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Diffuse interface methods

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Outline

- Diffuse interface methods

- Seven-equation models

- Six-equation models

- Five-equation models

- Numerical Methods

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Diffuse interface methods

- Unlike ghost fluid methods, diffuse interface methods are not a class of numerical technique, but a formulation of the underlying system of equations

- The key assumption behind these methods is that each computational cell can contain more than one material

- The equations governing the conservation of such a system can be expressed in a thermodynamically consistent manner

- This formulation allows for material interactions to be dealt with naturally

- Once we have this formulation, the numerical methods we have covered so far can (sort of) be used

- So the main challenge in implementing diffuse interface methods is to modify your code's material description (equation of state, flux functions, etc.)

Diffuse interfaces and naming

- (Almost) any boundary represented within a single system of equations, on an Eulerian mesh, will suffer from numerical smearing, hence **diffuse interface**

- However, these methods go by many different names, often based on the original application they were developed for

- And, unlike sharp interfaces, diffuse interface methods can be used to model both sharp material transitions and genuine transition regions

- Sometimes attempts are made to separate these transition models, but since they often use the same underlying mathematical formulations, and only differ through source terms, we shall lump all these methods together

- One this is clear though, we do not explicitly model the interface; these methods give an **implicit boundary representation**

Alternative names

- **Multi-fluid models** – the name originates from the assumption that finite volume methods are just used for computational 'fluid' dynamics

- However, the name originated with a specific application in mind, for modelling mixtures of homogeneous gases

- **Multi-phase models** – methods originally designed with two genuinely different phases

- However, sometimes two gases or two liquids are described as multi-phase, as are ghost fluid methods

- **Multi-material methods** – a bit more general, at least two gases are genuinely multi-material

- Though this term is often used for **all** multiphysics models

Methods without interfaces

- The three "multi-" names, although inconsistently used, do at least make the assumption that there doesn't need to be an interface when we have multiple materials per cell

- But, in general, if a system is left to settle, and there is still no visible interface (e.g. a mixture of oxygen and nitrogen molecules), then you could probably use a single equation of state for the entire mixture

- Not always, though, **two-fluid MHD** models electrons and ions separately, and due to their differing charge, there are strong effects between them, but they always form a mixture

- In such systems, however, you can model the two components completely separately, due to their very different masses (and also model electric and magnetic fields separately again)

- The key complexity in this case comes from source terms

Concepts of a diffuse interface method

- The concepts of conservation of **total** mass, momentum and energy still apply

- But we also have mass, momentum and energy to track for each material in our diffuse interface system

- Unless we allow for **phase change**, individual mass of each material will still be conserved

- But there will certainly be energy and momentum transfer between materials

- These models can be created for arbitrary numbers of materials, but for simplicity, we shall assume there are only two

- As a result, each cell could have two density values, two momentum values and two energy values

- What is needed to complete the system?

Mixture quantities and total quantities

- If the materials did not interact at all, this would be sufficient (but would not be multiphysics)

- For a finite volume cell, these two distributions are indistinguishable, we cannot assume knowledge of how material is distributed

- But if we say there is a 50-50 mix of materials, are we talking about mass or volume?

- And what do we mean by the density of one of these materials?

- We know it is mass per unit volume, but what volume? The whole cell, or the equivalent volume occupied by the material?
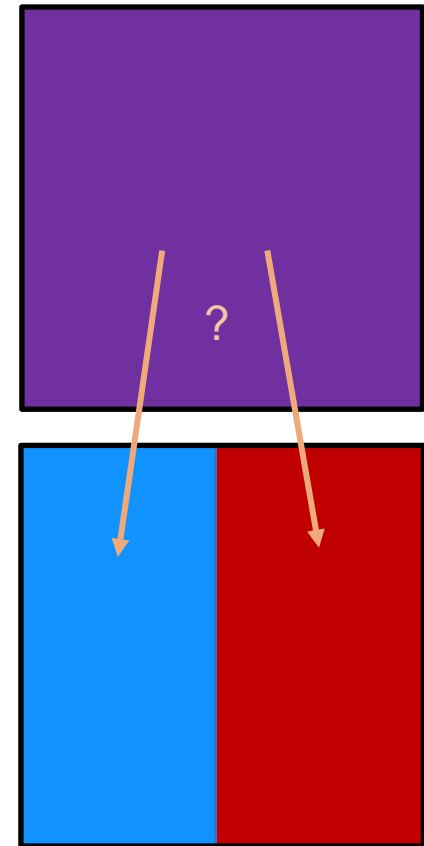
Volume fraction

- In these two configurations, we assume that the two materials are in the **same thermodynamic state**

- Equivalent to a moving contact discontinuity

- In this case, we have a single pressure across all materials, and since $p = p\left(\varepsilon, \rho\right)$, we need to have each material's density being measured per-volume-occupied

- This means that in order to complete this thermodynamic description of the materials, we need to know how much of each material is in the cell

- We need knowledge of the **volume fraction** of each material in the cell
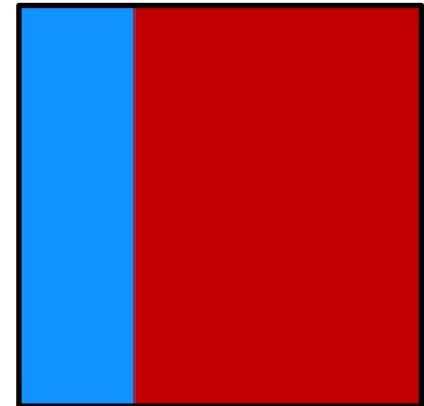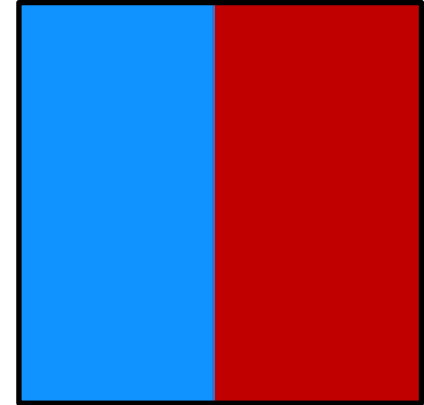
Volume fraction

- The standard convention is that any quantity which is per-region-occupied is given an index, e.g. ρ_1 and ρ_2

- We then have per-cell quantities, such as a total density (or total mass); these are given by quantities without an index, e.g. ρ

- In order to compute total density, we need to know each material's volume fraction, which is a quantity ranging from 0 to 1

- There is no standard symbol for volume fraction, α, z, λ and ϕ are commonly used in the literature – in these lectures I shall attempt to use α

- Since the total mass is just the sum of the individual masses within the volume, it is easy to show that

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

- Note that the two volume fractions are actually a single independent quantity, since they are related through

$$\alpha_1 + \alpha_2 = 1$$

Conserved quantities

- Total mass, and hence total density, **must** be conserved

- And clearly, individual densities are **not** conserved – these two configurations both have the same ρ_1 and ρ_2

- The **individual mass** of each material must still be conserved

- This implies that if there is no mass transfer, then $\alpha_1 \rho_1$ and $\alpha_2 \rho_2$ are conserved

- But what about the other variables?
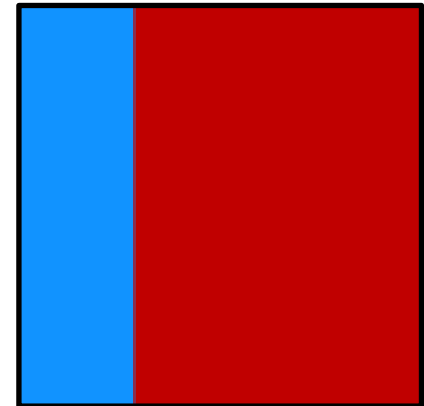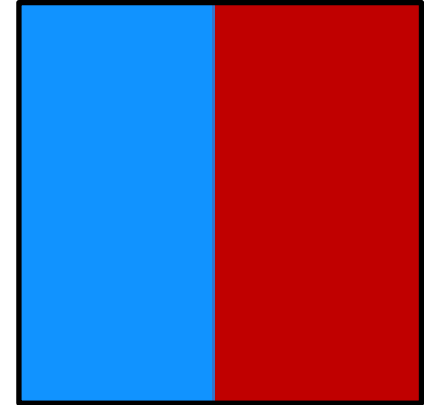
Other conserved variables

- We started with mass and density, because they are easy to visualise and intuitively understand

- There are equivalent concepts for the total momentum and the total energy in a cell too

$$\rho v = \alpha_1 \left(\rho v\right)_1 + \alpha_2 \left(\rho v\right)_2, \qquad E = \alpha_1 E_1 + \alpha_2 E_2$$

- The expression of a total quantity in a cell, in terms of the quantities for individual materials, is a **mixture rule**

- The total density, momentum and energy are **volume-weighted averages** of the individual material quantities

- Do we have the same mixture rule for all our **non-conserved** variables too?

- And we also need to know if quantities such as $\alpha_1 E_1$ are also conserved.

Mixture rules

- It is easy to show that not all quantities obey a volume weighted average

- Consider the total velocity

$$v = \frac{\rho v}{\rho} = \frac{\alpha_1 (\rho v)_1 + \alpha_2 (\rho v)_2}{\alpha_1 \rho_1 + \alpha_2 \rho_2} \neq \alpha_1 v_1 + \alpha_2 v_2$$

- Note that, as expected, $(\rho v)_1 = \rho_1 v_1$

- From this, we see that

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

- The quantities Y_1 and Y_2 are **mass fractions**, and velocity is therefore the **mass weighted average** of the individual velocities

- Various other weightings for total quantities exist

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Behaviour of the material properties

- The quantities $\alpha_1 \rho_1$ and $\alpha_2 \rho_2$ were conserved because we explicitly stated there was no way to transfer mass between materials (no phase change)

- Can we make the same statement about the other quantities?

- Consider a domain which is a liquid containing a lot of gas bubbles - if we have a large enough domain, this could be treated as a continuum

- If we start moving the liquid, do we expect the bubbles to move?

- Transfer of momentum and energy (e.g. kinetic energy in this case) cannot be neglected (assuming we actually want material interaction)

- It is also worth noting that one of the advantages of diffuse interface methods is that since they are a natural formulation for phase change or chemical reactions, we may want to drop the assumption that there is no transfer of mass too

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Do we have enough information?

- So far, we have given three conserved variables, ρ, $\rho\mathbf{v}$ and E, but seven independent quantities, $\mathbf{u}_1$, $\mathbf{u}_2$ and α_1 (or α_2)

- This is assuming we have equations of state for each material

- The key to closing the system of equations is that even though individual density, momentum and energy are not conserved, they are **in balance**

- In other words, the loss of momentum for one material, due to transfer, is the gain in momentum for the other

- If we know how to describe this transfer, then we can write seven **balance laws** for the unknown variables in this system

- We can think of this as the "conservation law with source terms" approach, but the source terms might well depend on what any two interacting materials are; they could be purely mechanical, but there might be chemistry or other thermodynamics

A one-dimensional example

- This example assumes only mechanical interaction between materials

Interfacial averages

Different interfacial averages

Relaxation terms

Pressure-induced interface movement

Drag effects

Equilibration effects

$$\frac{\partial \alpha_1}{\partial t} + v_I \frac{\partial \alpha_1}{\partial x} = \boxed{\mu}(p_1 - p_2)$$

$$\frac{\partial \alpha_1 \rho_1}{\partial t} + \frac{\partial \alpha_1 \rho_1 v_1}{\partial x} = 0$$

$$\frac{\partial \alpha_1 \rho_1 v_1}{\partial t} + \frac{\partial \alpha_1 \left(\rho_1 v_1^2 + p_1\right)}{\partial x} = p_I \frac{\partial \alpha_1}{\partial x} + \boxed{\lambda}(v_2 - v_1)$$

$$\frac{\partial \alpha_1 E_1}{\partial t} + \frac{\partial \alpha_1 \left(E_1 + p_1\right) v_1}{\partial x} = \boxed{p_I v_I} \frac{\partial \alpha_1}{\partial x} - \boxed{\mu p_I'} (p_1 - p_2) + \boxed{\lambda v_I'} (v_2 - v_1)$$

$$\frac{\partial \alpha_2 \rho_2}{\partial t} + \frac{\partial \alpha_2 \rho_2 v_2}{\partial x} = 0$$

$$\frac{\partial \alpha_2 \rho_2 v_2}{\partial t} + \frac{\partial \alpha_2 \left(\rho_2 v_2^2 + p_2\right)}{\partial x} = \boxed{p_I \frac{\partial \alpha_2}{\partial x}} - \boxed{\lambda (v_2 - v_1)}$$

$$\frac{\partial \alpha_2 E_2}{\partial t} + \frac{\partial \alpha_2 \left(E_2 + p_2\right) v_2}{\partial x} = p_I v_I \frac{\partial \alpha_2}{\partial x} + \boxed{\mu p_I' (p_1 - p_2)} - \lambda v_I' (v_2 - v_1)$$

The balance terms

- There is quite a lot of physics in these balance terms

- **Interfacial averages –** these are quantities which govern the physics of the interface

- For example, the effect of high-pressure water on low-pressure air is different to high-pressure air on low-pressure water; this allows for this 'one-sided' interaction

- **Pressure-induced interface movement –** if pressure is higher one side of the interface than the other, the resulting compression will move the interface, and hence alter volume fractions

- There is an important feature of diffuse interface methods here – we can have a **pressure jump across the interface**

Pressure jump

- When we considered sharp interfaces, we did technically also allow for a pressure jump, but this was in two cases; a shock wave hits the interface, or a rarefaction passes over it

- However, because there was only ever one material per cell, this did not require any special treatment

- Now, we have multiple materials in a cell, we have to consider what happens when **two materials have two different thermodynamic states**

- Over time, this will equilibrate, but there is a finite time scale to this behaviour, and whilst this is happening, the pressure difference will cause additional interface motion

- This is particularly true when we are modelling a true diffuse transition (the physics of a sharp interface should remain the same)

The balance terms (continued)

- In addition to the interface motion, we had two different relaxation effects, **drag** and **thermodynamic equilibration**

- The drag effects **equilibrate velocity**; as one material moves through another, it will transfer momentum to the other material, until both are moving at the same velocity

- Thermodynamic effects **equilibrate pressure**; one material will effectively compress the other until they are at the same pressure state

- There is no reason the interfacial average quantities are the same for the equilibration processes as for the interface motion, hence the two sets of average terms

- The relaxation terms λ and μ describe how fast the equilibration process is

Defining the balance terms

- Unfortunately, defining the balance terms is not easy

- Because they require knowledge of the physics between two materials, they may require a lot of experimental input, or may be genuinely unknown

- This is because, again unfortunately, interface physics is **sub-grid cell behaviour** – the distribution of the materials in the cell can actually have a substantial effect on these quantities

- For example, if we have a gas-liquid mixture, where the liquid (material $\mathbf{u}_2$) is suspended as bubbles with radius $R \ll \Delta x$, then we can define

$$\mu = \frac{\boxed{A_I}}{Z_1 + Z_2}, \quad A_I = \frac{3\alpha_2}{R}, \quad \boxed{Z_K} = \rho_K c_{s,K}$$

Specific interfacial area

Acoustic impedances

Defining the balance terms

$$\mu = \frac{A_I}{Z_1 + Z_2}, \quad A_I = \frac{3\alpha_2}{R}, \quad Z_K = \rho_K c_{s,K}$$

- This still does not give us everything; how do we know what radius our bubble have? And why should they be uniform?

- And we don't have the interfacial quantities either, and nor is there any single agreed definition for these

- It may seem that using this model is more trouble than it is worth

- Though this is application dependent – the first formulation was by Baer and Nunziato for granular explosives (granules of explosive surrounded by gas), which also had source terms for detonation chemistry

- In this case, at least uniform radius was both appropriate, and measurable

The Baer-Nunziato model

- Because of this initial work, seven-equation diffuse interface models are often referred to as **Baer-Nunziato-type** models

- And, despite the sheer number of uncertain parameters, in many cases, simple approximations have been shown to give good models capable of reproducing experimental data

- For example, we can often just use the pressure of the 'stiffest' material as the interface pressure (e.g. the liquid in a liquid-gas case)

- This formulation can therefore be very powerful if you have a good understanding of how your two materials mix

- Now we hopefully know it can describe the mathematics and physics well, how simple is it to solve numerically?

Numerical considerations

- We have a system of equations and some source terms; the first thing we would normally want to investigate is hyperbolicity

- But here, we have a few additional concerns; although density, momentum and energy equations are written in balance law form, what about volume fraction?

$$\frac{\partial \alpha_1}{\partial t} + v_I \frac{\partial \alpha_1}{\partial x} = \mu \left(p_1 - p_2 \right)$$

- Not only is this equation not in conservation form, we have first derivatives of volume fraction in many of the other equations

- Unlike sharp interface methods, this equation does not decouple from the system, and we **cannot** write the Baer-Nunziato equations in a conservative balance law form

- Instead, we must be **very careful** with numerical methods (which we will not worry about here)

Numerical considerations

- We are also not going to worry too much about how we deal with the source terms in the Baer-Nunziato system (because so much is unknown about them)

- They will, of course, introduce time step limitations, but there are other challenges too

- Relaxation is effectively 'converting' pressure or velocity from one material to another in a thermodynamically consistent manner; this often requires complex root finding problems using the equations of state

- We will consider a very specific example later, and one which also includes mass transfer (cavitation)

- For now, we analyse the equations in the absence of source terms, but we note that spatial derivatives of the volume fraction **cannot be considered** source terms here

Primitive variable form

- Fortunately, the equations are simple to express in primitive variable form, and this means the additional volume fraction derivatives are accounted for

$$\frac{\partial \mathbf{w}}{\partial t} + B\left(\mathbf{w}\right)\frac{\partial \mathbf{w}}{\partial x} = 0$$

$$\mathbf{w} = \left(\alpha_1, \rho_1, v_1, p_1, \rho_2, v_2, p_2\right)^T$$

$$B\left(\mathbf{w}\right) = \begin{pmatrix} v_I & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & v_1 & \rho_1 & 0 & 0 & 0 & 0 \\ \frac{p_1 - p_I}{\alpha_1} & 0 & v_1 & \frac{1}{\rho_1} & 0 & 0 & 0 \\ \frac{p_1 v_1 - p_I v_I}{\alpha_1} & 0 & \rho_1 c_{s,1}^2 & v_1 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & v_2 & \rho_2 & 0 \\ \frac{p_I - p_2}{1 - \alpha_1} & 0 & 0 & 0 & 0 & v_2 & \frac{2}{\rho_2} \\ \frac{p_I v_I - p_2 v_2}{1 - \alpha_1} & 0 & 0 & 0 & 0 & \rho_1 c_{s,1}^2 & v_1 \end{pmatrix}$$

Hyperbolicity and waves

- Although the volume fraction terms are a little messy, fortunately they all disappear from the calculation of the eigenvalues, and it is straightforward

$$\lambda_1 = v_I, \quad \lambda_2 = v_1 - c_{s,1}, \quad \lambda_3 = v_1, \quad \lambda_4 = v_1 + c_{s,1}$$

$$\lambda_5 = v_2 - c_{s,2}, \quad \lambda_6 = v_2, \quad \lambda_7 = v_2 + c_{s,2}$$

- We see there are seven waves, with (probably) seven different wave speeds

- Though since we don't know the interface velocity, this may be a degenerate wave

- However, it is a diagonalisable system, and we can consider characteristic variables

- The key difficulty in solving a Baer-Nunziato system, though, is that many numerical methods don't work well due to the lack of conservative form

Solving a Baer-Nunziato system

- Numerical methods do exist to solve the Baer-Nunziato equations, they need additional techniques to ensure that oscillations do not develop at sharp features

- One such technique is to use standard numerical methods for the conservative parts of the system, and then an alternative "upwind method" to deal with the rest, see, for example, Tokareva and Toro "A flux splitting method for the Baer-Nunziato equations of compressible two-phase flow"

- These follow our overall principles that you do not need to modify the methods you have already implemented, simply add to them

- However, the additional methods are not always straightforward

- Instead we consider an alternative which might make our life easier: do we always need to solve the Baer-Nunziato system for diffuse interface methods?

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Simplifying the system

- Although the Baer-Nunziato is a very powerful, and sometimes essential, multiphysics system, sometimes reasonable physical assumptions allow us to simplify both the system and the methods

- This is a matter of timescales – how long does it take for velocity or pressure to relax?

- We start with velocity – if one material starts moving, how long until the other material is moving at the same speed

- For most diffuse systems, we don't assume fixed particles of one material suspended in another, but either a true mixture at a molecular scale, or a diffuse representation of a sharp interface

- In either of these limits, we can often assume that velocity equilibrium is achieved very fast; faster than the hyperbolic scales of the problem

Relaxation time scales

- When we can assume velocity equilibrates rapidly, we are assuming an **instantaneous relaxation** of this quantity

- The relaxation parameters λ and μ are inversely related to the relaxation timescales

- $\lambda = 0$ implies no relaxation, the two materials are **completely independent** of each other

$$\frac{\partial \alpha_1 \rho_1 v_1}{\partial t} + \frac{\partial \alpha_1 \left(\rho_1 v_1^2 + p_1 \right)}{\partial x} = p_I \frac{\partial \alpha_1}{\partial x} + \lambda \left(v_2 - v_1 \right)$$

$$\frac{\partial \alpha_2 \rho_2 v_2}{\partial t} + \frac{\partial \alpha_2 \left(\rho_2 v_2^2 + p_2 \right)}{\partial x} = p_I \frac{\partial \alpha_2}{\partial x} - \lambda \left(v_2 - v_1 \right)$$

Instantaneous relaxation

- Instantaneous relaxation of velocity requires $\lambda \to \infty$

- Mathematically, we still want our equations to be well defined

- We can stop the relaxation source term from blowing up if we always have

$$v_2 - v_1 = 0$$

- In other words, we only have one velocity, we always have **velocity equilibrium**

$$\frac{\partial \alpha_1 \rho_1 v_1}{\partial t} + \frac{\partial \alpha_1 \left(\rho_1 v_1^2 + p_1 \right)}{\partial x} = p_I \frac{\partial \alpha_1}{\partial x} + \lambda \left(v_2 - v_1 \right)$$

$$\frac{\partial \alpha_2 \rho_2 v_2}{\partial t} + \frac{\partial \alpha_2 \left(\rho_2 v_2^2 + p_2 \right)}{\partial x} = p_I \frac{\partial \alpha_2}{\partial x} - \lambda \left(v_2 - v_1 \right)$$

Velocity equilibrium

- Whilst we could try to evolve the two momentum equations separately, things are much easier if we add them together

- This gives a single equation for momentum

$$\frac{\partial \rho v}{\partial t} + \frac{\partial \left(\rho v^2 + \alpha_1 p_1 + \alpha_2 p_2 \right)}{\partial x} = 0$$

- Sometimes, a **total pressure** is defined

$$p = \alpha_1 p_1 + \alpha_2 p_2$$

- At this stage, this is notational convenience, not necessarily a definition of a **total pressure** within a volume

Six-equation formulation

- Although we have velocity equilibrium, we may still want to add mass transfer terms, hence we do still include an interface velocity in the equations

$$\frac{\partial \alpha_1}{\partial t} + v_I \frac{\partial \alpha_1}{\partial x} = \mu \left(p_1 - p_2 \right)$$

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

$$\frac{\partial \alpha_2 \rho_2}{\partial t} + \frac{\partial \alpha_2 \rho_2 v}{\partial x} = 0$$

$$\frac{\partial \rho v}{\partial t} + \frac{\partial \left(\rho v^2 + \alpha_1 p_1 + \alpha_2 p_2 \right)}{\partial x} = 0$$

$$\frac{\partial \alpha_1 E_1}{\partial t} + \frac{\partial \alpha_1 \left(E_1 + p_1 \right) v}{\partial x} = p_I v_I \frac{\partial \alpha_1}{\partial x} - \mu p_I' \left(p_1 - p_2 \right)$$

$$\frac{\partial \alpha_2 E_2}{\partial t} + \frac{\partial \alpha_2 \left(E_2 + p_2 \right) v}{\partial x} = p_I v_I \frac{\partial \alpha_2}{\partial x} - \mu p_I' \left(p_1 - p_2 \right)$$

In many cases, though, this is simply the single velocity

Is this enough simplicifation?

- Unfortunately, the numerical methods for solving this equation are not much simpler than they were for the full Baer-Nunziato system

- There are, in fact, many different ways of formulating a six-equation system, and the way it is expressed is often dependent on the numerical method being used

- We shall revisit this model, however, when we consider cavitation

- For now, we make another assumption, which again assumes we have a sharp material interface, not one material in suspension

- Because pressure is transmitted from one material to another in this setup, we can assume pressure equilibrates instantaneously, i.e. $\mu \rightarrow \infty$

- This means we have $p_1 = p_2 = p$

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Five-equation formulation

- All source terms now cancel out when we add the two energy equations together

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

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

$$\frac{\partial \alpha_2 \rho_2}{\partial t} + \frac{\partial \alpha_2 \rho_2 v}{\partial x} = 0$$

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

$$\frac{\partial E}{\partial t} + \frac{\partial \alpha_1 \left(E + p\right) v}{\partial x} = 0$$

- We are now assuming no mass transfer – the interface velocity is the material velocity

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Is this a good model to use?

- The five-equation model allows us to get rid of all source terms, and associated time step (and other calculation) issues with these terms

- We only have one non-conservative equation; this doesn't immediately improve overall conservation properties of the system, but we shall discuss this more later

- Numerical methods are also significantly easier to implement

- But is the system hyperbolic?

- Each equation is something we have used to compute a primitive variable form

- This included pressure, with the equation

But what is this term?

$$\frac{\partial p}{\partial t} + \rho c_s^2 \frac{\partial v}{\partial x} + v \frac{\partial p}{\partial x} = 0$$
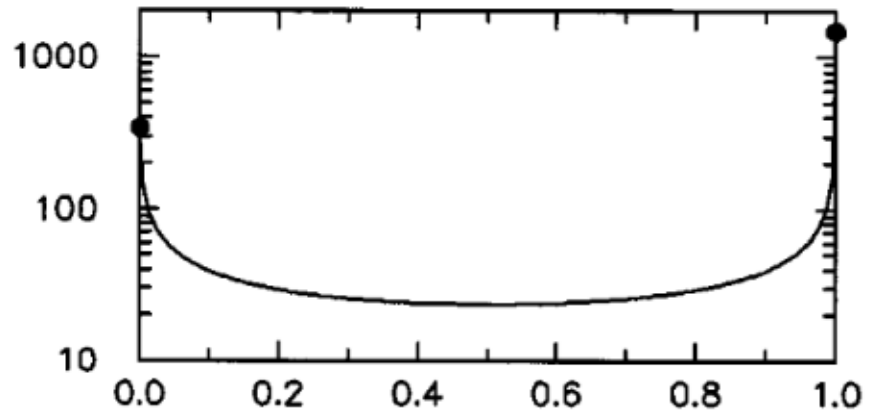
Sound speed of a mixture

- The sound speed of a mixture is a well-studied quantity

- Wood's textbook (1930) gives a mixture speed for air and water as

$$\frac{1}{\rho c_{s,eq}^2} = \frac{\alpha_1}{\rho_1 c_{s,1}^2} + \frac{\alpha_2}{\rho_2 c_{s,2}^2}$$

Equilibrium sound speed

Volume fraction of water

- The sound speed of a mixture can be **lower than that of either component**

Sound speed of a mixture

$$\frac{1}{\rho c_{s,\text{eq}}^2} = \frac{\alpha_1}{\rho_1 c_{s,1}^2} + \frac{\alpha_2}{\rho_2 c_{s,2}^2}$$

- What do we mean by equilibrium sound speed?

- This considers an equilibrium state in which two phases are at the **same pressure and temperature** and are fully mixed within a control volume

- Is this true if we are using a diffuse interface model to represent a sharp interface?

- Here we expect a sudden transition from one material to another - the acoustic speed across this volume would be much closer to some form of average of the two states

- One of the (seemingly major) disadvantages of the simplified diffuse interface equations is that sound speed is now underdetermined

- It can be shown that using the expression above causes oscillations at an interface

What do we need sound speed for?

- We have only really seen two uses of sound speed:

1. Calculating eigenvalues and hyperbolicity

2. Calculating the maximum wave speed

- If we can define a thermodynamically reasonable quantity as a mixture of known physical variables that also ensures the hyperbolicity of the system, we know we are solving a suitable set of equations for density, momentum and energy

- If this does not adversely affect time step calculations too, that would help

- This is an additional concept for **mixture quantities** - mathematically averaged quantities that do not permit thermodynamic violation and allow a stable solution despite the underdetermined sound speed

- In this case, we don't need to know the individual quantities, just their total value

Sound speed and hyperbolicity

- We now need to consider how a mixture sound speed is defined for the 5-equation model, and, at the same time, consider how we ensure we are solving a hyperbolic system

- We are looking at a specific 5-equation model, originally described (in more detail) by Allaire, Clerc and Kokh, "*A Five-Equation Model for the Simulation of Interfaces between Compressible Fluids*" and as a result, this model is often called **the Allaire model** within the group here

- Even within this paper, alternative forms of the equation are considered, e.g. temperature equilibrium, rather than pressure equilibrium

- In order to identify a mixture sound speed, we attempt to identify a primitive variable form of the 5-equation model

Primitive variable form of the 5-equation model

- Much like for the Euler equations, identifying the primitive variable forms for the momentum and the two density equations (as well as the volume fraction) are straightforward

- It is the energy equation which causes us trouble, recall for the Euler equations, we managed to rewrite the energy equation in terms of derivatives of pressure, giving

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

- We can do the same thing for the 5-equation model (see Allaire et al. for more detail) and we will get

Mixture specific enthalpy: $\rho h = \alpha_1 \rho_1 h_1 + \alpha_2 \rho_2 h_2 = \rho \varepsilon + p$

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

Enthalpy: $h_1 = \varepsilon_1 + p/\rho_1, \ h_2 = \varepsilon_2 + p/\rho_2$

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Primitive variable form of the 5-equation model

- This can be made to look like the primitive variable form for the Euler equations **if** we define

$$c_s^2 = h \frac{\partial p}{\partial (\rho \varepsilon)} + Y_1 \frac{\partial p}{\partial (\rho_1 \alpha_1)} + Y_2 \frac{\partial p}{\partial (\rho_2 \alpha_2)}$$

- At the moment, this is really just a quantity, which we can compute, which we are calling c_s^2 because of how the equations look if we do this

- If we are able to use this as a sound speed, we are then assuming that this quantity is greater than zero, something which depends on derivatives of the equation of state

- Potentially, the hyperbolicity of a system of equations **might** depend on the materials you are using (though not in this case)

Hyperbolicity of the 5-equation model

$$
\frac{\partial}{\partial t}
\begin{pmatrix} \alpha_1 \\ \rho_1 \\ \rho_2 \\ v \\ p \end{pmatrix}
+
\begin{pmatrix}
v & 0 & 0 & 0 & 0 \\
0 & v & 0 & \rho_1 & 0 \\
0 & 0 & v & \rho_2 & 0 \\
0 & 0 & 0 & v & \frac{1}{\rho} \\
0 & 0 & 0 & \rho c_s^2 & v
\end{pmatrix}
\frac{\partial}{\partial x}
\begin{pmatrix} \alpha_1 \\ \rho_1 \\ \rho_2 \\ v \\ p \end{pmatrix}
= 0
$$

- Once again, in primitive form, the eigenvalues are very easy to compute (and somewhat familiar)

$$
\lambda_1 = \lambda_2 = \lambda_3 = v, \quad \lambda_4 = v - c_s, \quad \lambda_5 = v + c_s
$$

- Even if we didn't call that quantity, c_s^2 the calculation would be just as easy, though it would take a little longer to write down

- So, provided c_s exists, we have a hyperbolic system, and now we know this, we can spend some time looking at this quantity

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Mixture sound speed

$$c_s^2 = h \frac{\partial p}{\partial(\rho\varepsilon)} + Y_1 \frac{\partial p}{\partial(\rho_1\alpha_1)} + Y_2 \frac{\partial p}{\partial(\rho_2\alpha_2)}$$

- Before we start, we need to decide how we are going to describe out total pressure quantity; what are we going to consider as independent variables

- It may initially seem that we have five independent variables in our pressure equation

$$p = \alpha_1 p_1 + \alpha_2 p_2 = \alpha_1 p_1(\rho_1, \varepsilon_1) + \alpha_2 p_2(\rho_2, \varepsilon_2) = p(\alpha_1, \rho_1, \varepsilon_1, \rho_2, \varepsilon_2)$$

- But, in our 5-equation system, we only have five total independent variables, and momentum (or velocity hasn't appeared here)

- In fact, we can always write total pressure as a function of four independent variables, e.g.

$$p = p(\varepsilon, \rho_1, \rho_2, \alpha_1) \text{ or } p = p(\alpha_1, \alpha_1\rho_1, \alpha_2\rho_2, \rho\varepsilon)$$

Mixture sound speed

$$c_s^2 = h \frac{\partial p}{\partial (\rho \varepsilon)} + Y_1 \frac{\partial p}{\partial (\rho_1 \alpha_1)} + Y_2 \frac{\partial p}{\partial (\rho_2 \alpha_2)}$$

- This definition does at least give us a very strong hint as to what variables we use:

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

- We then define a couple of quantities

$$\xi_1 = \left. \frac{\partial \rho_1 \varepsilon_1}{\partial p} \right|_{\rho_1}, \qquad \xi_2 = \left. \frac{\partial \rho_2 \varepsilon_2}{\partial p} \right|_{\rho_2}$$

$$\delta_1 = \left. \frac{\partial \rho_1 \varepsilon_1}{\partial \rho_1} \right|_p, \qquad \delta_2 = \left. \frac{\partial \rho_2 \varepsilon_2}{\partial \rho_2} \right|_p$$

- These are relatively straightforward derivatives of the equation of state, so this makes our derivation neater

Mixture sound speed

- Now we start our derivation by considering changes in internal energy

$$\mathrm{d}\left(\rho\varepsilon\right) = \mathrm{d}\left(\alpha_1\rho_1\varepsilon_1 + \alpha_2\rho_2\varepsilon_2\right)$$

- We use the product rule on this

$$\mathrm{d}\left(\rho\varepsilon\right) = \rho_1\varepsilon_1\mathrm{d}\alpha_1 + \rho_2\varepsilon_2\mathrm{d}\alpha_2 + \alpha_1\mathrm{d}\left(\rho_1\varepsilon_1\right) + \alpha_2\mathrm{d}\left(\rho_2\varepsilon_2\right)$$

$$= \rho_1\varepsilon_1\mathrm{d}\alpha_1 + \rho_2\varepsilon_2\mathrm{d}\alpha_2 + \alpha_1\left(\delta_1\mathrm{d}\rho_1 + \xi_1\mathrm{d}p\right) + \alpha_2\left(\delta_2\mathrm{d}\rho_2 + \xi_2\mathrm{d}p\right)$$

- And then rearrange for pressure

$$\mathrm{d}p = \frac{1}{\xi}\mathrm{d}\left(\rho\varepsilon\right) - \frac{\alpha_1\delta_1}{\xi}\mathrm{d}\rho_1 - \frac{\alpha_2\delta_2}{\xi}\mathrm{d}\rho_2 - \frac{\rho_1\varepsilon_1}{\xi}\mathrm{d}\alpha_1 - \frac{\rho_2\varepsilon_2}{\xi}\mathrm{d}\alpha_2$$

- Where we define $\xi = \alpha_1\xi_1 + \alpha_2\xi_2$

Mixture sound speed

$$dp = \frac{1}{\xi}d\left(\rho\varepsilon\right) - \frac{\alpha_1\delta_1}{\xi}d\rho_1 - \frac{\alpha_2\delta_2}{\xi}d\rho_2 - \frac{\rho_1\varepsilon_1}{\xi}d\alpha_1 - \frac{\rho_2\varepsilon_2}{\xi}d\alpha_2$$

- We keep simplifying this term, using $d\alpha_1\rho_1 = \rho_1 d\alpha_1 + \alpha_1 d\rho_1$ and $\alpha_1 + \alpha_2 = 1$

$$dp = \frac{1}{\xi}d\left(\rho\varepsilon\right) - \frac{\delta_1}{\xi}d\left(\alpha_1\rho_1\right) - \frac{\delta_2}{\xi}d\left(\alpha_2\rho_2\right) + \mathcal{M}d\alpha_1$$

$$\mathcal{M} = \frac{1}{\xi}\left[\rho_1\left(\delta_1 - \varepsilon_1\right) - \rho_2\left(\delta_2 - \varepsilon_2\right)\right]$$

- If we compare this to our original definition for c_s^2 , we see that the advantage here is that now the derivatives are very easy to compute

$$c_s^2 = h\frac{\partial p}{\partial\left(\rho\varepsilon\right)} + Y_1\frac{\partial p}{\partial\left(\rho_1\alpha_1\right)} + Y_2\frac{\partial p}{\partial\left(\rho_2\alpha_2\right)}$$

Mixture sound speed

- We how have

$$c_s^2 = \frac{1}{\xi}\left(h - Y_1\delta_1 - Y_2\delta_2\right)$$

- From our definition of mixture specific enthalpy, we have

$$\rho h = \alpha_1\rho_1 h_1 + \alpha_2\rho_2 h_2 \quad \Rightarrow \quad h = Y_1 h_1 + Y_2 h_2$$

- Giving

$$\xi c_s^2 = Y_1\left(h_1 - \delta_1\right) + Y_2\left(h_2 - \delta_2\right)$$

- We then use the definition of enthalpy, $h_1 = \varepsilon_1 + p/\rho_1$, and the definition of sound speed,

$$c_{s,1} = \sqrt{\left.\frac{\partial p}{\partial \rho_1}\right|_s} = \sqrt{\frac{p}{\rho_1^2 \frac{\partial \varepsilon_1}{\partial p}} - \frac{\frac{\partial \varepsilon_1}{\partial \rho_1}}{\frac{\partial \varepsilon_1}{\partial p}}}$$

to find

$$c_{s,1}^2 = \frac{h_1 - \delta_1}{\xi_1}, \qquad c_{s,2}^2 = \frac{h_2 - \delta_2}{\xi_2}$$

Mixture sound speed

$$\xi c_s^2 = Y_1 \left(h_1 - \delta_1 \right) + Y_2 \left(h_2 - \delta_2 \right)$$

- Eventually, we end up being able to write our mixture sound speed in terms of the individual material sound speeds

$$\xi c_s^2 = Y_1 \xi_1 c_{s,1}^2 + Y_2 \xi_2 c_{s,2}^2$$

- In other words, the thing we treated as a mixture sound speed is indeed a weighted average of the two material sound speeds

- It seems unlikely we could have guessed this weighting though

Outline

- Diffuse interface methods

- Seven-equation models

- Six-equation models

- Five-equation models

- Numerical Methods

Numerical methods for the 5-equation model

- In order to make sure the treatment of the non-conservative part of the equations doesn't give us problems, we need to be careful with our numerical methods

- Part of the popularity of the 5-equation system, though, is though the methods need care, they are not actually difficult, nor unfamiliar, and they don't have any timestep issues

- We need three things:

1. An HLLC solver, with no special corrections or consistency concerns for these equations (other approximate solvers could be used)

2. A **primitive-variable** MUSCL-Hancock solver (second order only)

3. A volume fraction equation which **looks like** a balance law, with some appropriate source term treatment

HLLC for the 5-equation system

- Although there is nothing too surprising about the HLLC solver for this system, we still have a few new terms to consider

- Volume fraction only jumps across the material interface under a sharp interface assumption, therefore, unsurprisingly, we have

$$\alpha_K^{\mathrm{HLLC}} = \alpha_K$$

- We also need an HLLC state for each of the density terms, which, given the result above, is also only a minor adjustment

$$(\alpha\rho)_{i,K}^{\mathrm{HLLC}} = (\alpha\rho)_{i,K} \left(\frac{S_K - v_K}{S_K - S^*} \right)$$

- The momentum and energy intermediate states do not change at all, and the wave speed estimates now use the mixture sound speed

Numerical treatment of the volume fraction

- We consider this before dealing with the primitive-variable MUSCL solver, since once we have a volume fraction update, we can immediately implement a first-order method

- First we express the equation in a balance law-like manner

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

- We can then use a Riemann problem-based method to get, using our HLLC solver, to get $\bar{\alpha_1}^{n+1}$

$$S_{i+1/2} = v^*_{i+1/2}$$

- Then we have a source term update step **specific to the system**

$$\alpha_{1,i}^{n+1} = \bar{\alpha_1}_i^{n+1} + \frac{\Delta t}{\Delta x}\alpha_{1,i}^n \left(S_{i+1/2} - S_{i-1/2}\right)$$

The update step uses the initial volume fraction

Primitive-variable MUSCL-Hancock scheme

- Although we didn't mention it at the time, there is more than one way of using a MUSCL-Hancock scheme – the name relates to the concept of reconstruction, half-timestep update and Godunov solve

- The primitive-variable scheme performs the reconstruction and half-timestep update on the primitive variables

$$\boldsymbol{\Delta}_i = \frac{1}{2}\boldsymbol{\Delta}_{i-1/2} + \frac{1}{2}\boldsymbol{\Delta}_{i+1/2}$$

$$\boldsymbol{\Delta}_{i-1/2} = \mathbf{w}_i^n - \mathbf{w}_{i-1}^n, \qquad \boldsymbol{\Delta}_{i+1/2} = \mathbf{w}_{i+1}^n - \mathbf{w}_i^n$$

$$\bar{\mathbf{w}}_i^L = \mathbf{w}_i^n - \frac{1}{2}\bar{\boldsymbol{\Delta}}_i = \mathbf{w}_i^n - \frac{1}{2}\xi(r)\boldsymbol{\Delta}_i$$

$$\bar{\mathbf{w}}_i^R = \mathbf{w}_i^n + \frac{1}{2}\bar{\boldsymbol{\Delta}}_i = \mathbf{w}_i^n + \frac{1}{2}\xi(r)\boldsymbol{\Delta}_i$$

- The limiters are unchanged, but the limiting variable might change – a standard choice is to limit each variable on itself

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Primitive-variable MUSCL-Hancock scheme

- Once we have our reconstructed states, we perform a half-timestep update

$$\bar{\mathbf{w}}_i^{L,n+1/2} = \bar{\mathbf{w}}_i^L - \frac{1}{2}\frac{\Delta t}{\Delta x} B\left(\mathbf{w}_i\right)\bar{\boldsymbol{\Delta}}$$

$$\bar{\mathbf{w}}_i^{R,n+1/2} = \bar{\mathbf{w}}_i^R - \frac{1}{2}\frac{\Delta t}{\Delta x} B\left(\mathbf{w}_i\right)\bar{\boldsymbol{\Delta}}$$

- We use the primitive variable form, where we have the derivative

$$\partial\mathbf{w}/\partial x = \bar{\boldsymbol{\Delta}}/\Delta x$$

- The primitive variable matrix is calculated using cell-centred values

- Although this is not normally a good form for evolving nonlinear systems, this is a **local update**, for which we have ensured a **suitably smooth** reconstruction

- Finally, we convert the updated variables to conservative ones, and use these in the Godunov step

Is this everything?

- The five-equation system we have introduced is a useful diffuse interface method for many physical systems

- It is even possible to compute a physically meaningful temperature (provided you have complete equations of state for your two materials)

$$T = \frac{\alpha_1 \rho_1 c_{V,1} T_1 + \alpha_2 \rho_2 c_{V,2} T_2}{\alpha_1 \rho_1 c_{V,1} + \alpha_2 \rho_2 c_{V,2}}$$

- Perhaps the main assumption that could need to be relaxed is the assumption that when we apply a force to a volume, both components 'get pushed out of the way' at the same speed

- In other words, each material in a cell is equally compressible

- This assumption holds for material interfaces, but will not be true for all material mixtures

Compaction

- Compressing one material in a volume more than another is known as **compaction**

- For example, in a water-air mixture, if the pressure on the edges of of a volume increases, we would expect more compression of the air than the water

- In other words, the volume fraction of water should increase as a result of pressure changes, not just advection with velocity

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

$$K = \frac{\alpha_1 \alpha_2 \left(\rho_2 c_{s,2}^2 - \rho_1 c_{s,1}^2 \right)}{\alpha_1 \rho_1 c_{s,1}^2 + \alpha_2 \rho_2 c_{s,2}^2}$$

- Additional numerical treatments may be needed for the stable evolution of this source term

Further models

- We have introduced a few of the most important diffuse interface models, many other formulations exist

- These include **single-density** models

- Some of these allow for closure by evolution of equation of state parameters, i.e. still have at least five equations

- However, they are designed with specific equations of state in mind (and, generally, two materials with comparable density)

- There are also models which do only solve four equations – similar to the one we introduced in the first lecture

- In order to achieve stability, a **correction step** is required - a (non-conservative) step to remove the oscillations we demonstrated with this simple system

Some notes on conservation

- We have now introduced two types of multiphysics model, both have the same undesirable property – **they are not conservative**

- We have previously said that non-conservative methods are guaranteed to get the position of shock waves wrong - why have we stopped worrying about this?

- In fact, for practical applications of many diffuse interface systems, extra work is needed to deal with shock waves, sometimes evolving additional variables to "fix" the solution

- This is particularly true for material transitions – for material interfaces, we typically get away with non-conservative methods

Some notes on conservation – sharp interfaces

- For sharp interface methods, the numerical methods for solving the individual phases are **still conservative**

- And provided the level set function remains smooth, we do not get errors here either

- The fact that there can only be one material in a computational cell is what causes mass gains and losses, as the interfacce moves

- Effectively, the conservation errors are a result of slightly changing the original problem, somewhat equivalent to altering one of the initial states in a Riemann problem

- We will still get a thermodynamically reasonable solution, with the correct shock speeds for this new case, it just won't be solution to the problem we started with

- It is clear that this becomes less of a problem with resolution

Some notes on conservation – diffuse interfaces

- Diffuse interface methods evolve a non-conservative system, they genuinely do have the risk of producing incorrect shock speeds

- We have said that we need to choose numerical methods carefully, we shall use the five-equation source term-free model as an example

- Here, only the volume fraction is evolved using a non-conservative method

- For most of the domain, we either have $\alpha_1 = 1$ or $\alpha_1 = 0$ – in these regions, the evolution equation for volume fraction does nothing and we avoid introducing convergence errors

- Numerical methods are then selected considering an isolated contact discontinuity

- They must ensure that in a situation with constant velocity, but changing density and volume fraction, this velocity **remains constant**

Some notes on conservation – diffuse interfaces

- This choice of numerical method deals with all behaviour away from an interface and continuous behaviour and contact discontinuities at an interface

- Although we cannot do anything about the method's convergence issues with shock waves, what we have done is made sure that these errors only impact a very small region of the computational domain

- For a few cells across the interface, there may be errors in shock speed, but these will be small enough not to be noticeable in the overall solution

- Additionally, as resolution increases, the interface width decreases, so these errors do converge away

- Techniques to sharpen a diffuse interface, such as the Tangent of Hyperbola INterface Capturing (THINC) method, which help further minimise these errors

- Provided we choose the correct numerical method, we can successfully cope with the conservation issues for diffuse interface methods