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Multiphysics Modelling for Four States of Matter

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Outline

- What do we mean by multiphysics?

- Methods for multiphysics

- Challenges of multiphysics modelling

- Multiphysics approaches

Multiphysics Modelling for Four States of Matter

- This course utilises the physics and numerical methods from Numerical Methods for Compressible Fluid Dynamics and Simulation of Matter Under Extreme Conditions, and considers how we can allow for **multiple materials in a single computational domain**

- The challenges in achieving this are largely in how we treat the boundaries between materials, whilst retaining the ability to work on a regular Cartesian mesh

- Six lectures and six practicals

- As is probably now expected, these will be recorded

- And similarly, the practical work has additional time scheduled for after exams, and may be helpful when choosing research projects

Multiphysics Modelling for Four States of Matter

- The Lectures:

1. Multiphysics Modelling for Four States of Matter

2. Level set methods

3. Ghost fluid methods (part 1)

4. Diffuse interface methods

5. Ghost fluid methods (part 2)

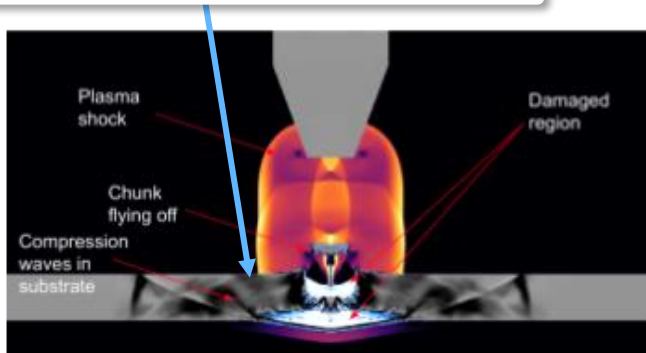6. Cavitation, surface tension and fracture

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- What do we mean by multiphysics?

- Methods for multiphysics

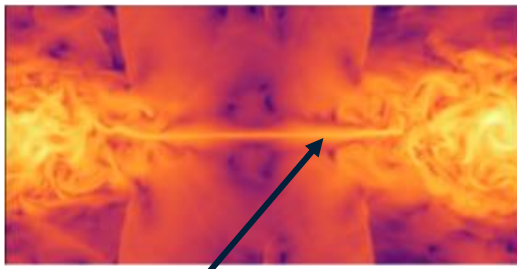- Challenges of multiphysics modelling

- Multiphysics approaches

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What do we mean by multiphysics?

Air

Helium
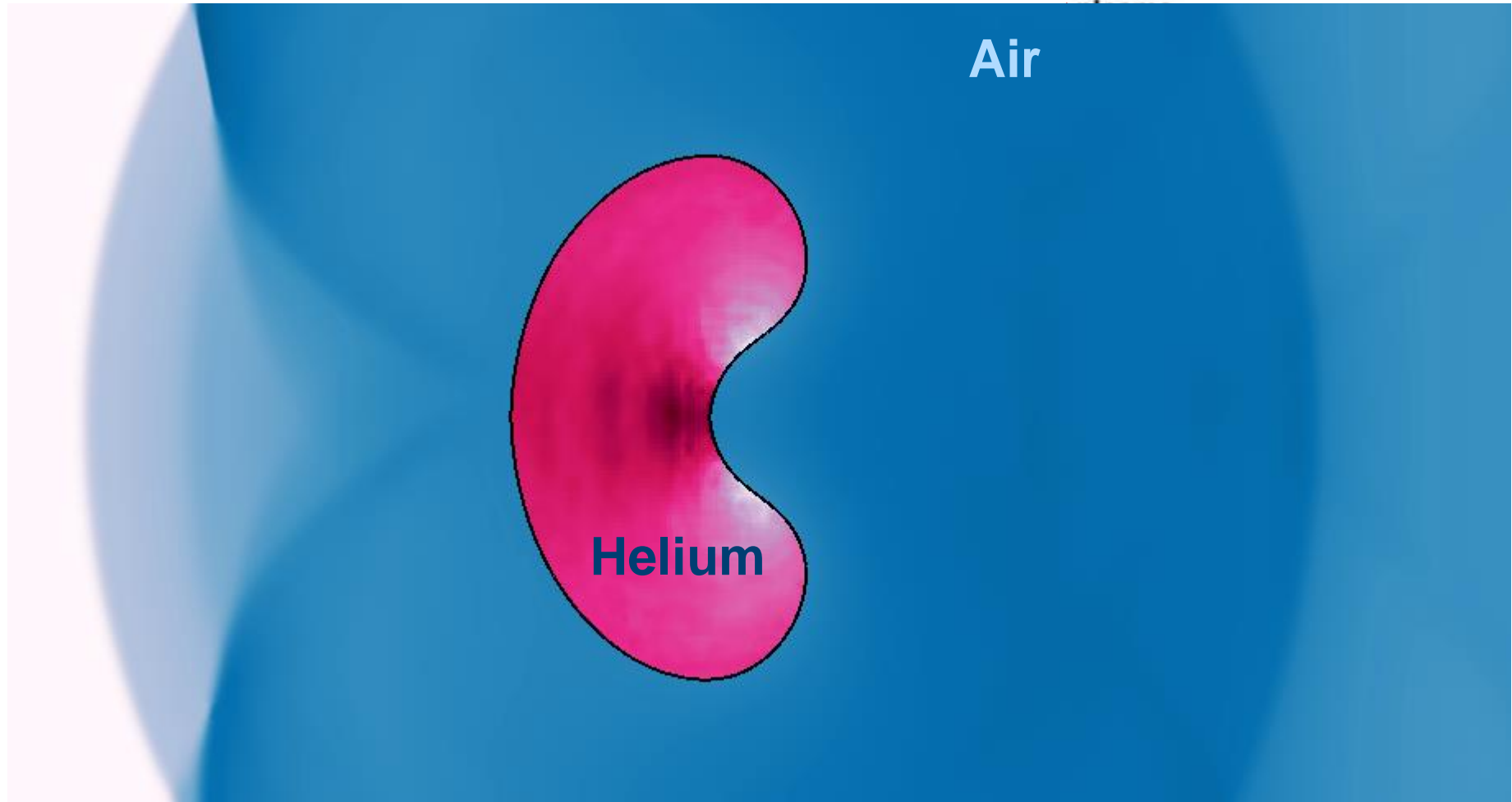
Multiphysics examples

Plasma-solid interaction

Air-solid interaction

Electron-ion interaction
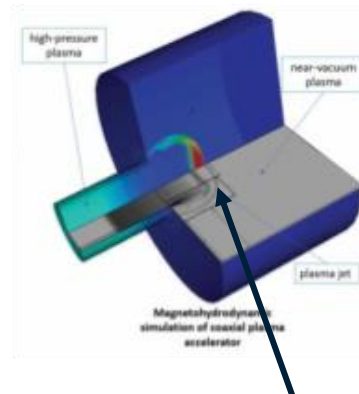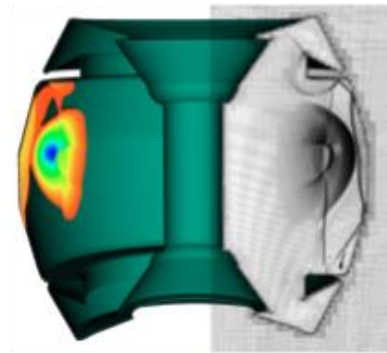
Plasma-vacuum interaction
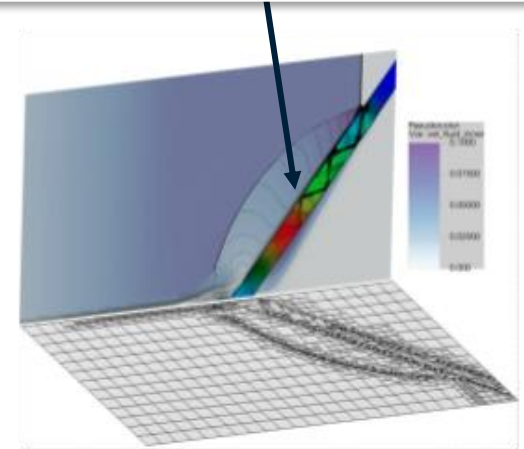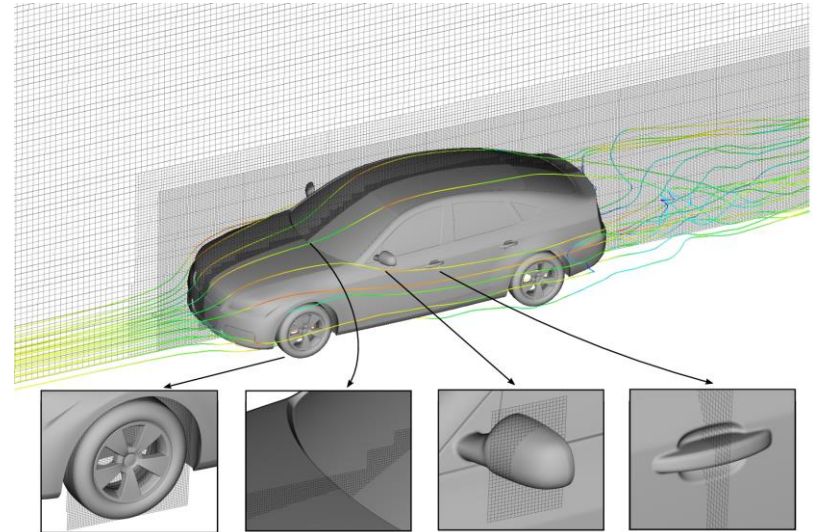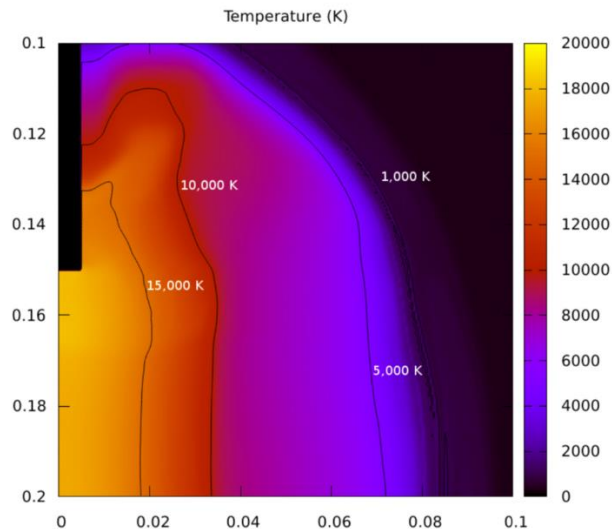
Material interactions without multiphysics

- Sometimes we have a material interface but don't need multiphysics methods

- The cut cell methods we have covered are a clear example of this

- In our lightning model, we have the transition from gas to plasma

- Whilst technically multiphysics, our EoS means we don't need to model the interactions that take place

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Multiphysics and two-way interaction

- When droplets impact surfaces at high speed, the jet forms much later than theoretical models suggest

1. The droplet impact sends shockwaves through the metal

2. The waves in the metal move faster than waves in the water and air
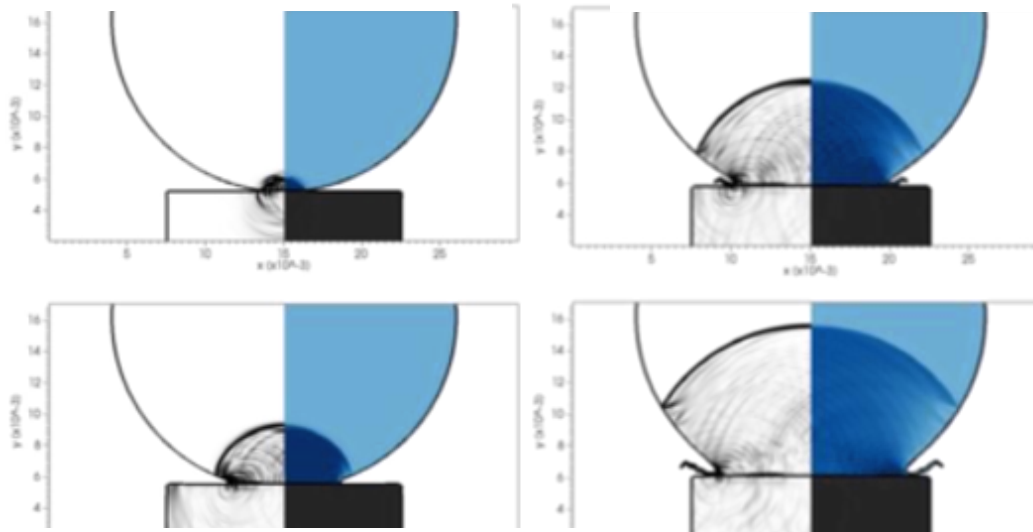
3. This alters the state of what theoretically is "ambient conditions"

4. As a result, the jet happens later, and damage to metal increases

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Multiphysics and two-way interaction

- Lightning attachment to an aircraft substrate is governed by their interaction

1. Current wants to take the shortest path through the substrate

2. Where it attaches, it damages the substrate, making it less conductive
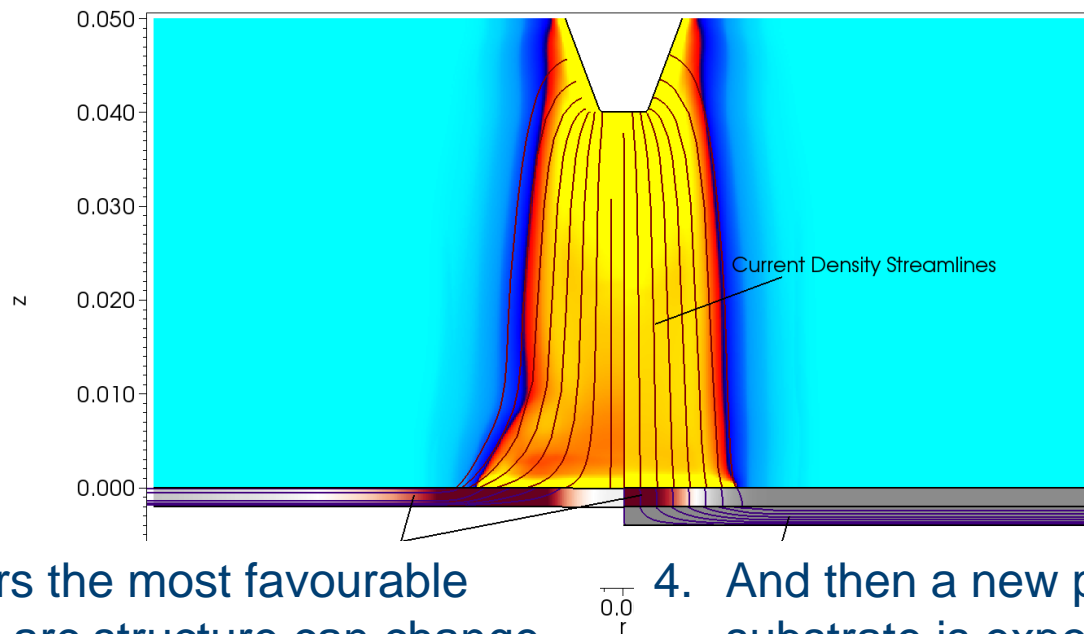
3. This alters the most favourable path; the arc structure can change

4. And then a new part of the substrate is exposed to high current

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Numerical multiphysics simulations

- These lectures consider the tools required for numerical simulation of multiphysics situations

- We focus on Eulerian 'single-code' models, after discussing the available methods

- Even within this restriction, there is no single 'best technique' to deal with multiphysics behaviour

- The choice of method depends on the physics of the situation and how the materials interact

- Development of these methods is still an active research area

- It may even be that multiple multiphysics models are used (multi-multiphysics?)

Techniques to model multiple materials

1. Each material is modelled using a separate code (or code instance) on its own mesh
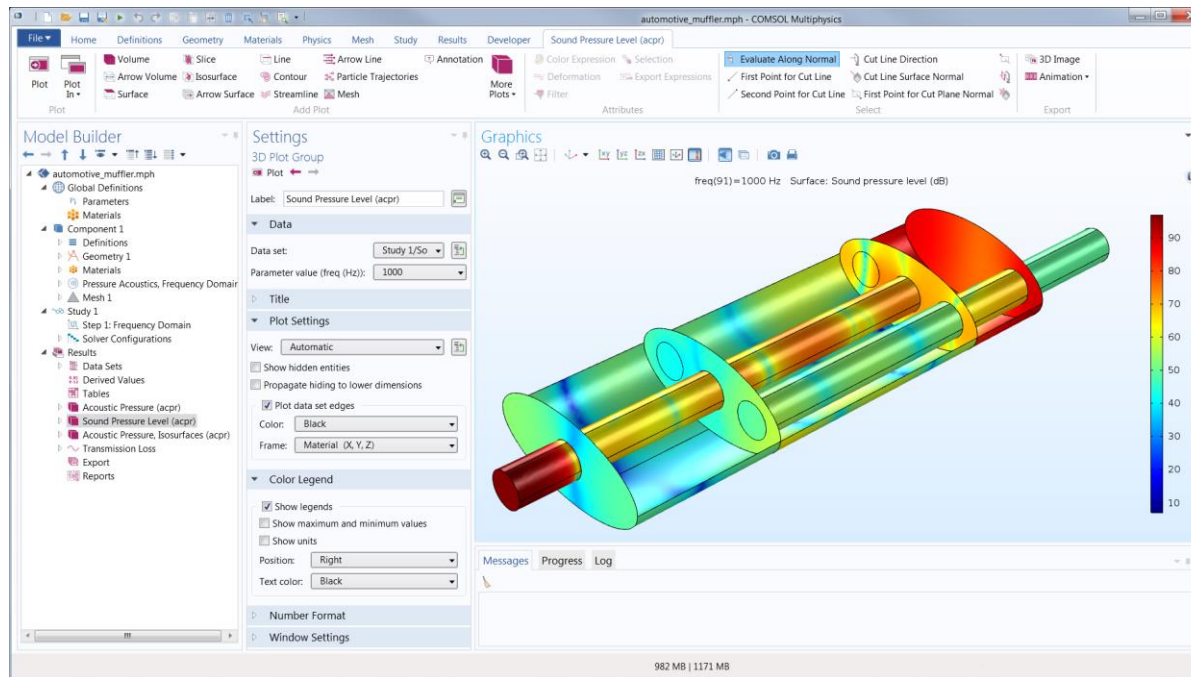
Source: COMSOL Multiphysics

- This is the typical approach when using commercial 'off-the-shelf' packages
- The **co-simulation** approach

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Techniques to model multiple materials

1. Each material is modelled using a separate code (or code instance) on its own mesh

Advantages:

- Simplicity – no need to write code

- Speed of implementation

Disadvantages:

- Passing information between models is difficult, and can introduce error

- Especially for two-way feedback

- If physics is missing from the code, it can be hard (or impossible) to add

- Lack of flexibility of your own code

Techniques to model multiple materials

2. Each material has its own Lagrangian mesh fitted to its own geometric configuration
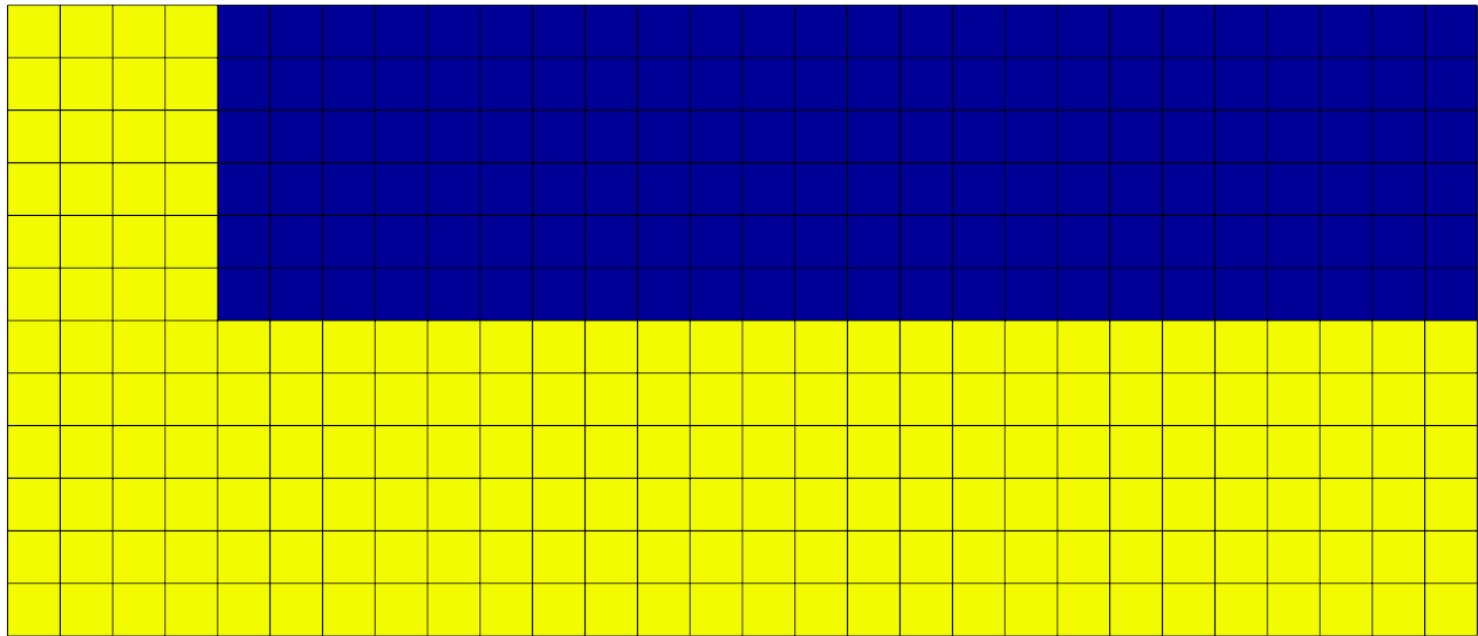
Source: LLNL BLAST

- This does, of course, require you to start with Lagrangian modelling

Techniques to model multiple materials

2. Each material has its own Lagrangian mesh fitted to its own geometric configuration

Advantages:

- An interface between materials is captured at the same time as meshing

- Interactions between materials can then be easily modelled

- These methods can be very accurate (high-order)

Disadvantages:

- All the disadvantages of Lagrangian meshes remain

- Stability can be harder to achieve

- Does not deal with the case where we might have a physical transition region between materials

Techniques to model multiple materials

3. All materials are represented on a single mesh, possibly with multiple materials existing in a given region

- Allows for an Eulerian description of material evolution

- Any material interfaces are referred to as **embedded**
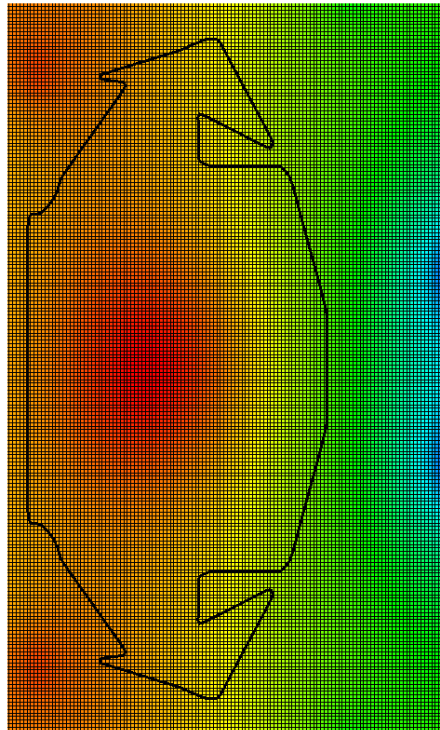
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Techniques to model multiple materials

3. All materials are represented on a single mesh, possibly with multiple materials existing in a given region

Advantages:

- Interactions can be modelled between materials, either with a distinct interface or a transition region

- Complex interface structures are only limited by mesh resolution

- And uniform meshes can be used; simple to generate and no remeshing

Disadvantages:

- Some technique to model where materials exist is now needed (more equations to solve)

- There can be accuracy issues at boundaries

- Not yet common in commercial codes – you'll have to write these methods yourself

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- Multiphysics approaches

What are the challenges of multiphysics modelling

- To illustrate the challenges, we consider a simple situation – two ideal gases

- As a wave passes through one material, it will eventually interact with the interface

- Our model needs to capture any waves transmitted, and any waves reflected when this interaction occurs

- This interaction will also give velocity to the interface
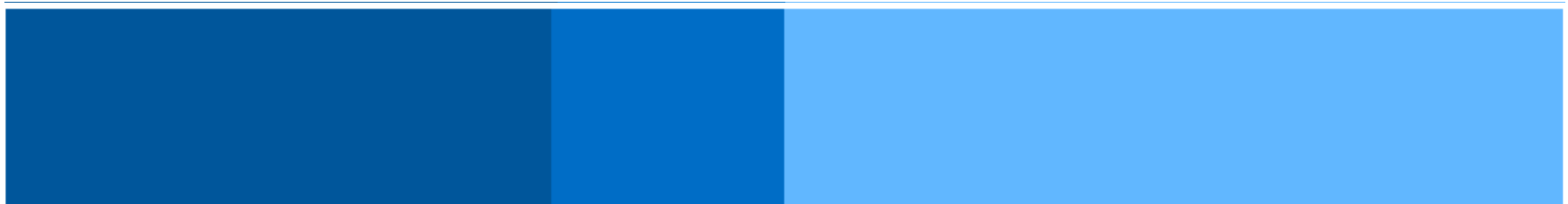
$$p = (\gamma_1 - 1)\,\rho e \qquad\qquad p = (\gamma_2 - 1)\,\rho e$$

Why are these challenges to model?

- It is worth considering why modelling the interaction between two materials is actually difficult

- To do this, we consider the simplest dynamic test case we can – the entire domain moving with a single velocity

- The physics of the material interface here is simple, it should also move with the material velocity

- So a simple assumption might be to have equation of state parameters being a function of space; governed by this velocity

$$p = (\gamma_1 - 1)\rho e \qquad\qquad p = (\gamma_2 - 1)\rho e$$

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Why are these challenges to model?

- The underlying evolution equations are straightforward; for the fluid variables, we just need the compressible Euler equations

$$\frac{\partial}{\partial t}\begin{pmatrix} \rho \\ \rho v \\ E \\ \gamma \rho \end{pmatrix} + \frac{\partial}{\partial x}\begin{pmatrix} \rho v \\ \rho v^2 + p \\ (E+p)\,v \\ \gamma \rho v \end{pmatrix} = 0$$

- If the equatic   another variable within our model, and thus we need an evolution equation to describe it
- We still have an ideal gas equation of state to close this system

- This is simple, since it beh $p = (\gamma - 1)\rho\varepsilon$ ₁ advective tracer

- But since γ is a variable, we have $\dfrac{\partial}{\partial t}(\gamma\rho) + \dfrac{\partial}{\partial x}(\gamma\rho v) = 0$

  $p = p(\rho, \varepsilon, \gamma)$

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Why is this the equation for a material interface?

- A material interface in thermodynamic equilibrium is defined by having a constant pressure and velocity, and a jump in density

- A contact discontinuity is defined by having a constant pressure and velocity, and a jump in density

- From previous lectures, a contact discontinuity moves at the speed of the material, i.e.

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

- When a wave interacts with an interface, we assume (for now) that there is no change in phase, or change in material, of either of the two initial states, i.e. there is no mass transfer over the interface

- Again, the only wave for which this property holds is the contact discontinuity

Testing this approach

- The full initial data for a moving contact discontinuity is

	ρ	v	p	γ
$x \leq x_I$	ρ_L	v	p	γ_L
$x > x_I$	ρ_R	v	p	γ_R

- Two different materials at constant pressure (without thermal diffusion) should simply move at velocity v without generating additional waves

- Numerical diffusion of density is expected, as with any contact discontinuity

- We will also see this diffusion in the equation of state parameter, however, since we would physically expect some mixture region between the gases, this might be reasonable

- To test our simple model, we consider initial data

|	ρ	v	p	γ
$x \leq 0.2495$	1	1	1	1.4
$x > 0.2495$	0.5	1	1	1.67

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The expected result

- The exact solution to this initial data is known, the initial density discontinuity should just propagate to the right
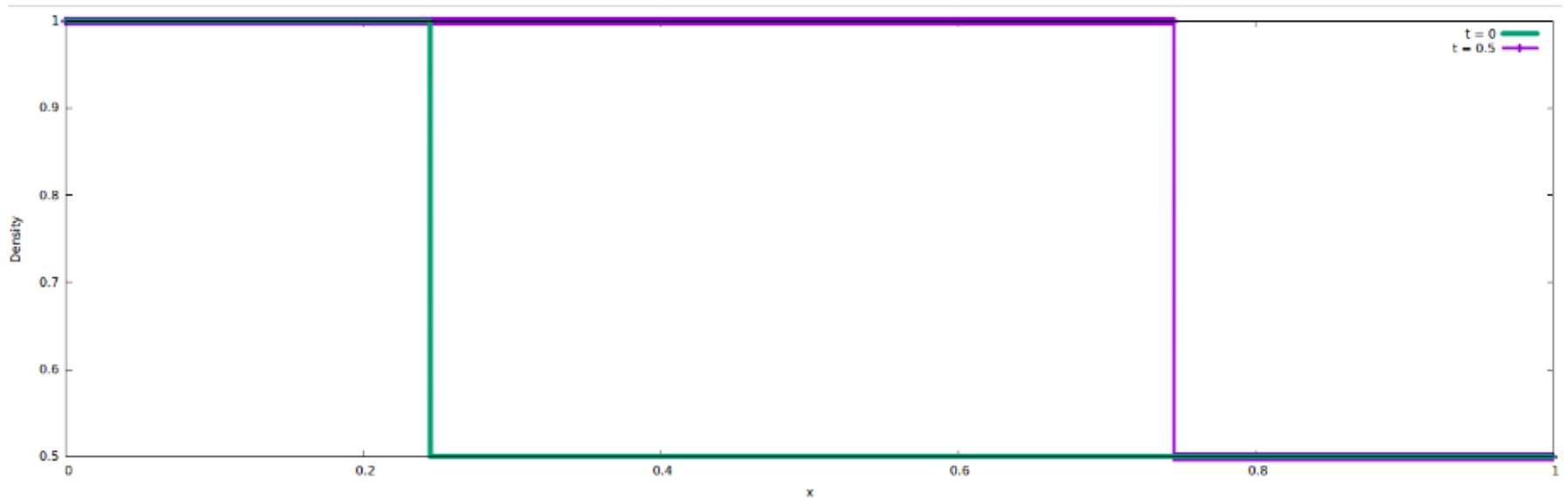
- We attempt to simulate this using our four-equation model

After a very short time…

- Density and velocity are plotted after $t = 0.005$ the evolution should have moved the interface to $x_I = 0.25$

- Unphysical oscillations are seen - it is possible that they will decrease with increased resolution though.
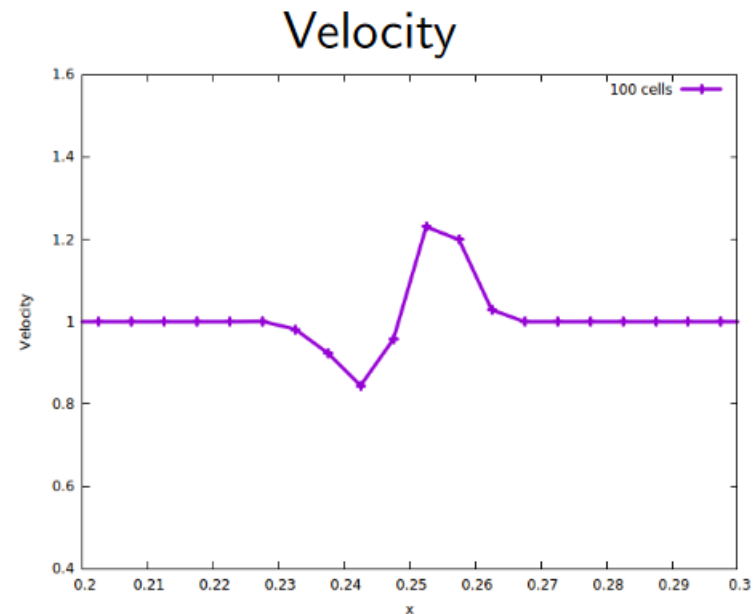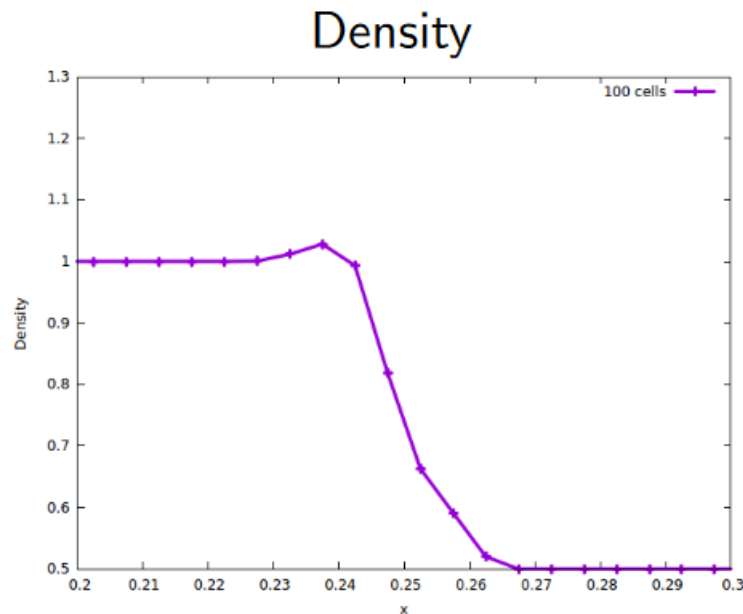
After a very short time…

- We re-run the test case with 800 cells, compared to 100 cells for the original run

- The oscillations are not converging (in fact, the 800 cell simulation crashed shortly after this point)
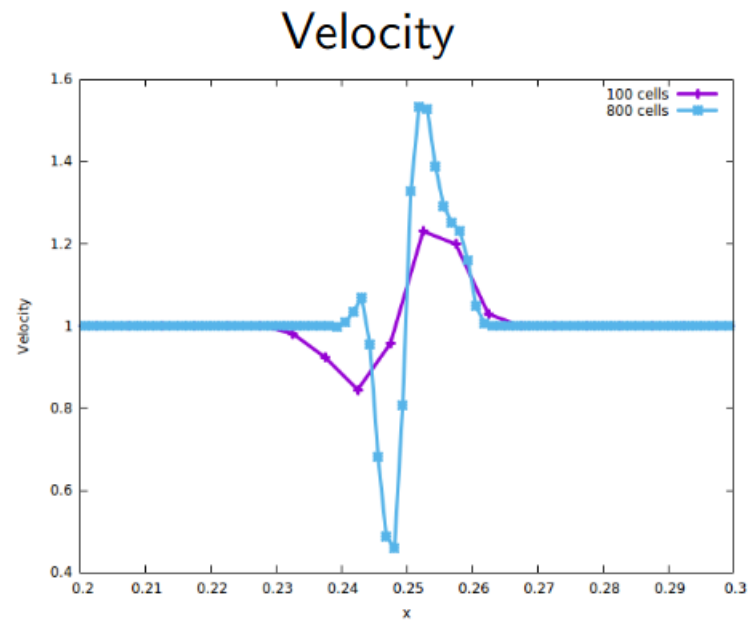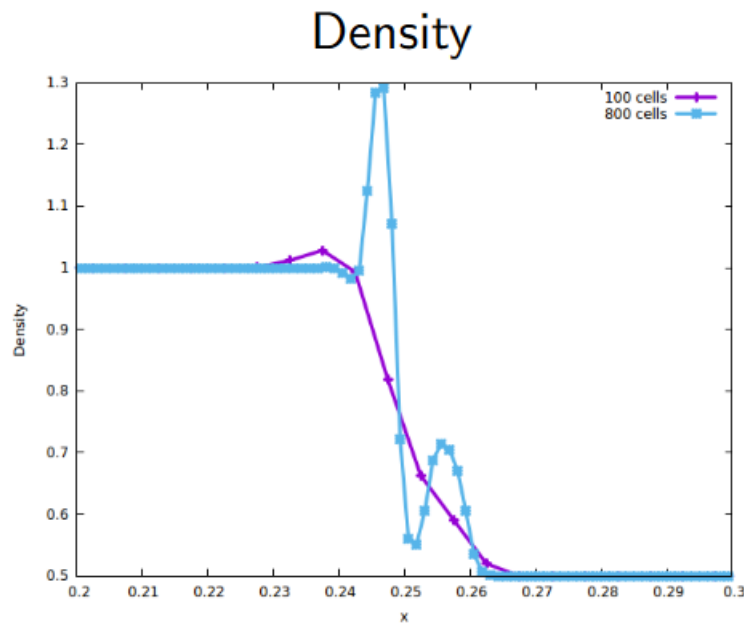
After a very short time…

- The growth of oscillations with resolution demonstrates an instability; something has gone wrong

- We can plot the result using a successful numerical method in green; we see the expected smearing, but no oscillation and a perfectly smooth velocity profile
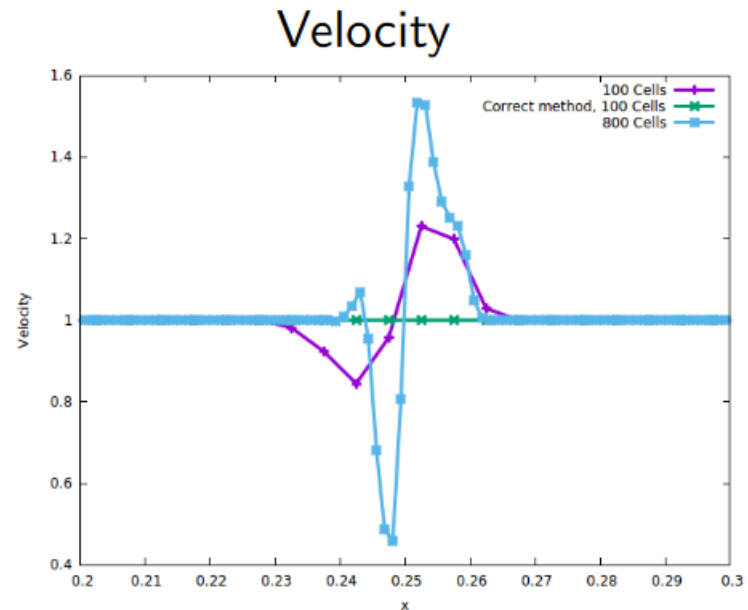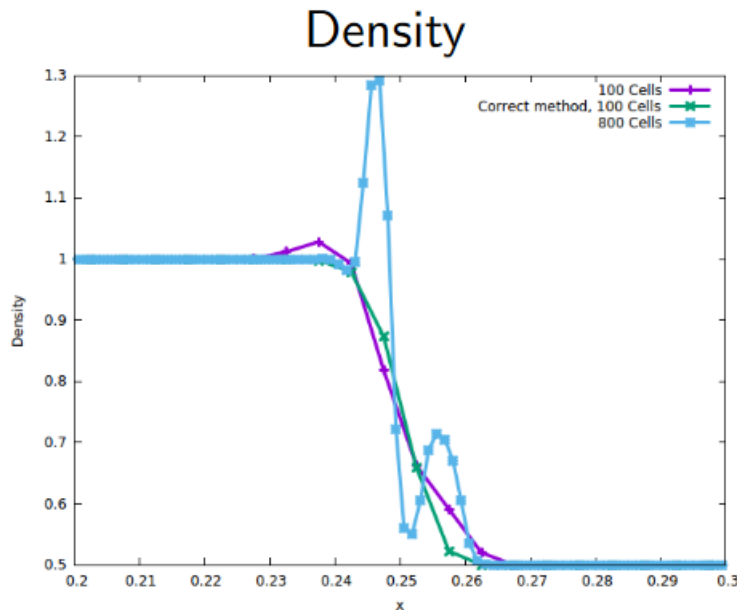
Why does this approach fail?

- By allowing the equation of state to smear, we make the assumption that the ideal gas coefficient for a mixture of our two materials is an average of each individual coefficient

- The results suggest that there are problems with this assumption

- In fact, we can show that we have an under-determined system

- We can demonstrate this by considering the behaviour at the first time step

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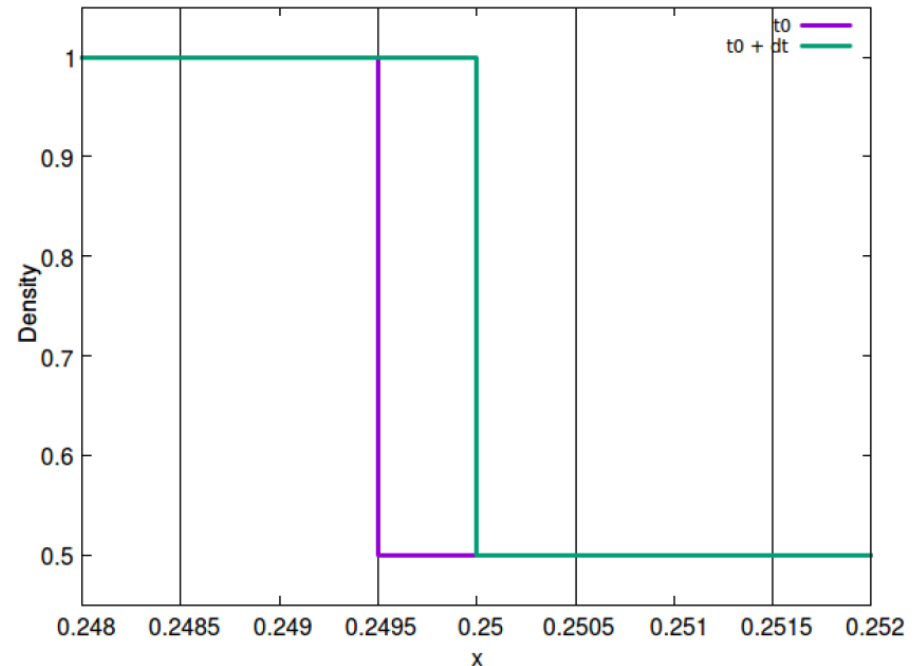
Why does this approach fail?

- We consider a case where we have chosen a time step such that our discontinuity has moved half a cell

- The exact solution in this case would be the discontinuity reaches $x_i = 0.25$

- Under the finite volume representation, we would not see this, of course

- Instead we would have $\rho(x_i) = 0.75$
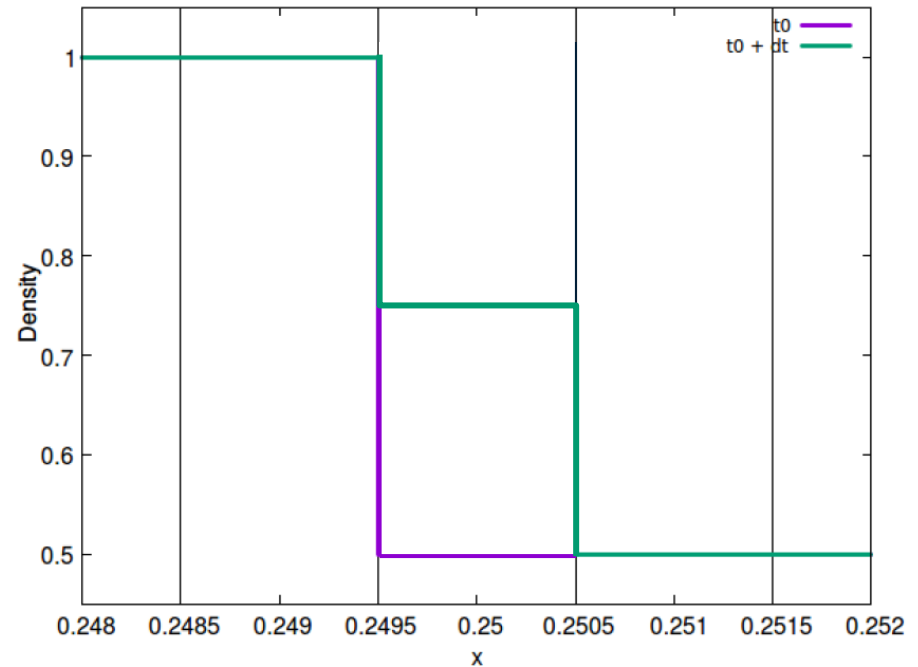
Why does this approach fail?

- For a mixture of chemically non-interacting ideal gases, it is possible to determine an adiabatic mixture constant

$$\gamma_M = \frac{\sum_i n_i \frac{\gamma_i}{\gamma_i+1}}{\sum_i n_i \frac{1}{\gamma_i+1}}$$

- The materials we have chosen: $\gamma = 1.4$ is air and $\gamma = 1.67$ is a monatomic gas

- Both argon and helium are commonly used in experiments

- We can also work out the mixture γ for the evolved cell, using the conserved quantity $\gamma\rho$
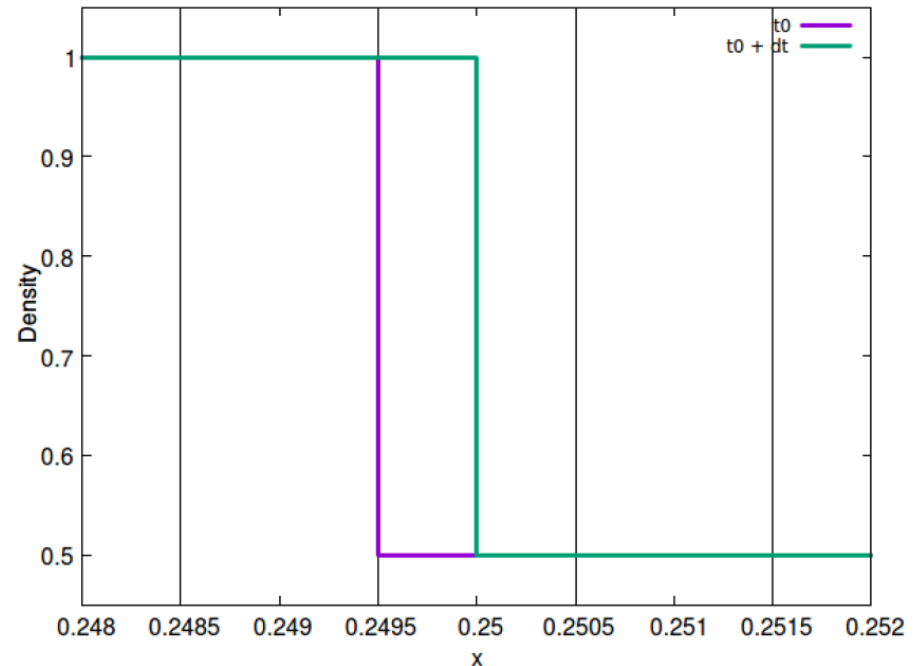
Why does this approach fail?

- As discussed, the interface (and hence $\gamma\rho$) moves with the fluid velocity, and thus has also moved half a cell

- Therefore:

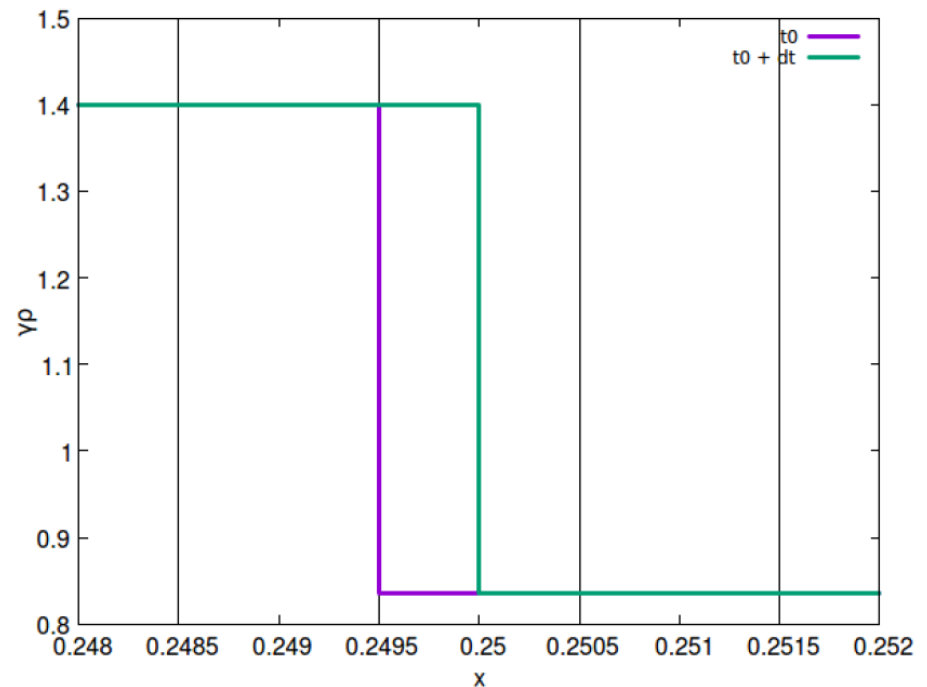$$\gamma\rho = 1.1175$$

- Which means we can compute the mixture value, $\gamma = 1.49$

- Does this correspond to the expected mixture value?

$$\gamma_M = \frac{\sum_i n_i \frac{\gamma_i}{\gamma_i+1}}{\sum_i n_i \frac{1}{\gamma_i+1}}$$

Why does this approach fail?

- In order to compute the mixture adiabatic index, we need to know the number of moles of material within our volume, n_i

- This is where we start to see some issues – we haven't said which noble gas we are using

- This didn't matter for our model, but it does for reality!

- Because argon is heavier than helium, for a given density, we have a different n_i
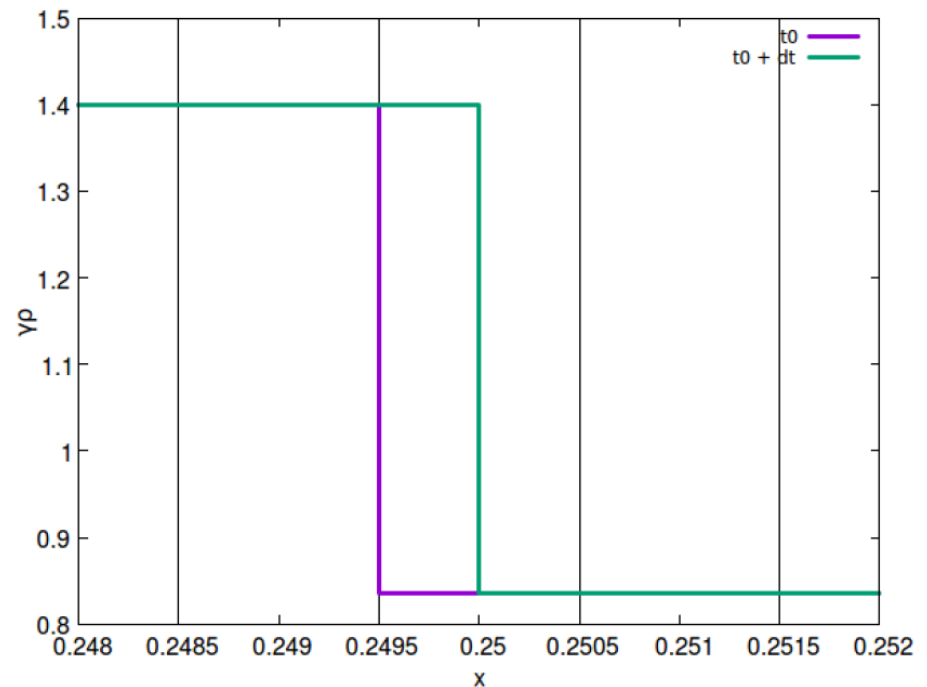
Why does this approach fail?

- The mathematical model we constructed gave us an answer, but this was for an **underdetermined system**

- As a result, this result could well be meaningless

- If we assume our noble gas is argon, then for this mixuture, we have $\gamma = 1.467$

- Since $1.467 \neq 1.49$, this model has clearly been unable to solve for an air-argon interface correctly
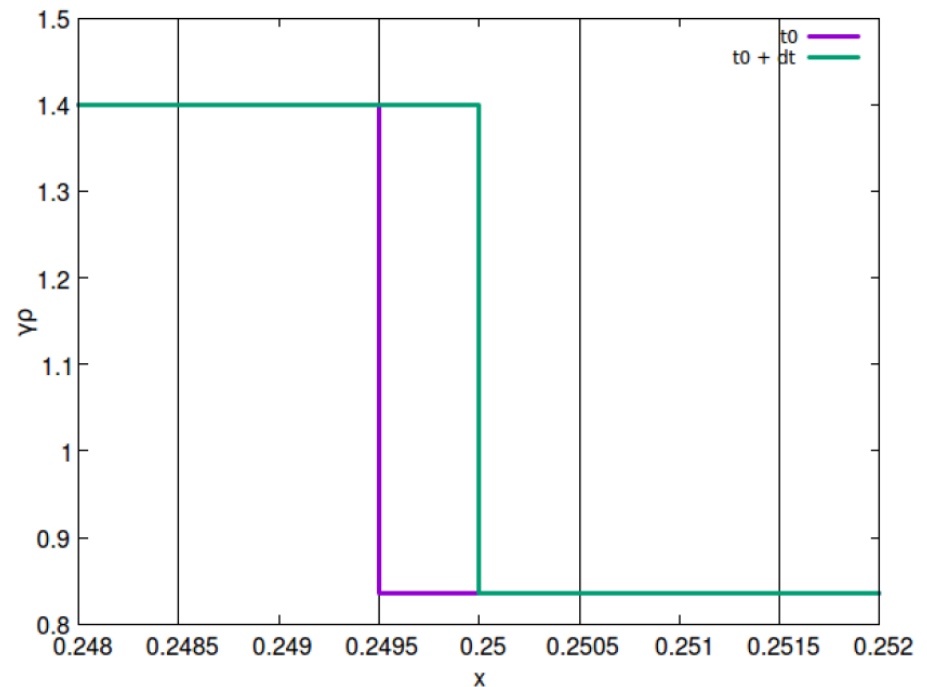
Thermodynamic inconsistency

- We have demonstrated that this naive model leads to an incorrect prediction of γ
- In a coupled system, an error in one variable propagates through, causing errors globally
- The reason for this is clear, an incorrect value of γ leads to a spontaneous change in entropy, which, following the laws of thermodynamics, provides unphysical energy input or removal from the system

$$s \propto \left(\frac{p}{\rho}\right)^{\gamma} \qquad T\mathrm{d}S = p\mathrm{d}V + \mathrm{d}U$$

- This is a **thermodynamic inconsistency** in the underlying equations
- This results in the oscillations seen in the simulation
- The challenge in any multiphysics method is therefore to achieve thermodynamic consistency at the interface between two materials

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Dealing with multiple materials

- Multiphysics methods are those that can deal with material interactions whilst maintaining thermodynamic consistency

- We shall now give an overview of the methods available, before looking at many of them in detail

- First, however, comes a little terminology with how we refer to material interactions, and the methods for simulating them

- Material interactions can either be a sharp **interface**, or a discrete **transition** (on a continuum scale)

- And multiphysics methods can either consider a sharp **jump**, or a **diffuse** region

- There is not a 1-1 mapping between these though

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Material interactions

Sharp transition:
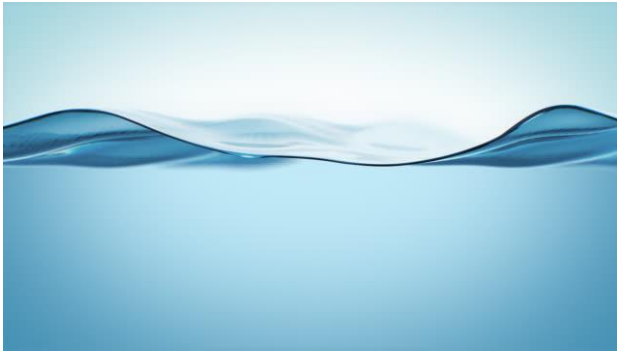
Sharp interface method:
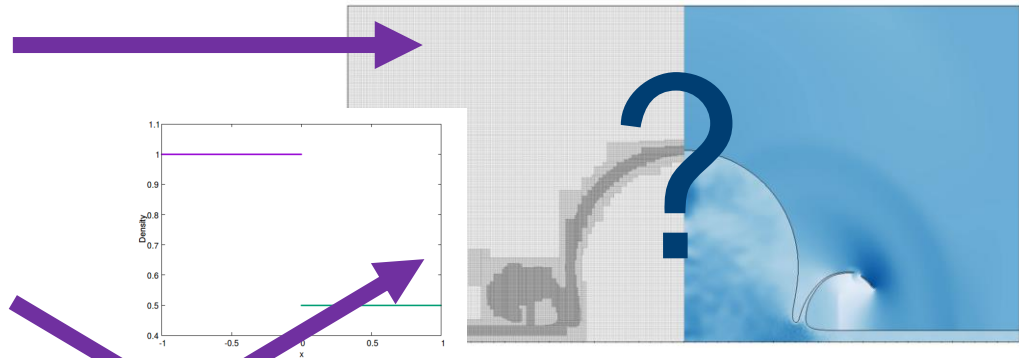
Diffuse transition:

Diffuse interface method:
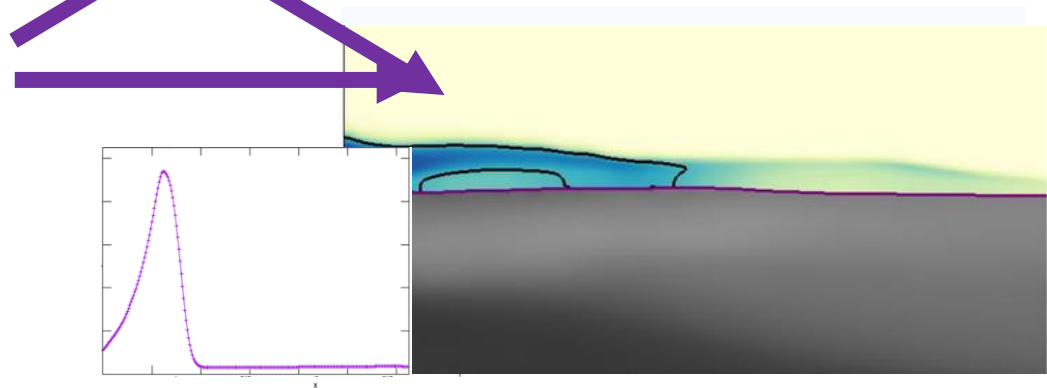
Multiphysics methods

- Both sharp and diffuse interface methods are widely used

- Both have their advantages and disadvantages; their use is often situation-dependent

- And both require additional techniques to be implemented on top of our existing models

- And part of the reason both are still very successful is that they can be used in extremely complex scenarios

Diffuse interface methods
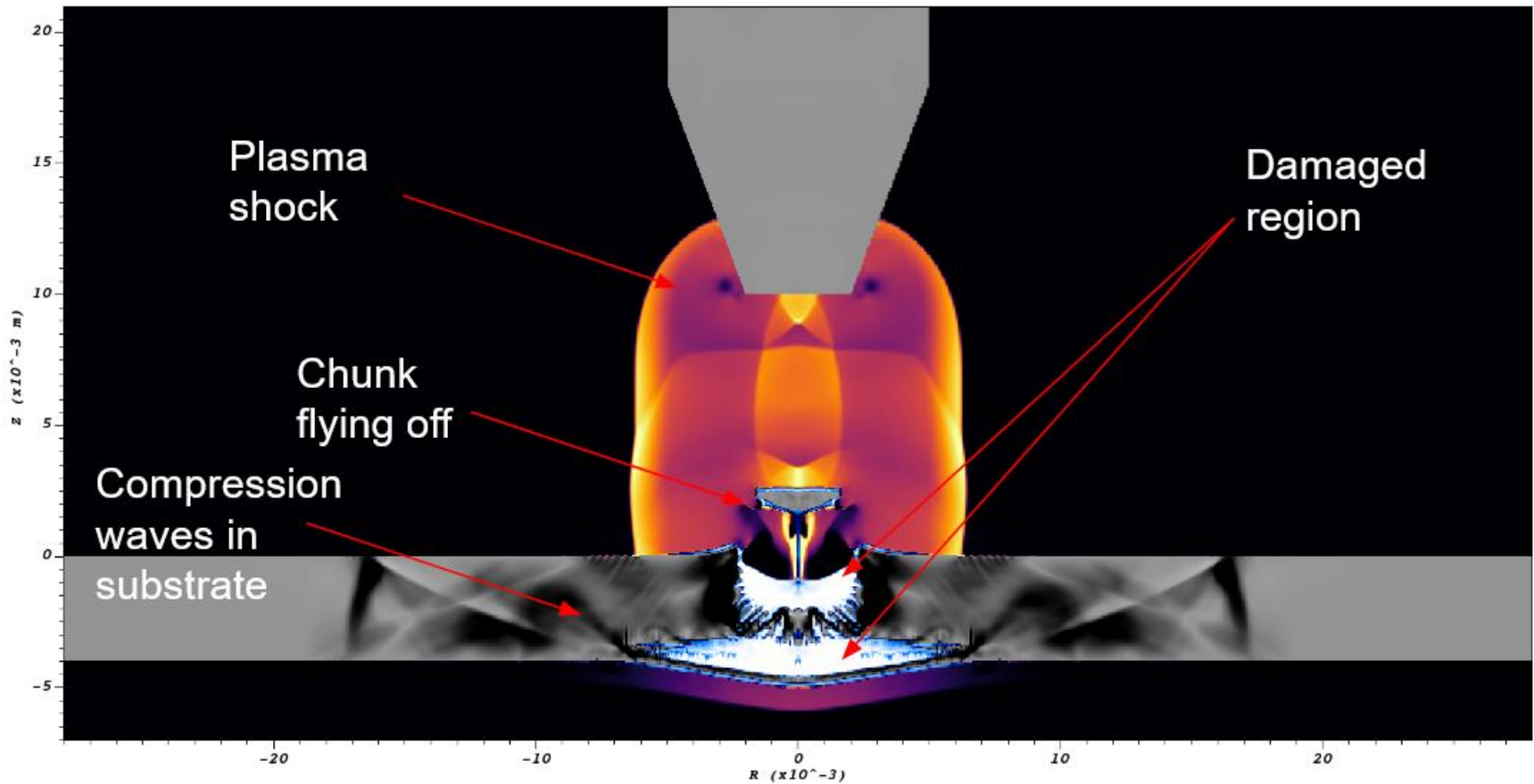
Diffuse interface methods

- Diffuse interface methods use a **single system of equations** to solve multiphysics problems

- This then means that there is numerical evolution of what should be a sharp interface, and hence there will be some smearing, i.e. it becomes a **diffuse interface**

- This results in a **mixture region**; the formulation of the equations is such that this mixture is thermodynamically consistent
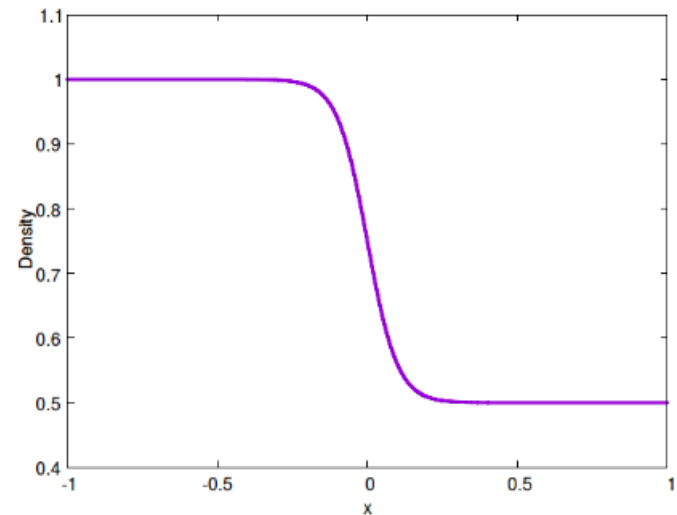
An example diffuse interface formulation

- Many different formulations exist, with different numbers of equations; here we have a **six-equation model**

The amount of material in each computational cell is computed by evolving a **volume fraction** (or a **mass fraction)**

Total quantities are computed through **mixture rules,** e.g. total density

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

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

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

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

$$\frac{\partial}{\partial t}(\alpha_1\rho_1\varepsilon_1) + \frac{\partial}{\partial x}(\alpha_1\rho_1\varepsilon_1 v) + \alpha_1 p_1\frac{\partial v}{\partial x} = 0$$

$$\frac{\partial}{\partial t}(\alpha_2\rho_2\varepsilon_2) + \frac{\partial}{\partial x}(\alpha_2\rho_2\varepsilon_2 v) + \alpha_2 p_2\frac{\partial v}{\partial x} = 0$$

$$\rho = \sum_i \alpha_i\rho_i,$$

At every point in space, **all materials can exist**, with their own density, pressure and/or velocity

Advantages of diffuse interfaces

- The entire system is solved as a single system of equations – dealing with the material interaction is handled by the formulation

- No additional techniques are required to find the interface either, this is part of the formulation

- Allowing both materials to exist within a cell means this is a natural approach to deal with material chemistry and phase change; effectively we 'adjust' the quantities of each material according to the physics

- Forcing terms on the interface, such as surface tension, can be included as source terms for the system

Disadvantages of diffuse interfaces

- There are always some terms in the system of equations which cannot be written in conservative form – this requires additional care in choice of numerical method

$$\frac{\partial}{\partial t}\left(\alpha_1 \rho_1 \varepsilon_1\right) + \frac{\partial}{\partial x}\left(\alpha_1 \rho_1 \varepsilon_1 v\right) + \alpha_1 p_1 \frac{\partial v}{\partial x} = 0$$
$$\frac{\partial}{\partial t}\left(\alpha_2 \rho_2 \varepsilon_2\right) + \frac{\partial}{\partial x}\left(\alpha_2 \rho_2 \varepsilon_2 v\right) + \alpha_2 p_2 \frac{\partial v}{\partial x} = 0$$

- Dealing with these non-conservative terms may then require additional techniques to be implemented

- Because the interface is artificially diffuse, and always spread over more than one cell, there may be situations where this increases error in behaviour at the interface

- Each combination of materials requires its own formulation, it may be difficult to move between them (e.g. suddenly incorporating a solid material)

Sharp interface methods
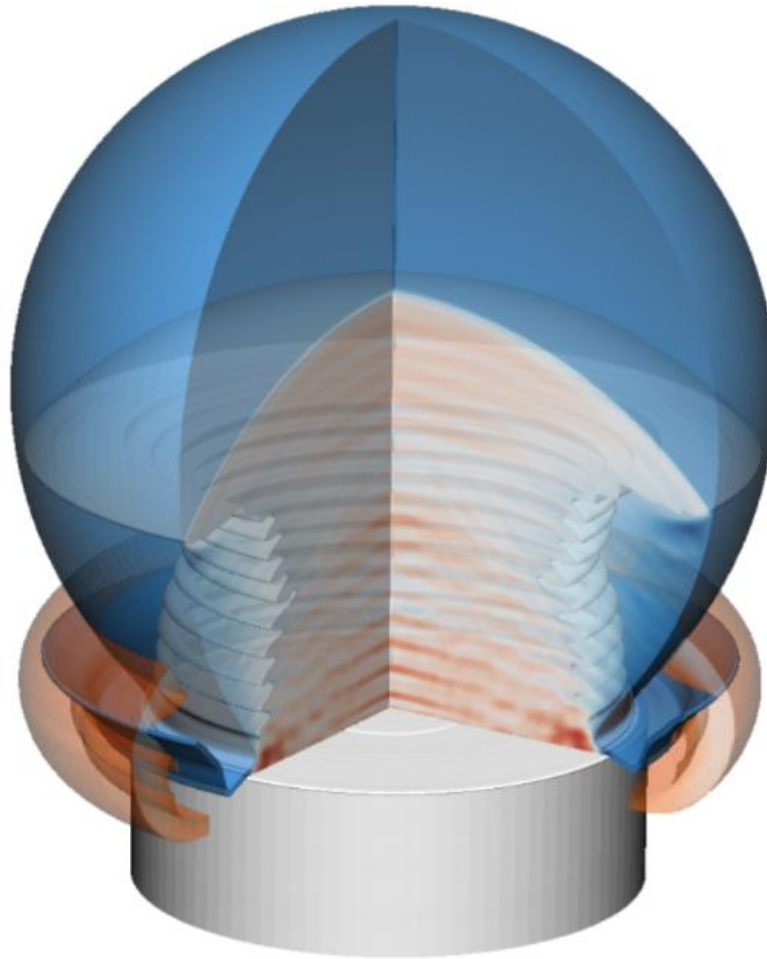
Sharp interface methods

- Sharp interface methods model each material within the system with **its own system of equations**

- An additional method is then required to identify where material interfaces exist

- This method gives every computational cell a unique material (at a given point in time)

- We then need to be able to describe how materials interact with each other
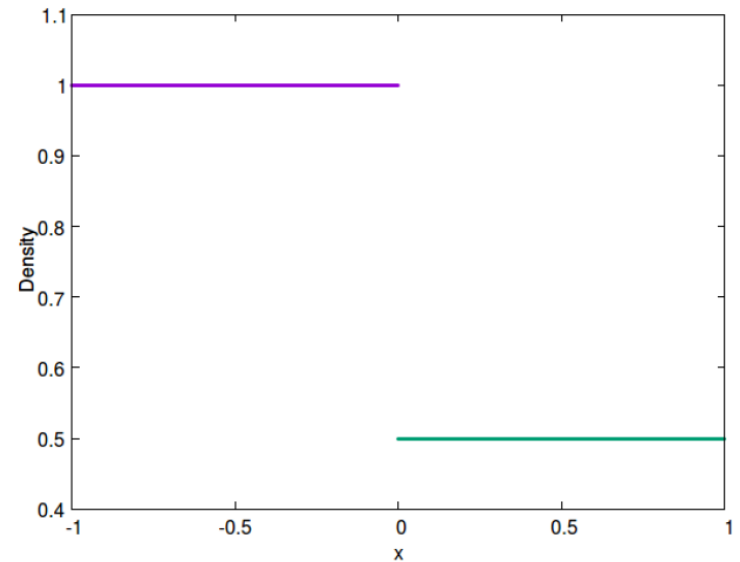
An example sharp interface formulation

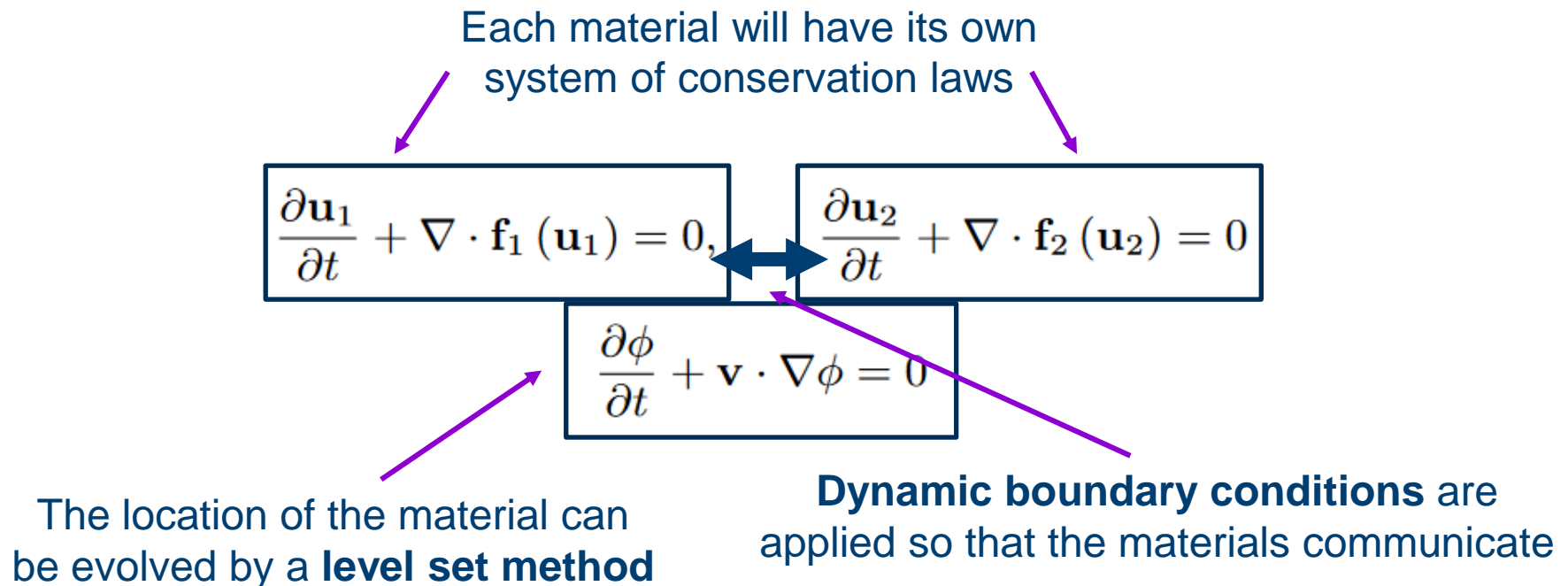- Sharp interface methods are a collection of methods, for dealing with materials and their interfaces, which can be pieced together as needed

Each material will have its own system of conservation laws

$$\frac{\partial \mathbf{u}_1}{\partial t} + \nabla \cdot \mathbf{f}_1\left(\mathbf{u}_1\right) = 0, \qquad \frac{\partial \mathbf{u}_2}{\partial t} + \nabla \cdot \mathbf{f}_2\left(\mathbf{u}_2\right) = 0$$

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

The location of the material can be evolved by a **level set method**

Dynamic boundary conditions are applied so that the materials communicate

Advantages of sharp interfaces

- The numerical methods for each individual material are straightforward – if you have implemented it by itself, it is ready to use

- The methods for each material don't need to be the same either, whatever was easiest/best to implement

- This makes it particularly useful if you need to deal with complex systems of equations, you don't need to work out how e.g. pressure in a liquid and stress in a solid 'mix'

- Because the interface remains sharp, it is easier to capture fine behaviour along it, especially where you wouldn't expect mixing to occur

Disadvantages of sharp interfaces

- Because each cell contains only one material, and this material can change over time, sharp interface methods are not conservative

- This treatment can also lead to a 'stepped' appearance to the interface, which can potentially generate additional waves, especially for slow flows

- Because each cell contains only one material, there is no easy way to model phase change or mixing – techniques exist but are very complex

- You need to be able to describe how any two materials interact – this involves deriving boundary conditions, and you may need to know the characteristic behaviour of your underlying equations

What method is best?

- The best method to use depends on your application, the amount of time you have to implement things, and what you feel most comfortable with

- For phase change and chemistry, diffuse interface methods will always have the advantage

- For fine interface features such as water droplet jetting, or for very complex systems, sharp interface methods have the advantage

- And the two methods can be combined, such as the cativating water droplet (diffuse) impacting a metal substrate (sharp)

- And advanced techniques, such as material fracture, blend these descriptions to some extent within a single interface

What else is there

- In this course, we shall cover diffuse interface methods and dynamic boundary conditions for sharp interfaces (ghost fluid methods)

- There are other options, which we don't have time to go into

1. **Volume-of-fluid** methods – an alternative technique to locating the material interface – can be harder to find interface properties, but common in older work
2. **Arbitrary Eulerian-Lagrangian** methods – attempting to mix the best of both Eulerian behaviour for compression and Lagrangian interface motion – requires understanding of both methods
3. **Multi-material cut cell** methods – use the advantages of cut cell methods to describe material interfaces – still a research area and some of the challenges (material break-up) start to become apparent again

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