the mixture sound speed.

(g) Stiffened gas EoS:

$$p = (\gamma - 1)\rho\varepsilon - \gamma p_\infty$$

Since material 1 and material 2 are identical, $\rho_1 = \rho_2 = \rho$, and p is independent of $\alpha_1\rho_1$ and $\alpha_2\rho_2$,

$$\begin{aligned}
\rho h \frac{\partial p}{\partial \rho\varepsilon} + \alpha_1\rho_1 \frac{\partial p}{\partial \alpha_1\rho_1} + \alpha_2\rho_2 \frac{\partial p}{\partial \alpha_2\rho_2} &= \rho h \frac{\partial p}{\partial \rho\varepsilon} \\
&= \rho h(\gamma - 1) \\
&= (\gamma - 1)(\rho\varepsilon + p) \\
&= (\gamma - 1)\left(\frac{p + \gamma p_\infty}{\gamma - 1} + p\right) \\
&= (\gamma - 1)\left(\frac{p + \gamma p_\infty + \gamma p - p}{\gamma - 1}\right) \\
&= \rho\frac{\gamma(p + p_\infty)}{\rho} = \rho c_s^2
\end{aligned}$$

(h) **Incorporating additional physics into diffuse interface model - compaction**
Compaction is compressing one material in a volume more than the other.

For example, in a water-air mixture, if the pressure in a cell increase, we would expect more compression of the air than the water. This means that volume fraction of water should increase because of pressure changes, not just advection with velocity. This can be captured by including the compaction source term in the volume fraction equation:

$$\frac{\partial \alpha_1}{\partial t} + v\frac{\partial \alpha_1}{\partial x} + K\boldsymbol{\nabla}\cdot\boldsymbol{v} = 0$$

where:

$$K = \alpha_1\alpha_2\frac{\rho_1 c_1^2 - \rho_2 c_2^2}{\alpha_1\rho_1 c_1^2 + \alpha_2\rho_2 c_2^2}$$

(i) **Drawbacks of Allaire model over other diffuse interface models**.

- It is constructed assuming a sharp interface, but treated in a diffuse manner.
- Ideal gas will start mixing and the assumption by Allaire model is no longer accurate.
- However, it is timescale dependent. Over very short times, this assumption holds, since moving would be minimal.

6.3 Q3

3. (a) Take x-derivative:

$$\frac{\partial}{\partial x}\left(\frac{\partial \phi}{\partial t}\right)+\frac{\partial}{\partial x}H\left(\frac{\partial \phi}{\partial x}\right)=0$$

$$\frac{\partial}{\partial t}\left(\frac{\partial \phi}{\partial x}\right)+\frac{\partial}{\partial x}\left[H\left(\frac{\partial \phi}{\partial x}\right)\right]=0$$

$$\frac{\partial u}{\partial t}+\frac{\partial H(u)}{\partial x}=0$$

where $u=\frac{\partial \phi}{\partial x}$.

(b) Combining level set evolution with conservation of mass:

$$\rho\frac{\partial \phi}{\partial t}+\rho v\frac{\partial \phi}{\partial x}+\phi\frac{\partial \rho}{\partial t}+\phi\frac{\partial \rho v}{\partial x}=0$$

$$\frac{\partial \rho\phi}{\partial t}+\frac{\partial \rho\phi v}{\partial x}=0$$

(c)
- **Argument why Hamilton-Jacobi is a good form.**
  Part (a) is conservation law for spatial derivative of ϕ. It shows that the HJ equation is an integral solution to a conservation law. The level set function will only have discontinuity if the solution from the conservation law is a delta function. However, physically, we are unlikely to get a delta function. This means we can solve the HJ directly, without worrying about discontinuities arising from smooth initial data.

- Part (b) is a way to put the level set equation in conservative form for material interfaces. Density is discontinuous between liquid and gas i.e. contact discontinuity, so we get unnecessary smearing error at the interface, which is the only place we need the method to be accurate.

  And the whole point of the level set method is to identify the motion of the interface between two materials.
- It is far more accurate to use a non-conservative, non-discontinuous form of the equation that automatically introduce a discontinuity there and revert to first-order methods.

(d) Reinitialisation returns a level set function to a signed-distance function, while maintaining the position of the zero-contour. Advection of ϕ with non-constant material velocity may cause it to become too smeared or too steep. If too steep, it resembles a discontinuity and our non-conservation method fails. If too smeared, it is easy to introduce errors.

(e) Reinitialisation involves solving:

$$|\boldsymbol{\nabla}\phi|=1$$

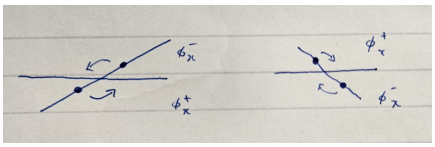
which is a form of Eikonal equation.

- It is a steady state hyperbolic equation. For the level set equation, information propagates out from the boundary with speed 1.
- It has applications in describing path of light in complex medium.

(f) τ is the fictitious time. We achieve reinitialisation by evolving a solution to a steady state. At steady state, the time derivative vanishes, hence we have found a solution that satisfies the Eikonal equation.

(g) **Iterative reinitialisation**

- We approximate the derivatives to first-order, since we are aiming for a first-order numerical method.
- The PDE will evolve to a steady state provided the slopes of ϕ are always calculated in the upwind direction (remember: information propagate outward from the interface).



- The sign of $\text{sgn}(\phi)\frac{\partial \phi}{\partial x}$ tells us which is the upwind direction.

$$\phi_x = \begin{cases} \phi^-_{x,i} = \frac{\phi_{i,j}-\phi_{i-1,j}}{\Delta x} & \text{, if } \text{sgn}(\phi)\frac{\partial \phi}{\partial x} \geq 0 \\ \phi^+_{x,i} = \frac{\phi_{i+1,j}-\phi_{i,j}}{\Delta x} & \text{, if } \text{sgn}(\phi)\frac{\partial \phi}{\partial x} < 0 \end{cases}$$

- Similarly for the y-direction, the sign of $\text{sgn}(\phi)\frac{\partial \phi}{\partial y}$ tells us which is the upwind direction.

$$\phi_y = \begin{cases} \phi^-_{y,j} = \frac{\phi_{i,j}-\phi_{i,j-1}}{\Delta y} & \text{, if } \text{sgn}(\phi)\frac{\partial \phi}{\partial y} \geq 0 \\ \phi^+_{y,j} = \frac{\phi_{i,j+1}-\phi_{i,j}}{\Delta y} & \text{, if } \text{sgn}(\phi)\frac{\partial \phi}{\partial y} < 0 \end{cases}$$

-

$$\frac{\phi^{n+1}_{i,j} - \phi^n_{i,j}}{\Delta t} + \frac{\text{sgn}(\phi)}{\sqrt{\phi_x^2 + \phi_y^2}}\left(\phi_x^2 + \phi_y^2\right) = \text{sgn}(\phi)$$

$$\frac{\phi^{n+1}_{i,j} - \phi^n_{i,j}}{\Delta t} = \text{sgn}(\phi)\left[1 - \frac{\phi_x^2 + \phi_y^2}{\sqrt{\phi_x^2 + \phi_y^2}}\right]$$

$$\phi^{n+1}_{i,j} = \phi^n_{i,j} + \Delta t \times \text{sgn}(\phi)\left[1 - \frac{\phi_x^2 + \phi_y^2}{\sqrt{\phi_x^2 + \phi_y^2}}\right]$$

- Perform this iteration until a steady state is obtained:

$$|\phi^{n+1}_{i,j} - \phi^n_{i,j}| < \epsilon$$

where ϵ is a self-defined small number.

(h) Using second-order or higher method will increase spatial accuracy by providing better numerical approximation to ϕ_x^- and ϕ_x^+.

- Central differencing is unstable with forward Euler time discretisation and the usual CFL condition with $\Delta t \sim \Delta x$.
- ENO/WENO
- We can achieve stability with a higher-order temporal discretisation such as third-order accurate Runge-Kutta method

Yes, it is used in practice as it is easy to code and can be extended to higher orders easily.

7 2024-25 (Mock)

7.1 Q1

1. (a) Zero-strength left-moving wave, same state as the left state:

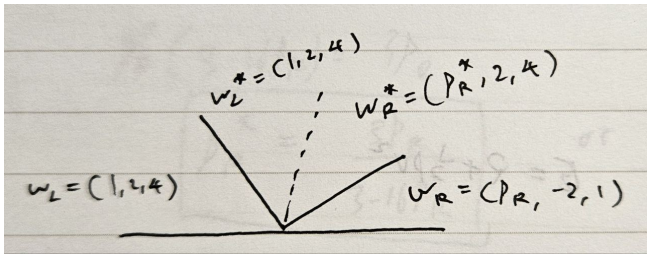
$$\boldsymbol{w}_L^* = (1, 2, 4)^T$$

(b)

$$\frac{\partial}{\partial t}\underbrace{\begin{pmatrix}\rho\\ \rho v\\ E\end{pmatrix}}_{\boldsymbol{u}} + \frac{\partial}{\partial x}\underbrace{\begin{pmatrix}\rho v\\ \rho v^2 + p\\ (E+p)v\end{pmatrix}}_{\boldsymbol{f}} = 0$$

S is the shock speed.

(c)



$$E = \frac{p}{\gamma - 1} + \frac{1}{2}\rho v^2 = p + \frac{1}{2}\rho v^2$$

Write RH conditions in vector form:

$$\begin{pmatrix}2\rho_R^*\\ 4\rho_R^* + 4\\ (8 + \frac{1}{2}\cdot 4\rho_R^*)\cdot 2\end{pmatrix} - \begin{pmatrix}-2\rho_R\\ 4\rho_R + 1\\ (2 + \frac{1}{2}\cdot 4\rho_R)\cdot(-2)\end{pmatrix} = S\left[\begin{pmatrix}\rho_R^*\\ 2\rho_R^*\\ 4 + \frac{1}{2}\cdot 4\rho_R^*\end{pmatrix} - \begin{pmatrix}\rho_R\\ -2\rho_R\\ 1 + \frac{1}{2}\cdot 4\rho_R\end{pmatrix}\right]$$

$$\begin{pmatrix}2(\rho_R^* + \rho_R)\\ 4(\rho_R^* - \rho_R) + 3\\ 4(4 + \rho_R^* + 1 + \rho_R)\end{pmatrix} = S\begin{pmatrix}\rho_R^* - \rho_R\\ 2\rho_R^* + 2\rho_R\\ 3 + 2\rho_R^* - 2\rho_R\end{pmatrix}$$

$$\begin{pmatrix}2(\rho_R^* + \rho_R)\\ 4(\rho_R^* - \rho_R) + 3\\ 4(5 + \rho_R^* + \rho_R)\end{pmatrix} = S\begin{pmatrix}\rho_R^* - \rho_R\\ 2\rho_R^* + 2\rho_R\\ 3 + 2\rho_R^* - 2\rho_R\end{pmatrix}$$

From (1):

$$S = 2\frac{\rho_R^* + \rho_R}{\rho_R^* - \rho_R}$$

Substitute S into (2):

$$4(\rho_R^* - \rho_R) + 3 = 2\frac{\rho_R^* + \rho_R}{\rho_R^* - \rho_R}\cdot 2(\rho_R^* + \rho_R)$$

$$4(\rho_R^* - \rho_R)^2 + 3(\rho_R^* - \rho_R) = 4(\rho_R^* + \rho_R)^2$$
$$-8\rho_R^*\rho_R + 3(\rho_R^* - \rho_R) = 8\rho_R^*\rho_R$$
$$3\rho_R^* - 3\rho_R = 16\rho_R^*\rho_R$$
$$\rho_R^*(3 - 16\rho_R) = 3\rho_R$$
$$\rho_R^* = \frac{3\rho_R}{3 - 16\rho_R}$$

Substitute S into (3):

$$4(5 + \rho_R^* + \rho_R) = 2\frac{\rho_R^* + \rho_R}{\rho_R^* - \rho_R}(3 + 2\rho_R^* - 2\rho_R)$$
$$20(\rho_R^* - \rho_R) + \cancel{4(\rho_R^* + \rho_R)(\rho_R^* - \rho_R)} = 6(\rho_R^* + \rho_R) + \cancel{4(\rho_R^* + \rho_R)(\rho_R^* - \rho_R)}$$
$$14\rho_R^* = 26\rho_R$$
$$\rho_R^* = \frac{13}{7}\rho_R$$

Hence,

$$\frac{13}{7}\rho_R = \frac{3\rho_R}{3 - 16\rho_R}$$
$$\frac{21}{13} = 3 - 16\rho_R$$
$$\rho_R = \frac{1}{16}\left(3 - \frac{21}{13}\right) = \frac{9}{104}$$

Then,

$$\rho_R^* = \frac{9}{56}$$
$$\boldsymbol{w}_R^* = \left(\frac{9}{56}, 2, 4\right)$$

And,

$$S = \frac{20}{3}$$

(d) GFM provides dynamics boundary conditions at the interface between two materials, at which the interface is sharp and implicitly represented.
Advantages: allows for an interface between two material with different equation of state. Single-material solution might introduce error from smearing.
Disadvantages: ...

(e) Pressure and velocity is copied.

$$p_G = 1$$

Constant entropy extrapolation, from $s = c_v \ln p + c_p \ln v + \text{const} = c_v \ln p + \gamma c_v \ln v + \text{const}$:

$$\frac{p}{\rho^\gamma} = \text{const}$$
$$\frac{p_G}{\rho_G^\gamma} = \frac{p_I}{\rho_I^\gamma}$$

$$\rho_G = \rho_I \left(\frac{p_G}{p_I}\right)^{1/\gamma}$$

Ghost fluid of the left material to the right of the interface:

$$\rho_{G,L} = 1\left(\frac{1}{4}\right)^{1/2} = \frac{1}{2}$$

$$\boldsymbol{w}_{G,L} = \left(\frac{1}{2}, -2, 1\right)$$

Ghost fluid of the right material to the left of the interface:

$$\rho_{G,R} = \frac{1}{10}\left(\frac{4}{1}\right)^{1/2} = \frac{1}{5}$$

$$\boldsymbol{w}_{G,R} = \left(\frac{1}{5}, 2, 4\right)$$

(f) For $\frac{1}{10}$, we get two shocks, the basic ghost fluid method would fail to give a correct solution as entropy jumps across the shock, violating the assumption of the basic GFM.

For $\frac{1}{12}$, we get left-moving rarefaction and right-moving shock, it gives correct behaviour for the rarefaction but not the shock wave.

(g) Yes, the exact Riemann solver can give the correct solution for shock wave.

(h) No, HLL does not include contact discontinuity which needs to be included.

7.2 Q2

2. Same question as 2022-23 (MOCK) Q2. Link

7.3 Q3

3. Same question as 2021-22(EXAM) Q3. Link

8 Appendix

8.1 Allaire Model

It is well known that the seven-equation model is the most complete and general model although it exhibits a complex wave pattern as a consequence of the source terms nature. Relaxation procedure are employed to deal with the different length and time scales for velocity and pressure equilibration. Kapila proposed an asymptotic reduction of the seven equation model under stiff mechanical relaxation in order to obtain a model with a single velocity and a single pressure. The result is a five equation model, with a non-conservative volume fraction transport equation, two mass balances, and one momentum and energy balance equation.

$$\frac{\partial \alpha_1}{\partial t} + \boldsymbol{u} \cdot \boldsymbol{\nabla} \alpha_1 + K \boldsymbol{\nabla} \cdot \boldsymbol{u} = 0$$

$$\frac{\partial \alpha_1 \rho_1}{\partial t} + \boldsymbol{\nabla} \cdot (\alpha_1 \rho_1 u) = 0 \quad , \quad \frac{\partial \alpha_2 \rho_2}{\partial t} + \boldsymbol{\nabla} \cdot (\alpha_2 \rho_2 u) = 0$$

$$\frac{\partial \rho \boldsymbol{u}}{\partial t} + \boldsymbol{\nabla} \cdot (\rho \boldsymbol{u} \otimes \boldsymbol{u} + p \boldsymbol{I}) = 0$$

$$\frac{\partial \rho e}{\partial t} + \boldsymbol{\nabla} \cdot [(E + p) v] = 0$$

However, the five-equation is not closed. A possible way to understand how this missing closure relation acts in the system is to recognise that it is not possible to compute the pressure p with the sole knowledge of conserved quantities. The primitive variable formulation to attain closure is by defining a mixture EoS:

$$p = p(\alpha_1, \alpha_1 \rho_1, \alpha_2 \rho_2, \rho \varepsilon)$$

Remarks:

- If the volume fraction takes only values 0 or 1, it means it describes a sharp interface. Then, Equation (1), (2) and (5) are redundant (only 2 of them are independent). The five-equation model reduces to the four-equation model.
- Always conserves mass.
- The model can be easily extended to treat more than two fluids by adding a mass conservation equation and a volume fraction advection equation for each new fluid.

Determination of sound speed not trivial

$$\text{Wood's formula:} \quad \frac{1}{\rho c_{eq}^2} = \frac{\alpha_1}{\rho_1 c_1^2} + \frac{\alpha_2}{\rho_2 c_2^2}$$

This expression assumes the two phases are fully mixed at the same pressure and temperature. It is non-monotonic and the mixture equilibrium sound speed can eventually become smaller than the ones in pure fluid. Sound speed is now undermined. Using this expression for the sound speed cause oscillations at the interface. We need to identify the correct mixutre sound speed. Link

Numerical Method Algorithm

1. Build the primitive variable
2. Use MUSCL (or WENO) to reconstruct the primitive variable (linear reconstruction and half-timestep update).

$$\bar{\boldsymbol{w}}_i^R = \boldsymbol{w}_i^n + \frac{1}{2}\xi(r)\boldsymbol{\Delta}_i \quad \text{and} \quad \bar{\boldsymbol{w}}_i^L = \boldsymbol{w}_i^n - \frac{1}{2}\xi(r)\boldsymbol{\Delta}_i$$

where $\boldsymbol{\Delta}_i = \frac{1}{2}\boldsymbol{\Delta}_{i-1/2} + \frac{1}{2}\boldsymbol{\Delta}_{i+1/2}$, such that $\boldsymbol{\Delta}_{i-1/2} = \boldsymbol{w}_i^n - \boldsymbol{w}_{i-1}^n$ and $\boldsymbol{\Delta}_{i+1/2} = \boldsymbol{w}_{i+1}^n - \boldsymbol{w}_i^n$

$$\bar{\boldsymbol{w}}_i^{R,n+1/2} = \boldsymbol{w}_i^R - \frac{1}{2}\frac{\Delta t}{\Delta x}B(\boldsymbol{w}_i)\xi(r)\boldsymbol{\Delta}_i \quad \text{and} \quad \bar{\boldsymbol{w}}_i^{L,n+1/2} = \boldsymbol{w}_i^L - \frac{1}{2}\frac{\Delta t}{\Delta x}B(\boldsymbol{w}_i)\xi(r)\boldsymbol{\Delta}_i$$

where $B(\boldsymbol{w}_i)$ is the primitive variable matrix.

3. Build the conserved variables, $\boldsymbol{q}_i^R$ and $\boldsymbol{q}_i^L$ from the reconstructed primitive variables.
4. Use the adapted HLLC approximate Riemann solver to compute the numerical flux.

$$\boldsymbol{f}_{i+1/2}^n = \boldsymbol{f}_{i+1/2}^n\left(\bar{\boldsymbol{q}}_i^R, \bar{\boldsymbol{q}}_{i+1}^L\right)$$

$$\boldsymbol{q}_K^* = \left(\frac{S_K - u_K}{S_K - S^*}\right)\begin{pmatrix} \alpha_{1K} \\ (\alpha_1\rho_1)_K \\ (\alpha_2\rho_2)_K \\ \rho_K S^* \\ E_K + (S^* - u_K)\left(\rho_K S^* + \frac{p_K}{S_K - u_K}\right) \end{pmatrix}$$

where:

$$S^* = \frac{p_R - p_L + \rho_L u_L(S_L - u_L) - \rho_R u_R(S_R - u_R)}{\rho_L(S_L - u_L) - \rho_R(S_R - u_R)}$$

with $S^+ = \max(|u_L| + c_{s,L}, |v_R| + c_{s,R})$ and $S_L = -S^+$, $S_R = S^+$

Finally,

$$\boldsymbol{f}_{i+1/2}^{HLLC} = \begin{cases} \boldsymbol{f}_L & , 0 \le S_L \\ \boldsymbol{f}_L + S_L(\boldsymbol{q}_L^* - \boldsymbol{q}_L) & , S_L < 0 \le S^* \\ \boldsymbol{f}_R + S_R(\boldsymbol{q}_R^* - \boldsymbol{q}_R) & , S^* < 0 \le S_R \\ \boldsymbol{f}_R & , 0 > S_R \end{cases}$$

5. March forward in time.

$$\boldsymbol{q}_i^{n+1} = \boldsymbol{q}_i^n - \frac{\Delta t}{\Delta x}(\boldsymbol{f}_{i+1/2}^{HLLC} - \boldsymbol{f}_{i-1/2}^{HLLC})$$

Also, perform a source term update for the volume fraction equation:

$$\frac{\partial \alpha_1}{\partial t} + \boldsymbol{\nabla}\cdot(\alpha_1\boldsymbol{u}) = \alpha_1\boldsymbol{\nabla}\cdot\boldsymbol{u}$$

$$\alpha_{1,i}^{n+1} = \bar{\alpha}_i^{n+1} + \frac{\Delta t}{\Delta x}a_{1,i}^n(S_{i+1/2} - S_{i-1/2})$$

8.2 Hamilton-Jacobi Equations

$$\phi_t + H(\boldsymbol{\nabla}\phi) = 0 \quad \Rightarrow \quad \phi_t + H(\phi_x, \phi_y, \phi_z) = 0$$

By taking spatial derivative of the entire equation, we can show that the solution ϕ to a Hamilton-Jacobi equation is the integral of a solution, u, to a conservation law, $u_t + H(u)_x = 0$.

- Integral of discontinuity is a kink (i.e. discontinuity in the first derivative), so solutions to HJ can develop kinks in the solution even if the data are initially smooth.
- Solutions to HJ equations cannot generally develop a discontinuity unless the corresponding conservation law develops a delta function, which is physically unlikely. Thus, solution ϕ are typically smooth.

Numerical discretisation

$$\frac{\phi^{n+1} - \phi^n}{\Delta t} + \hat{H}^n(\phi_x^-, \phi_x^+, \phi_y^-, \phi_y^+, \phi_z^-, \phi_z^+) = 0$$

CFL condition $C = \frac{a\Delta t}{\Delta x} \leq 1$:

$$\Delta t \max_i \left(\frac{|H_i^x|}{\Delta x} + \frac{|H_i^y|}{\Delta y} + \frac{|H_i^z|}{\Delta z} \right) < 1$$

How should we approximate $\hat{H}$? (assuming 2D)

1. Lax-Friedrichs Schemes:

$$\hat{H} = H\left(\frac{\phi_x^- + \phi_x^+}{2}, \frac{\phi_y^- + \phi_y^+}{2} \right) - \alpha^x \left(\frac{\phi_x^+ - \phi_x^-}{2} \right) - \alpha^y \left(\frac{\phi_y^+ - \phi_y^-}{2} \right)$$

   where $\alpha^{x,y}$ are dissipation coefficients that control the amount of numerical viscosity.

$$\alpha^x = \max_i |H^x(\phi_x, \phi_y)| \quad , \quad \alpha^y = \max_i |H^y(\phi_x, \phi_y)|$$

   Further extensions such as Local Lax-Friedrichs (LLF) and Local Local Lax-Friedrichs (LLLF) are designed to further reduce numerical dissipation.

2. Roe-Fix Schemes:

$$\hat{H} = H(\phi_x^*, \phi_y^*) - \alpha^x \left(\frac{\phi_x^+ - \phi_x^-}{2} \right) - \alpha^y \left(\frac{\phi_y^+ - \phi_y^-}{2} \right)$$

3. Godunov's Scheme:

$$\hat{H} = \text{ext}_x \text{ext}_y H(\phi_x, \phi_y)$$

8.3 Hamilton-Jacobi ENO/WENO Method

$$\text{Level set equation: } \frac{\phi_i^{n+1}-\phi_i^n}{\Delta t}+v_{x,i}^n\left(\frac{\partial\phi}{\partial x}\right)_i^n+v_{y,i}^n\left(\frac{\partial\phi}{\partial y}\right)_i^n+v_{z,i}^n\left(\frac{\partial\phi}{\partial z}\right)_i^n=0$$

First-order upwind difference:

$$\left(\frac{\partial\phi}{\partial x}\right)_i^n=\begin{cases}\phi_{x,i}^+=D_{i+1/2}^1 & ,\text{if } v_{x,i}<0\\ \phi_{x,i}^-=D_{i-1/2}^1 & ,\text{if } v_{x,i}>0\end{cases}$$

Numerical methods for HJ equation is still just a matter of choosing approximations for $\phi_{x,y,z}^{\pm}$. We get to higher-order spatial accuracy by providing better numerical approximations to ϕ_x^- and ϕ_x^+.

Divided difference notation:

$$D_i^0=\phi_i \quad \text{(at grid nodes)}$$

$$D_{i+1/2}^1\phi=\frac{D_{i+1}^0\phi-D_i^0\phi}{\Delta x}=\frac{\phi_{i+1}-\phi_i}{\Delta x} \quad \text{(midway grid nodes)}$$

$$D_i^2\phi=\frac{D_{i+1/2}^1\phi-D_{i-1/2}^1\phi}{2\Delta x}=\frac{\frac{D_{i+1}^0\phi-D_i^0\phi}{\Delta x}-\frac{D_i^0\phi-D_{i-1}^0\phi}{\Delta x}}{2\Delta x}=\frac{\phi_{i+1}-2\phi_i+\phi_{i-1}}{2\Delta x^2} \quad \text{(at grid nodes)}$$

$$D_{i+1/2}^3\phi=\frac{D_{i+1}^2\phi-D_i^2\phi}{3\Delta x}=\frac{\frac{\phi_{i+2}-2\phi_{i+1}+\phi_i}{2\Delta x^2}-\frac{\phi_{i+1}-2\phi_i+\phi_{i-1}}{2\Delta x^2}}{3\Delta x}=\frac{\phi_{i+2}-3\phi_{i+1}+3\phi_i-\phi_{i-1}}{3!\Delta x^3} \quad \text{(midway)}$$

Hamilton-Jacobi ENO method

Origin: Harten proposed the idea of essentially nonoscillatory (ENO) polynomial interpolation of data for the numerical solution of C. laws. The basic idea was to compute the numerical flux functions using the smoothest possible polynomial interpolants. After Osher and Sethain realise that the HJ equations in 1D are integrals of conservation laws, they applied the ENO method to HJ equations.

Goal of HJ ENO: Choose the single approximation with the least error by selecting the smoothest stencil for approximation of ϕ (differentiate to get ϕ_x) thus avoiding undue oscillations.

$$\phi_{x,i}=Q_1'(x_i)+Q_2'(x_i)+Q_3'(x_i)$$

To find ϕ_x^- $(v_{x,i}>0)$, we start with $k=i-1$, and to find ϕ_x^+ $(v_{x,i}<0)$ we start with $k=i$.

$$Q_1'(x_i)=D_{k+1/2}^1\phi \quad \text{(First-order contribution)}$$

Second-order accurate correction: choose $D_k^2\phi$ or $D_{k+1}^2\phi$? We want to avoid interpolating near large variations such as discontinuities or steep gradients, since they cause overshoots in the interpolating function, leading to numerical errors in the approximation of the derivative.

$$(c,k^*)=\begin{cases}(D_k^2\phi,\ k-1) & ,\text{if } |D_k^2\phi|\le|D_{k+1}^2\phi|\\ (D_{k+1}^2\phi,\ k) & ,\text{otherwise}\end{cases}$$

$$Q_2(x)=c(x-x_k)(x-x_{k+1}) \quad \Rightarrow \quad Q_2'(x_i)=c[2(i-k)-1]\Delta x$$

Proof:

$$\begin{aligned} Q_2'(x) &= c(x - x_k) + c(x - x_{k+1}) \\ &= c(2x - x_k - x_{k+1}) \\ Q_2'(x_i) &= c(2x_i - x_k - x_{k+1}) \\ &= c(2i - 2k - 1)\Delta x \end{aligned}$$

Third-order correction:

$$c^* = \begin{cases} D^3_{k^*+1/2}\phi & \text{, if } |D^3_{k^*+1/2}\phi| \leq |D^3_{k^*+3/2}\phi| \\ D^3_{k^*+3/2}\phi & \text{, otherwise} \end{cases}$$

$$Q_3(x) = c^*(x - x_{k^*})(x - x_{k^*+1})(x - x_{k^*+2}) \quad \Rightarrow \quad Q_3'(x_i) = c^* \left[3(i - k^*)^2 - 6(i - k^*) + 2\right](\Delta x)^2$$

Proof:

$$\begin{aligned} Q_3'(x) &= c^*(x - x_{k^*})(x - x_{k^*+1}) + c^*(x - x_{k^*})(x - x_{k^*+2}) + c^*(x - x_{k^*+1})(x - x_{k^*+2}) \\ Q_3'(x_i) &= c^* \left[(x_i - x_{k^*})(x_i - x_{k^*+1}) + (x_i - x_{k^*})(x_i - x_{k^*+2}) + (x_i - x_{k^*+1})(x_i - x_{k^*+2})\right] \\ &= c^* \left[(i - k^*)(i - k^* - 1) + (i - k^*)(i - k^* - 2) + (i - k^* - 1)(i - k^* - 2)\right](\Delta x)^2 \\ &= c^* \left[3(i - k^*)^2 - (i - k^*) - 2(i - k^*) - 3(i - k^*) + 2\right](\Delta x)^2 \\ &= c^* \left[3(i - k^*)^2 - 6(i - k^*) + 2\right](\Delta x)^2 \end{aligned}$$

Hamilton-Jacobi WENO method

The numerical stencil for $\phi^-_{x,i}$ is $\{\phi_{i-3}, \phi_{i-2}, \phi_{i-1}, \phi_i, \phi_{i+1}, \phi_{i+2}\}$. In fact, there are exactly 3 possible HJ ENO approximations for them. Combining all these possible options gives us the WENO method. For $\phi^-_{x,i}$:

$$v_1 = D^-\phi_{i-2} = D^1_{i-5/2}\ ,\ v_2 = D^-\phi_{i-1}\ ,\ v_3 = D^-\phi_i = D^1_{i-1/2}\ ,\ v_4 = D^-\phi_{i+1}\ ,\ v_5 = D^-\phi_{i+2}$$

The three potential HJ ENO approximations to ϕ^-_x are:

$$\phi^1_x = \frac{1}{3}v_1 - \frac{7}{6}v_2 + \frac{11}{6}v_3 \quad , \quad \phi^2_x = -\frac{1}{6}v_2 + \frac{5}{6}v_3 + \frac{1}{3}v_4 \quad , \quad \phi^3_x = \frac{1}{3}v_3 + \frac{5}{6}v_4 - \frac{1}{6}v_5$$

Proof ($k = i - 1$ and $k^* = i - 2$ and $D^3_{k^*+1/2}\phi$):

$$\begin{aligned} \phi^1_{x,i} &= D^1_{i-1/2}\phi + D^2_{i-1}\phi[2(1) - 1]\Delta x + D^3_{i-3/2}\phi[3(2)^2 - 6(2) + 2](\Delta x)^2 \\ &= D^1_{i-1/2}\phi + D^2_{i-1}\phi\Delta x + 2D^3_{i-3/2}\phi(\Delta x)^2 \\ &= v_3 + \frac{1}{2}(v_3 - v_2) + \frac{2}{3}(D^2_{i-1}\phi - D^2_{i-2}\phi)\Delta x \\ &= v_3 + \frac{1}{2}(v_3 - v_2) + \frac{1}{3}(v_3 - v_2 - v_2 + v_1) \\ &= \frac{11}{6}v_3 - \frac{7}{6}v_2 + \frac{1}{3}v_1 \end{aligned}$$

Motivation for HJ Weighted ENO: instead of choosing exactly one candidate stencils (overkill in smooth regions), take a convex combination of the three ENO approximations.

If any of the three approximations interpolates across a discontinuity, it is given minimal weight in the convex combination to minimise its contribution and the resulting errors. Otherwise, in smooth regions, all three approximations are allowed to make significant contribution in a way that improves the local accuracy from third-order up to fifth-order.

$$\phi_x = \omega_1 \phi_x^1 + \omega_2 \phi_x^2 + \omega_3 \phi_x^3$$

where $0 \leq \omega_k \leq 1$ and $\omega_1 + \omega_2 + \omega_3 = 1$.

In smooth regions, the optimal weights are:

$$\omega_1 = 0.1 \quad , \quad \omega_2 = 0.6 \quad , \quad \omega_3 = 0.3$$

we get the fifth-order approximation to $\phi_{x,i}$ and is known to provide the smallest truncation error.

To sustain both accuracy and essentially non-oscillatory property, the weights are defined according to two principles:

1. If ϕ is smooth on the whole stencil, then we require:

$$\omega_1 = 0.1 + C_1(\Delta x^2) \quad , \quad \omega_2 = 0.6 + C_2(\Delta x^2) \quad , \quad \omega_3 = 0.3 + C_3(\Delta x^2)$$

   in which case the WENO approximation is still fifth order accurate. Proof:

$$\text{Associated error: } \cancel{(C_1 + C_2 + C_3)}(\Delta x^2)(\phi_x^{1,E}) + \mathcal{O}(\Delta x^2)\mathcal{O}(\Delta x^3) = \mathcal{O}(\Delta x^5)$$

2. If the stencil contains a singularity of ϕ (discontinuity), we are better off with digital ($\omega_k = 0, 1$) weights that choose a single approximation for ϕ_x (revert to ENO) i.e. digital HJ ENO weights.

To compute the weights, we estimate the smoothness of the stencils as:

$$\begin{aligned}
S_1 &= \frac{13}{12}(v_1 - 2v_2 + v_3)^2 + \frac{1}{4}(v_1 - 4v_2 + 3v_3)^2 \\
S_2 &= \frac{13}{12}(v_2 - 2v_3 + v_4)^2 + \frac{1}{4}(v_2 - v_4)^2 \\
S_3 &= \frac{13}{12}(v_3 - 2v_4 + v_5)^2 + \frac{1}{4}(3v_3 - 4v_4 + v_5)^2
\end{aligned}$$

Define:

$$\alpha_1 = \frac{0.1}{(S_1 + \epsilon)^2} \quad , \quad \alpha_2 = \frac{0.6}{(S_2 + \epsilon)^2} \quad , \quad \alpha_3 = \frac{0.3}{(S_3 + \epsilon)^2}$$

with $\epsilon = 10^{-6}$ to avoid division by zero in the case of perfect smoothness. (a smooth solution has small variation leading to small S_k) The actual weights are obtained by normalising α_k:

$$\omega_i = \frac{\alpha_i}{\alpha_1 + \alpha_2 + \alpha_3}$$

- Nearly optimal weights are obtained as long as all the S_k are approximately the same size, as is the case for sufficiently smooth data.
- If the data is not smooth, as indicated by large S_k, then the corresponding α_k will be small compared to the other α_k's, giving that particular stencil limited influence.
- If two of the S_k are relatively large, then their corresponding α_k's will both be small, and the scheme will rely most heavily on a single stencil similar to the digital behaviour of HJ ENO.
- If all three S_k are large, the data are poorly conditioned, and none of the stencils are particularly useful. Fortunately, this usually occurs only locally in space and time, allowing the methods to repair themselves after the situation subsides.

TVD Runge-Kutta for time

EJ WENO and HJ ENO allow us to discretise the spatial terms to fifth-order accuracy, while the forward Euler time discretisation is only first-order accurate in time. In this case, spurious oscillations are often seen. This is when a higher-order temporal discretisation is necessary in order to obtain accurate numerical solutions.

- First-order accurate RK (= forward Euler method):

$$\frac{\phi_i^{n+1} - \phi_i^n}{\Delta t} + v^n \cdot \boldsymbol{\nabla} \phi^n = 0$$

- Second-order accurate RK (= Heun's predictor-corrector method): advance solution to time $t^n + \Delta t$ and $t^n + 2\Delta t$

$$\frac{\phi_i^{n+1} - \phi_i^n}{\Delta t} + v^n \cdot \boldsymbol{\nabla} \phi^n = 0 \quad , \quad \frac{\phi_i^{n+2} - \phi_i^{n+1}}{\Delta t} + v^{n+1} \cdot \boldsymbol{\nabla} \phi^{n+1} = 0$$

  followed by an averaging step:

$$\phi^{n+1} = \frac{1}{2}(\phi^n + \phi^{n+2})$$

- Third-order accurate RK: advance the solution to time $t^n + \Delta t$ and $t^n + 2\Delta t$, followed by an averaging step:

$$\phi^{n+1/2} = \frac{3}{4}\phi^n + \frac{1}{4}\phi^{n+2}$$

  Then, advance solution to time $t^n + \frac{3}{2}\Delta t$,

$$\frac{\phi_i^{n+3/2} - \phi_i^{n+1/2}}{\Delta t} + v^{n+1/2} \cdot \boldsymbol{\nabla} \phi^{n+1/2} = 0$$

  followed by a second averaging step:

$$\phi^{n+1} = \frac{1}{3}\phi^n + \frac{2}{3}\phi^{n+3/2}$$

8.4 Primitive-variable Form of Baer–Nunziato Equations

Baer–Nunziato equations:

$$\partial_t \boldsymbol{U} + \partial_x \boldsymbol{F}(\boldsymbol{U}) + \boldsymbol{B}(\boldsymbol{U})\partial_x \alpha_1 = \boldsymbol{S}(\boldsymbol{U})$$

Ignore source terms,

$$\frac{\partial \alpha_1}{\partial t} + v_I \frac{\partial \alpha_1}{\partial x} = 0$$
$$\frac{\partial \alpha_1 \rho_1}{\partial t} + \frac{\partial \alpha_1 \rho_1 v_1}{\partial x} = 0$$
$$\frac{\partial \alpha_1 \rho_1 v_1}{\partial t} + \frac{\partial \alpha_1 (\rho_1 v_1^2 + p_1)}{\partial x} = p_I \frac{\partial \alpha_1}{\partial x}$$
$$\frac{\partial \alpha_1 E_1}{\partial t} + \frac{\partial \alpha_1 (E_1 + p_1) v_1}{\partial x} = p_I v_I \frac{\partial \alpha_1}{\partial x}$$
$$\frac{\partial \alpha_2 \rho_2}{\partial t} + \frac{\partial \alpha_2 \rho_2 v_2}{\partial x} = 0$$
$$\frac{\partial \alpha_2 \rho_2 v_2}{\partial t} + \frac{\partial \alpha_2 (\rho_2 v_2^2 + p_2)}{\partial x} = p_I \frac{\partial \alpha_2}{\partial x}$$
$$\frac{\partial \alpha_2 E_2}{\partial t} + \frac{\partial \alpha_2 (E_2 + p_2) v_2}{\partial x} = p_I v_I \frac{\partial \alpha_2}{\partial x}$$

With $\boldsymbol{\omega} = (\alpha_1, \rho_1, v_1, p_1, \rho_2, v_2, p_2)$,

For α_1: trivial.

For ρ_1:

$$\alpha_1 \frac{\partial \rho_1}{\partial t} + \rho_1 \frac{\partial \alpha_1}{\partial t} + \alpha_1 \frac{\partial \rho_1 v_1}{\partial x} + \rho_1 v_1 \frac{\partial \alpha_1}{\partial x} = 0$$
$$\alpha_1 \frac{\partial \rho_1}{\partial t} - \rho_1 v_I \frac{\partial \alpha_1}{\partial x} + \alpha_1 \rho_1 \frac{\partial v_1}{\partial x} + \alpha_1 v_1 \frac{\partial \rho_1}{\partial x} + \rho_1 v_1 \frac{\partial \alpha_1}{\partial x} = 0$$
$$\frac{\partial \rho_1}{\partial t} + \frac{\rho_1}{\alpha_1}(v_1 - v_I)\frac{\partial \alpha_1}{\partial x} + v_1 \frac{\partial \rho_1}{\partial x} + \rho_1 \frac{\partial v_1}{\partial x} = 0$$

For v_1:

$$\cancel{v_1 \frac{\partial \alpha_1 \rho_1}{\partial t}} + \alpha_1 \rho_1 \frac{\partial v_1}{\partial t} + \cancel{v_1 \frac{\partial (\alpha_1 \rho_1 v_1)}{\partial x}} + \alpha_1 \rho_1 v_1 \frac{\partial v_1}{\partial x} + \frac{\partial \alpha_1 p_1}{\partial x} - p_I \frac{\partial \alpha_1}{\partial x} = 0$$
$$\alpha_1 \rho_1 \frac{\partial v_1}{\partial t} + \alpha_1 \rho_1 v_1 \frac{\partial v_1}{\partial x} + p_1 \frac{\partial \alpha_1}{\partial x} + \alpha_1 \frac{\partial p_1}{\partial x} - p_I \frac{\partial \alpha_1}{\partial x} = 0$$
$$\alpha_1 \rho_1 \frac{\partial v_1}{\partial t} + \alpha_1 \rho_1 v_1 \frac{\partial v_1}{\partial x} + (p_1 - p_I)\frac{\partial \alpha_1}{\partial x} + \alpha_1 \frac{\partial p_1}{\partial x} = 0$$
$$\frac{\partial v_1}{\partial t} + \frac{p_1 - p_I}{\alpha_1 \rho_1}\frac{\partial \alpha_1}{\partial x} + v_1 \frac{\partial v_1}{\partial x} + \frac{1}{\rho_1}\frac{\partial p_1}{\partial x} = 0$$

For p_1:

$$E_1 = \rho_1\varepsilon_1 + \frac{1}{2}\rho_1 v_1^2$$

$$\frac{\partial \alpha_1\rho_1\varepsilon_1}{\partial t} + \frac{1}{2}\frac{\partial \alpha_1\rho_1 v_1^2}{\partial t} + \frac{\partial \alpha_1\rho_1\varepsilon_1 v_1}{\partial x} + \frac{1}{2}\frac{\partial \alpha_1\rho_1 v_1^3}{\partial x} + \frac{\partial \alpha_1 p_1 v_1}{\partial x} = p_I v_I \frac{\partial \alpha_1}{\partial x}$$

$$\frac{\partial \alpha_1\rho_1\varepsilon_1}{\partial t} + \frac{\partial \alpha_1\rho_1\varepsilon_1 v_1}{\partial x} + \frac{1}{2}\frac{\partial \alpha_1\rho_1 v_1^2}{\partial t} + \frac{1}{2}\frac{\partial \alpha_1\rho_1 v_1^3}{\partial x} + \frac{\partial \alpha_1 p_1 v_1}{\partial x} = p_I v_I \frac{\partial \alpha_1}{\partial x}$$

Spot conservation of mass,

$$\frac{\partial \alpha_1\rho_1\varepsilon_1}{\partial t} + \frac{\partial \alpha_1\rho_1\varepsilon_1 v_1}{\partial x} + \frac{1}{2}\alpha_1\rho_1\frac{\partial v_1^2}{\partial t} + \frac{1}{2}\alpha_1\rho_1 v_1\frac{\partial v_1^2}{\partial x} + \frac{\partial \alpha_1 p_1 v_1}{\partial x} = p_I v_I \frac{\partial \alpha_1}{\partial x}$$

$$\frac{\partial \alpha_1\rho_1\varepsilon_1}{\partial t} + \frac{\partial \alpha_1\rho_1\varepsilon_1 v_1}{\partial x} + \alpha_1\rho_1 v_1\frac{\partial v_1}{\partial t} + \alpha_1\rho_1 v_1^2\frac{\partial v_1}{\partial x} + \frac{\partial \alpha_1 p_1 v_1}{\partial x} = p_I v_I \frac{\partial \alpha_1}{\partial x}$$

Spot conservation of mass again,

$$\alpha_1\rho_1\frac{\partial \varepsilon_1}{\partial t} + \alpha_1\rho_1 v_1\frac{\partial \varepsilon_1}{\partial x} + \alpha_1\rho_1 v_1\frac{\partial v_1}{\partial t} + \alpha_1\rho_1 v_1^2\frac{\partial v_1}{\partial x} + \frac{\partial \alpha_1 p_1 v_1}{\partial x} = p_I v_I \frac{\partial \alpha_1}{\partial x}$$

$$\alpha_1\rho_1\frac{\partial \varepsilon_1}{\partial t} + \alpha_1\rho_1 v_1\frac{\partial \varepsilon_1}{\partial x} + \alpha_1\rho_1 v_1\frac{\partial v_1}{\partial t} + \alpha_1\rho_1 v_1^2\frac{\partial v_1}{\partial x} + \alpha_1 v_1\frac{\partial p_1}{\partial x} + p_1\frac{\partial \alpha_1 v_1}{\partial x} = p_I v_I \frac{\partial \alpha_1}{\partial x}$$

Divide throughout by α_1

$$\rho_1\frac{\partial \varepsilon_1}{\partial t} + \rho_1 v_1\frac{\partial \varepsilon_1}{\partial x} + \rho_1 v_1\frac{\partial v_1}{\partial t} + \rho_1 v_1^2\frac{\partial v_1}{\partial x} + v_1\frac{\partial p_1}{\partial x} + \frac{p_1}{\alpha_1}\frac{\partial \alpha_1 v_1}{\partial x} = \frac{p_I v_I}{\alpha_1}\frac{\partial \alpha_1}{\partial x}$$

$$\rho_1\frac{\partial \varepsilon_1}{\partial t} + \rho_1 v_1\frac{\partial \varepsilon_1}{\partial x} + \rho_1 v_1\frac{\partial v_1}{\partial t} + \cancel{\rho_1 v_1^2\frac{\partial v_1}{\partial x}} + \cancel{v_1\frac{\partial p_1}{\partial x}} + p_1\frac{\partial v_1}{\partial x} + \cancel{\frac{p_1 v_1}{\alpha_1}\frac{\partial \alpha_1}{\partial x}} = \frac{p_I v_I}{\alpha_1}\frac{\partial \alpha_1}{\partial x}$$

Using v_1:

$$\frac{\partial v_1}{\partial t} = -\frac{p_1 - p_I}{\alpha_1\rho_1}\frac{\partial \alpha_1}{\partial x} - v_1\frac{\partial v_1}{\partial x} - \frac{1}{\rho_1}\frac{\partial p_1}{\partial x}$$

$$\rho_1 v_1\frac{\partial v_1}{\partial t} = -\frac{v_1(p_1 - p_I)}{\alpha_1}\frac{\partial \alpha_1}{\partial x} - \cancel{\rho_1 v_1^2\frac{\partial v_1}{\partial x}} - \cancel{v_1\frac{\partial p_1}{\partial x}}$$

After cancelling the terms, we have:

$$\rho_1\frac{\partial \varepsilon_1}{\partial t} + \rho_1 v_1\frac{\partial \varepsilon_1}{\partial x} + \frac{p_I v_1}{\alpha_1}\frac{\partial \alpha_1}{\partial x} + p_1\frac{\partial v_1}{\partial x} = \frac{p_I v_I}{\alpha_1}\frac{\partial \alpha_1}{\partial x}$$

Consider $\varepsilon_1 = \varepsilon_1(\rho_1, p_1)$,

$$\frac{\partial \varepsilon_1}{\partial t} = \frac{\partial \varepsilon_1}{\partial \rho_1}\frac{\partial \rho_1}{\partial t} + \frac{\partial \varepsilon_1}{\partial p_1}\frac{\partial p_1}{\partial t} \quad , \quad \frac{\partial \varepsilon_1}{\partial x} = \frac{\partial \varepsilon_1}{\partial \rho_1}\frac{\partial \rho_1}{\partial x} + \frac{\partial \varepsilon_1}{\partial p_1}\frac{\partial p_1}{\partial x}$$

$$\rho_1\frac{\partial \varepsilon_1}{\partial \rho_1}\left(\frac{\partial \rho_1}{\partial t} + v_1\frac{\partial \rho_1}{\partial x}\right) + \frac{\partial \varepsilon_1}{\partial p_1}\left(\rho_1\frac{\partial p_1}{\partial t} + \rho_1 v_1\frac{\partial p_1}{\partial x}\right) + \frac{p_I v_1}{\alpha_1}\frac{\partial \alpha_1}{\partial x} + p_1\frac{\partial v_1}{\partial x} = \frac{p_I v_I}{\alpha_1}\frac{\partial \alpha_1}{\partial x}$$

$$\rho_1\frac{\partial\varepsilon_1}{\partial\rho_1}\left(\frac{\partial\rho_1}{\partial t}+v_1\cancel{\frac{\partial\rho_1}{\partial x}}\right)+\frac{\partial\varepsilon_1}{\partial p_1}\left(\rho_1\frac{\partial p_1}{\partial t}+\rho_1 v_1\frac{\partial p_1}{\partial x}\right)+\frac{p_I v_1}{\alpha_1}\frac{\partial\alpha_1}{\partial x}+p_1\frac{\partial v_1}{\partial x}=\frac{p_I v_I}{\alpha_1}\frac{\partial\alpha_1}{\partial x}$$

Using ρ_1:

$$\frac{\partial\rho_1}{\partial t}=-\frac{\rho_1}{\alpha_1}(v_1-v_I)\frac{\partial\alpha_1}{\partial x}-v_1\cancel{\frac{\partial\rho_1}{\partial x}}-\rho_1\frac{\partial v_1}{\partial x}$$

$$\rho_1\frac{\partial\varepsilon_1}{\partial\rho_1}\left(-\frac{\rho_1}{\alpha_1}(v_1-v_I)\frac{\partial\alpha_1}{\partial x}-\rho_1\frac{\partial v_1}{\partial x}\right)+\frac{\partial\varepsilon_1}{\partial p_1}\left(\rho_1\frac{\partial p_1}{\partial t}+\rho_1 v_1\frac{\partial p_1}{\partial x}\right)+\frac{p_I v_1}{\alpha_1}\frac{\partial\alpha_1}{\partial x}+p_1\frac{\partial v_1}{\partial x}=\frac{p_I v_I}{\alpha_1}\frac{\partial\alpha_1}{\partial x}$$

$$\rho_1\frac{\partial\varepsilon_1}{\partial p_1}\frac{\partial p_1}{\partial t}+\left(-\frac{\rho_1^2(v_1-v_I)}{\alpha_1}\frac{\partial\varepsilon_1}{\partial\rho_1}+\frac{p_I v_1}{\alpha_1}-\frac{p_I v_I}{\alpha_1}\right)\frac{\partial\alpha_1}{\partial x}+\left(-\rho_1^2\frac{\partial\varepsilon_1}{\partial\rho_1}+p_1\right)\frac{\partial v_1}{\partial x}+\rho_1 v_1\frac{\partial\varepsilon_1}{\partial p_1}\frac{\partial p_1}{\partial x}=0$$

Note:

$$c^2=\frac{p}{\rho^2\frac{\partial\varepsilon}{\partial p}}-\frac{\frac{\partial\varepsilon}{\partial\rho}}{\frac{\partial\varepsilon}{\partial p}}=\frac{1}{\frac{\partial\varepsilon}{\partial p}}\left(\frac{p}{\rho^2}-\frac{\partial\varepsilon}{\partial\rho}\right)$$

Divide by ρ_1,

$$\frac{\partial\varepsilon_1}{\partial p_1}\frac{\partial p_1}{\partial t}+\left(-\frac{\rho_1(v_1-v_I)}{\alpha_1}\frac{\partial\varepsilon_1}{\partial\rho_1}+\frac{p_I v_1}{\rho_1\alpha_1}-\frac{p_I v_I}{\rho_1\alpha_1}\right)\frac{\partial\alpha_1}{\partial x}+\left(-\rho_1\frac{\partial\varepsilon_1}{\partial\rho_1}+\frac{p_1}{\rho_1}\right)\frac{\partial v_1}{\partial x}+v_1\frac{\partial\varepsilon_1}{\partial p_1}\frac{\partial p_1}{\partial x}=0$$

$$\frac{\partial\varepsilon_1}{\partial p_1}\frac{\partial p_1}{\partial t}+\frac{\rho_1}{\alpha_1}\left(-(v_1-v_I)\frac{\partial\varepsilon_1}{\partial\rho_1}+\frac{p_I v_1}{\rho_1^2}-\frac{p_I v_I}{\rho_1^2}\right)\frac{\partial\alpha_1}{\partial x}+\rho_1\left(\frac{p_1}{\rho_1^2}-\frac{\partial\varepsilon_1}{\partial\rho_1}\right)\frac{\partial v_1}{\partial x}+v_1\frac{\partial\varepsilon_1}{\partial p_1}\frac{\partial p_1}{\partial x}=0$$

Factoring,

$$\frac{\partial\varepsilon_1}{\partial p_1}\frac{\partial p_1}{\partial t}+\frac{\rho_1}{\alpha_1}\left(-\frac{\partial\varepsilon_1}{\partial\rho_1}+\frac{p_I}{\rho_1^2}\right)(v_1-v_I)\frac{\partial\alpha_1}{\partial x}+\rho_1\left(\frac{p_1}{\rho_1^2}-\frac{\partial\varepsilon_1}{\partial\rho_1}\right)\frac{\partial v_1}{\partial x}+v_1\frac{\partial\varepsilon_1}{\partial p_1}\frac{\partial p_1}{\partial x}=0$$

$$\frac{\partial\varepsilon_1}{\partial p_1}\frac{\partial p_1}{\partial t}+\frac{\rho_1}{\alpha_1}\left(\frac{p_I}{\rho_1^2}-\frac{\partial\varepsilon_1}{\partial\rho_1}\right)(v_1-v_I)\frac{\partial\alpha_1}{\partial x}+\rho_1\left(\frac{p_1}{\rho_1^2}-\frac{\partial\varepsilon_1}{\partial\rho_1}\right)\frac{\partial v_1}{\partial x}+v_1\frac{\partial\varepsilon_1}{\partial p_1}\frac{\partial p_1}{\partial x}=0$$

$$\frac{\partial p_1}{\partial t}+\frac{\rho_1 c_{1I}^2}{\alpha_1}(v_1-v_I)\frac{\partial\alpha_1}{\partial x}+\rho_1 c_1^2\frac{\partial v_1}{\partial x}+v_1\frac{\partial p_1}{\partial x}=0$$

Hence, in primitive variable form:

$$\frac{\partial\boldsymbol{w}}{\partial t}+B(\boldsymbol{w})\frac{\partial\boldsymbol{w}}{\partial x}=0$$

with $\boldsymbol{\omega}=(\alpha_1,\rho_1,v_1,p_1,\rho_2,v_2,p_2)$.

$$B(\boldsymbol{w})=\begin{pmatrix}
v_I & 0 & 0 & 0 & 0 & 0 & 0\\
\frac{\rho_1}{\alpha_1}(v_1-v_I) & v_1 & \rho_1 & 0 & 0 & 0 & 0\\
\frac{p_1-p_I}{\alpha_1\rho_1} & 0 & v_1 & \frac{1}{\rho_1} & 0 & 0 & 0\\
\frac{\rho_1 c_{1I}^2}{\alpha_1}(v_1-v_I) & 0 & \rho_1 c_1^2 & v_1 & 0 & 0 & 0\\
\frac{\rho_2}{\alpha_2}(v_I-v_2) & 0 & 0 & 0 & v_2 & \rho_2 & 0\\
\frac{p_2-p_I}{\alpha_2\rho_2} & 0 & 0 & 0 & 0 & v_2 & \frac{1}{\rho_2}\\
\frac{\rho_1 c_{2I}^2}{\alpha_2}(v_I-v_2) & 0 & 0 & 0 & 0 & \rho_2 c_2^2 & v_2
\end{pmatrix}$$

8.5 Level Set Equations

Advection:

$$\frac{\partial \phi}{\partial t} + \boldsymbol{v} \cdot \boldsymbol{\nabla} \phi = 0$$

Normal motion ($\boldsymbol{v} = v_n \hat{\boldsymbol{n}}$):

$$\frac{\partial \phi}{\partial t} + \underbrace{v_n |\boldsymbol{\nabla} \phi|}_{H(\boldsymbol{\nabla}\phi)} = 0 \quad \Rightarrow \quad \phi_t + v_n \frac{\boldsymbol{\nabla}\phi}{|\boldsymbol{\nabla}\phi|} \cdot \boldsymbol{\nabla}\phi = 0$$

$$H_x = \frac{\partial H}{\partial \phi_x} = v_n \phi_x |\nabla \phi|^{-1}$$

where $\phi_x = \frac{\partial \phi}{\partial x}$.

If ϕ is SDF,

$$\frac{\partial \phi}{\partial t} = -v_n$$

$$\phi^{n+1} = \phi^n - v_n \Delta t \quad \text{(discretised)} \quad , \quad \phi(t) = \phi_0 - v_n t \quad \text{(exact)}$$

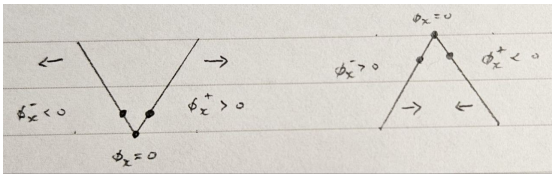
- Taking gradient:

  $$\nabla \phi^{n+1} = \nabla \phi^n - \cancel{\nabla (v_n \Delta t)}$$

  If ϕ^n is initially a signed distance function ($|\boldsymbol{\nabla}\phi| = 1$), it stays an SDF for all time.

- If ϕ_0 is an SDF, we can write down the exact solution for all time. On the other hand, when ϕ_0 is not an SDF, we need so solve it numerically by treating it as a Hamilton-Jacobi equation.

- Upwinding discretisation (approximating ϕ_x with ϕ_x^+ or ϕ_x^-): when ϕ_x^+ and ϕ_x^- have the same sign, assuming $a > 0$, choose ϕ_x^- when $a\phi_x > 0$, choose ϕ_x^+ when $a\phi_x < 0$.However, when ϕ_x^+ and ϕ_x^- have different signs (sonic point), need to be careful to ensure that the correct solution is obtained.



- Alternatives: Lax-Friedrichs method adds some numerical dissipation and uses central differencing to treat the ambiguity near sonic points. Or even better, use Godunov scheme:

$$\phi_x^2 = \max(\max(\phi_x^-, 0)^2, \min(\phi_x^+, 0)^2) \quad \text{if} \quad a > 0$$

$$\phi_x^2 = \max(\min(\phi_x^-, 0)^2, \max(\phi_x^+, 0)^2) \quad \text{if} \quad a < 0$$

Curvature-driven motion ($\boldsymbol{v} = -b\kappa\hat{\boldsymbol{n}}$):
Consider motion by mean curvature where the interface moves in the normal direction with a velocity proportional to its curvature. When $b > 0$, the interface moves in the direction of the concavity, so that circles (2D) shrink to a single point and disappear. When $b < 0$, the interface moves in the direction of convexity, so that circles grow instead of shrink. This growing-circle effects lead to the growth of small perturbations in the front including those due to round-off errors. $b < 0$ allows small erroneous perturbations to incorrectly grow into $\mathcal{O}(1)$ features so it is ill-posed, and we neglect it.

$$\frac{\partial \phi}{\partial t} - b\kappa|\boldsymbol{\nabla}\phi| = 0 \quad \Rightarrow \quad \frac{\partial \phi}{\partial t} - b\left[\boldsymbol{\nabla} \cdot \left(\frac{\nabla \phi}{|\nabla \phi|}\right)\right]|\boldsymbol{\nabla}\phi| = 0$$

It contains second derivatives of ϕ, so it is not a Hamilton-Jacobi equation. It is a parabolic term.

When ϕ is the signed distance function, we obtain the heat equation:

$$\phi_t = b\nabla^2\phi$$

To use the heat equation form, it is particularly important to perform reinitialisation of ϕ.

Discretisation:

- Parabolic equation needs to be discretised using central differencing since the domain of dependence includes information from all spatial directions, as opposed to hyperbolic equations, where information flows in the direction of characteristics only.
- $\nabla^2\phi$ is discretised using $D_i^2\phi$.
- Stable time step:

$$\Delta t\left(\frac{2b}{\Delta x^2} + \frac{2b}{\Delta y^2} + \frac{2b}{\Delta z^2}\right) < 0$$

  We can see that $\Delta t \sim \mathcal{O}(\Delta x^2)$ which is significantly more stringent than the hyperbolic case, where $\Delta t \sim \mathcal{O}(\Delta x)$.

Modelling burning flame fronts

$$\phi_t + \underbrace{\boldsymbol{v} \cdot \boldsymbol{\nabla}\phi + v_n|\boldsymbol{\nabla}\phi|}_{\text{hyperbolic HJ part}} = \underbrace{b\kappa|\boldsymbol{\nabla}\phi|}_{\text{parabolic}}$$

It has advection term, normal motion term and curvature-driven term. The advection terms accounts for the velocity of the unburnt material. Most flames burn with a speed in the normal direction plus extra heating and cooling effects due to the curvature of the front.

To discretise the Hamilton-Jacobi part, we identify partial derivatives of H with respect to $\nabla\phi$ i.e. $H^x = \frac{\partial H}{\partial \phi_x}$ and $H^y = \frac{\partial H}{\partial \phi_y}$.

$$H^x = v_x + v_n\phi_x|\nabla\phi|^{-1} \quad \text{and} \quad H^y = v_y + v_n\phi_y|\nabla\phi|^{-1}$$

8.6 Ghost Fluid Methods Overview

Aim: capture the correct behaviour at the interface, by suitably populating the ghost cells with flow properties such that the real fluid together with the corresponding ghost fluid depict the interface properties and conditions precisely. Improvements are made to deal with strong shock waves or different material properties across the interface.

1. **Original GFM**

   - Populate the ghost cells based on the fact that the pressure and velocity are continuous across the contact discontinuity. This enables us to define a fluid that has the pressure and velocity of the real fluid at each point, but the entropy of some other fluid.
   - Consider the case of air and water. In order to solve for the air, we replace the water with ghost air that acts like the water in every way (pressure and velocity) but appears to be air (entropy). In order to solve for the water, we replace the air with ghost water that acts like the air in every way (pressure and velocity) but appears to be water (entropy). Since the ghost fluids behave in a fashion consistent with the real fluids that they are replacing, the appropriate boundary conditions are captured.
   - Work well for shock tube problems and even a not-very-strong shock impacting on an interface. However, it does not work very efficiently in the application to a strong shock wave impacting on an interface.
   - In such a situation, the pressure, velocity and entropy at the interface may experience a sudden jump; the sudden jump of pressure, velocity and entropy across the interface implies that the real fluid pressure and velocity may not readily be taken as "reasonably acceptable" ghost fluid pressure and velocity and thus these have to be predicted separately and correctly before the GFM is applied.

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2. **Modified GFM**

   - Sometimes the original GFM predicts a reflected rarefaction when there should be a reflected shock wave. So MGFM was specifically designed to address the problems suffered when a strong shock wave impacts an interface.
   - Looking at Riemann problem solution can give information about when this would happen.
   - It uses characteristic equations to approximate RP solution.
   - Non-physical shock refraction still cannot be avoided for a shock impacting on a gaseous interface under critical condition.

3. **Interface GFM**

   - Similar to modified GFM, still using the characteristic jumps, $dp \pm \rho c_s du = 0$.
   - It attempts to inform the real-ghost interaction by first obtaining interface conditions from real-real fluid interaction, and then setting them to be the final states after the real-ghost interaction. We then proceed to solve for the ghost states.

4. **Explicit simplified interface GFM**

   - Original GFM cannot handle entropy gradients across the interface.
   - Physically, ESIM allows GFM to deal with temperature gradients.
   - ESIM uses jump conditions of derivatives to allow linear extrapolation of entropy.

   A correction to the real fluid nodes next to the interface is deemed necessary to accurately take into account such influence.

---

5. **Real GFM**

   - Similar to modified GFM, solves a Riemann problem at the interface to obtain the solution.
   - In this case, the entire intermediate state of the mixed-material RP is computed, using the fact the standard equation for a Riemann problem is actually a general equation for multiple materials:
   $$f_L(p_I, \boldsymbol{u}_L) + f_R(p_I, \boldsymbol{u}_R) + \Delta v = 0$$
   - This ensures that we have a thermodynamically reasonable state within the ghost cell.
   - The real fluid states next to the interface instead of the ghost fluid states will be predicted by solving a Riemann problem and the ghost fluid states are then obtained by solving an advection equation. This will result in the complete modification and redefinition of the real fluid next to the interface.

6. **Riemann GFM**

   - Uses a Riemann solver to predict ghost-cell states adjacent to the interface.
   - However, the Riemann problem solution is an evolved state of the problem ($t > t^n$) so using this as the ghost fluid state at time t^n is incorrect.

7. **Practical GFM**

   - Improves upon the Riemann GFM by finding a state for the ghost fluid region $\boldsymbol{u}_{G,L}$ such that the interaction between $\boldsymbol{u}_{G,L}$ and $\boldsymbol{u}_L$ results in $\boldsymbol{u}_L^*$.
   - Ghost fluid states are set as reflective boundary conditions, with $v_g = 2v_I - v_{real}$.
   - The ghost cell and the real cell are equidistant from the interface.
   - Correct for entropy errors in the ghost fluid states.

8.7 Extrapolating Entropy

Starting from second law of thermodynamics,

$$d\varepsilon = Tds - pdv \quad \Rightarrow \quad Tds = d\varepsilon + pdv$$

Constant entropy is by setting $ds = 0$,

$$d\varepsilon + pdv = 0$$

For **ideal gas** $p = (\gamma - 1)\rho\varepsilon$ and we want $s = s(p, v)$ i.e. a function of pressure and density,

$$d\varepsilon = \frac{vdp + pdv}{\gamma - 1}$$

Then,

$$\frac{v}{\gamma - 1}dp + \left(\frac{1}{\gamma - 1} + 1\right)pdv = 0$$

$$vdp + \gamma pdv = 0$$

$$\frac{1}{p}dp + \gamma\frac{1}{v}dv = 0$$

$$\ln(pv^\gamma) = \ln\left(\frac{p}{\rho^\gamma}\right) = \text{constant}$$

For stiffened gas, $p = (\gamma - 1)\rho\varepsilon - \gamma p_\infty$ and we want $s = s(p, v)$,

$$\varepsilon = \frac{(p + \gamma p_\infty)v}{\gamma - 1}$$

$$d\varepsilon = \frac{(p + \gamma p_\infty)dv}{\gamma - 1} + \frac{vdp}{\gamma - 1}$$

Then, in a similar process to ideal gas,

$$\frac{(p + \gamma p_\infty)dv}{\gamma - 1} + \frac{vdp}{\gamma - 1} + pdv = 0$$

$$(p + \gamma p_\infty + \gamma p - p)dv + vdp = 0$$

$$\gamma(p_\infty + p)dv + vdp = 0$$

$$\gamma\frac{1}{v}dv + \frac{1}{p + p_\infty}dp = 0$$

$$\ln v^\gamma + \ln(p + p_\infty) = \text{const}$$

$$\ln\left(\frac{p + p_\infty}{\rho^\gamma}\right) = \text{const}$$

For JWL EoS, we do the same things for finding an expression for $\varepsilon = \varepsilon(p, v)$.

8.8 Cavitation Model

Cavitation is pressure-induced phase change of a liquid into a gas, which occurs when pressure drops below the saturated vapour pressure. It occurs on an acoustic timescale.

Requirements:

- Need phase change: use diffuse interface formulation.
- Need to know when water has reached the saturation pressure and will cavitate: need two pressures in our model.
- Assume velocity equilibrium between water and vapour: use 6-equation model.

$$
\begin{aligned}
\frac{\partial \alpha_g \rho_g}{\partial t} + \frac{\partial \alpha_g \rho_g v_x}{\partial x} &= 0 \\
\frac{\partial \alpha_l \rho_l}{\partial t} + \frac{\partial \alpha_l \rho_l v_x}{\partial x} &= 0 \\
\frac{\partial \rho v_x}{\partial t} + \frac{\partial (\rho v_x^2 + p)}{\partial x} &= 0 \\
\frac{\partial \alpha_g}{\partial t} + v_x \frac{\partial \alpha_g}{\partial x} &= \mu(p_g - p_l) \\
\frac{\partial \alpha_g \rho_g \varepsilon_g}{\partial t} + \frac{\partial \alpha_g \rho_g \varepsilon_g v_x}{\partial x} + \alpha_g p_g \frac{\partial v_x}{\partial x} &= -p_I \mu(p_g - p_L) \\
\frac{\partial \alpha_l \rho_l \varepsilon_l}{\partial t} + \frac{\partial \alpha_l \rho_l \varepsilon_l v_x}{\partial x} + \alpha_l p_l \frac{\partial v_x}{\partial x} &= p_I \mu(p_g - p_L)
\end{aligned}
$$

Extra energy equation: by also evolving the conserved quantity of total energy, we can "correct" for conservation errors in specific internal energy:

$$\frac{\partial E}{\partial t} + \frac{\partial (E + p) v_x}{\partial x} = 0$$

Note: this model assumes that cavitation does not result from mass transfer. Cavitation pockets appear as the volume fraction increases for a small amount of gas present initially. Cavitation is thus modelled as a mechanical relaxation process, occurring at infinite rate. (not as a mass transfer process)

Further assumption: make instantaneous relaxation assumption, $\mu \to \infty$, as we assume the timescale over which cavitation occurs is fast. Relaxation is effectively converting pressure or velocity from one material to another in a thermodynamically consistent manner.

Pressure relaxation step:

$$\frac{\partial \alpha_g}{\partial t} = \mu(p_g - p_l) \quad , \quad \frac{\partial \alpha_g \rho_g \varepsilon_g}{\partial t} = -p_I \mu(p_g - p_l) \quad , \quad \frac{\partial \alpha_l \rho_l \varepsilon_l}{\partial t} = p_I \mu(p_g - p_l)$$

$$\frac{\partial \alpha_g \rho_g}{\partial t} = 0 \quad , \quad \frac{\partial \alpha_l \rho_l}{\partial t} = 0 \quad , \quad \frac{\partial \rho v_x}{\partial t} = 0$$

Closure is achieved by the pressure equilibrium condition, we know the solution must give $p_l = p_g$.

1. Remove μ by combining equation for α_g and $\alpha_g \rho_g \varepsilon_g$:

$$\varepsilon_g \frac{\partial \alpha_g \cancel{\rho_g}}{\cancel{\partial t}} + \alpha_g \rho_g \frac{\partial \varepsilon_g}{\partial t} = -p_I \frac{\partial \alpha_g}{\partial t}$$

$$\begin{aligned}
\frac{\partial \varepsilon_g}{\partial t} &= -\frac{p_I}{\alpha_g \rho_g} \frac{\partial}{\partial t}\left(\frac{\alpha_g \rho_g}{\rho_g}\right) \\
&= -\frac{p_I}{\alpha_g \rho_g}\left[\alpha_g \rho_g \frac{\partial}{\partial t}\left(\frac{1}{\rho_g}\right) + \frac{1}{\rho_g}\frac{\partial \alpha_g \cancel{\rho_g}}{\cancel{\partial t}}\right] \\
&= -p_I \frac{\partial \nu_g}{\partial t}
\end{aligned}$$

   We aim to write the source term as a relationship between specific internal energy and density, so we can use the EoS to equilibrate pressure.

2. Integrate:

$$\varepsilon_i - \varepsilon_i^0 = -\hat{p}_{I,i}(\nu_i - \nu_i^0) \quad \text{where,} \quad \hat{p}_{I,i} = \frac{1}{\nu_i - \nu_i^0}\int_0^{\Delta t} p_I \frac{\partial \nu_i}{\partial t} dt$$

   We need an approximation to compute $\hat{p}_{I,i}$. We can assume $\hat{p}_{I,i} = p$, the relaxed pressure that both liquid and gas reach through cavitation. This approximation is consistent with instantaneous relaxation, where the interfacial pressure immediately becomes the relaxed pressure.

3. Form a system of equations:

$$\begin{cases}
\varepsilon_i(p, \nu_i) - \varepsilon_i^0(p_i^0, \nu_i^0) + p(\nu_i - \nu_i^0) = 0 \\
\varepsilon_i(p, \nu_i) = \frac{p_i + \gamma_i p_{\infty,i}}{\gamma_i - 1}\nu_i \quad \text{(EoS)} \\
\alpha_g + \alpha_l = (\alpha\rho)_g \nu_g + (\alpha\rho)_l \nu_l = 1 \quad \text{(saturation constraint)}
\end{cases}$$

4. Solve system of equation for p:

$$\frac{1}{\gamma_i - 1}\nu_i(p + \gamma_i p_{\infty,i}) - \frac{1}{\gamma_i - 1}\nu_i^0(p_i^0 + \gamma_i p_{\infty,i}) + p(\nu_i - \nu_i^0) = 0$$

$$\nu_i\left[\cancel{p} + \gamma_i p_{\infty,i} + (\gamma_i - \cancel{1})p\right] = \nu_i^0\left[p_i^0 + \gamma_i p_{\infty,i} + (\gamma_i - 1)p\right]$$

$$\nu_i(p) = \frac{p_i^0 + \gamma_i p_{\infty,i} + (\gamma_i - 1)p}{\gamma_i(p + p_{\infty,i})}$$

Then,

$$(\alpha\rho)_i\nu_i = \frac{a_i + b_i p}{c_i + \gamma_i p}$$

where a_i, b_i, c_i are just some constants.

$$\frac{a_g + b_g p}{c_g + \gamma_g p} + \frac{a_l + b_l p}{c_l + \gamma_l p} - 1 = 0$$

which is a quadratic in p.

5. Solve the quadratic to find relaxed pressure p, and also we know the phase's specific volume ν_i.
6. **Correction/reinitialisation step**: first compute mixture pressure using conservation of total energy evolution equation.

$$p_{\text{mix}} = \frac{E - \frac{1}{2}\rho v^2 - \sum_i \frac{\alpha_i}{\gamma_i - 1} \cdot \gamma_i p_{\infty,i}}{\sum_i \frac{\alpha_i}{\gamma_i - 1}}$$

Once the mixture pressure is determined, the internal energies of the phases are reinitialised with the help of their respective EOS before going to the next time step.

$$\varepsilon_i = \varepsilon_i \left(p_{\text{mix}}, \frac{(\alpha\rho)_i}{\alpha_i} \right) \quad \text{(EoS)}$$

In summary, numerical method process:

1. At each cell boundary, solve the Riemann problem of the 6-equation system free of relaxation terms, with a favourite solver such as HLLC.
2. Evolve all flow variables with the Godunov type method i.e. finite volume conservative update.
3. Relaxation step: solving the source term ODE. Determine the relaxed pressure by solving:

$$\sum_k (\alpha\rho)_k \nu_k(p) = 1 \quad \text{with} \quad \nu_k(p) = \nu_k^0 \frac{p^0 + \gamma_k p_{\infty,k} + (\gamma_k - 1)\hat{p}_I}{p + \gamma_k p_{\infty,k} + (\gamma_k - 1)\hat{p}_I}$$

after which we can find the phase's specific volume and volume fraction. The Newton method is appropriate for this task.

4. Compute the mixture pressure:

$$p_{\text{mix}} = \frac{\rho\varepsilon - \left(\frac{\alpha_1}{\gamma_1 - 1} \cdot \gamma_1 p_{\infty,1} + \frac{\alpha_2}{\gamma_2 - 1} \cdot \gamma_2 p_{\infty,2} \right)}{\frac{\alpha_1}{\gamma_1 - 1} + \frac{\alpha_2}{\gamma_2 - 1}}$$

5. Reinitialisation step: reset the internal energies with the mixture pressure with the help of their respective EoS.
6. Restart for the next time step.

8.9 Recommended Papers to Read

1. **Allaire 5-equation model**: Allaire, G., Clerc, S. & Kokh, S. A Five-Equation Model for the Simulation of Interfaces between Compressible Fluids. Journal of Computational Physics 181, 577–616 (2002). Link
2. **Diffuse Interface Modelling**: Maltsev, V., Skote, M. & Tsoutsanis, P. High-order methods for diffuse-interface models in compressible multi-medium flows: A review. Physics of Fluids 34, 021301 (2022). Link
3. **Numerical Method for Allaire Model 1**: Coralic, V. & Colonius, T. Finite-volume WENO scheme for viscous compressible multicomponent flows. J Comput Phys 274, 95–121 (2014). Link
4. **Numerical Method for Allaire Model 2**: Johnsen, E. & Colonius, T. Implementation of WENO schemes in compressible multicomponent flow problems. Journal of Computational Physics 219, 715–732 (2006). Link
5. **The Level Set Methods and Dynamic Implicit Surfaces**: Osher, S. & Fedkiw, R. The Level Set Methods and Dynamic Implicit Surfaces. in Applied Mechanics Reviews vol. 57 xiv+273 (2004).Link
6. **Hamilton-Jacobi WENO**: Jiang, G.-S. & Peng, D. Weighted ENO Schemes for Hamilton–Jacobi Equations. SIAM J. Sci. Comput. 21, 2126–2143 (2000). Link
7. **Baer-Nunziato Model Primitive Variable Form**: Saurel, R. & Abgrall, R. A Multiphase Godunov Method for Compressible Multifluid and Multiphase Flows. Journal of Computational Physics 150, 425–467 (1999). Link
8. **Original Ghost Fluid Method**: Fedkiw, R. P., Aslam, T., Merriman, B. & Osher, S. A Non-oscillatory Eulerian Approach to Interfaces in Multimaterial Flows (the Ghost Fluid Method). Journal of Computational Physics 152, 457–492 (1999). Link
9. **Modified Ghost Fluid Method**: Liu, T. G., Khoo, B. C. & Yeo, K. S. Ghost fluid method for strong shock impacting on material interface. Journal of Computational Physics 190, 651–681 (2003). Link
10. **Interface Ghost Fluid Method**: Hu, X. Y. & Khoo, B. C. An interface interaction method for compressible multifluids. Journal of Computational Physics 198, 35–64 (2004). Link
11. **Explicit Simplified Interface Ghost Fluid method**: Lombard, B. & Donat, R. The Explicit Simplified Interface Method for Compressible Multicomponent Flows. SIAM J. Sci. Comput. 27, 208–230 (2005). Link
12. **Real Ghost Fluid method**: Wang, C. W., Liu, T. G. & Khoo, B. C. A Real Ghost Fluid Method for the Simulation of Multimedium Compressible Flow. SIAM J. Sci. Comput. 28, 278–302 (2006). Link

13. **Riemann Ghost Fluid method**: Sambasivan, S. K. & UdayKumar, H. S. Ghost Fluid Method for Strong Shock Interactions Part 1: Fluid-Fluid Interfaces. AIAA Journal 47, 2907–2922 (2009). Link

14. **Practical Ghost Fluid method**: 1. Xu, L., Feng, C. & Liu, T. Practical Techniques in Ghost Fluid Method for Compressible Multi-Medium Flows. Communications in Computational Physics 20, 619–659 (2016). Link

15. **Mixed-Material Riemann Ghost Fluid Method**: Michael, L. & Nikiforakis, N. A multi-physics methodology for the simulation of reactive flow and elastoplastic structural response. Journal of Computational Physics 367, 1–27 (2018). Link

16. **Cavitaion Model** Richard Saurel, Petitpas, F. & Berry, R. A. Simple and efficient relaxation methods for interfaces separating compressible fluids, cavitating flows and shocks in multiphase mixtures. Journal of Computational Physics 228, 1678–1712 (2009). Link

17. **Fracture Modelling** Wallis, T., Barton, P. T. & Nikiforakis, N. A Flux-enriched Godunov Method for Multi-material Problems with Interface Slide and Void Opening. Journal of Computational Physics 442, 110499 (2021). Link