

Cavitation, surface tension and fracture

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Outline

- Cavitating flows
- Surface forces
- Fracture

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- Surface forces
- Fracture

What is cavitation?

- Cavitation is pressure-induced phase change of a liquid into a gas (vapour)
- Cavitation occurs when pressure drops (below the **saturated vapour pressure**)
- Different mechanism to boiling, which requires temperature to reach **saturation temperature**
- This means a timescale difference – acoustic timescales, not thermal ones



Why do we want to model cavitation

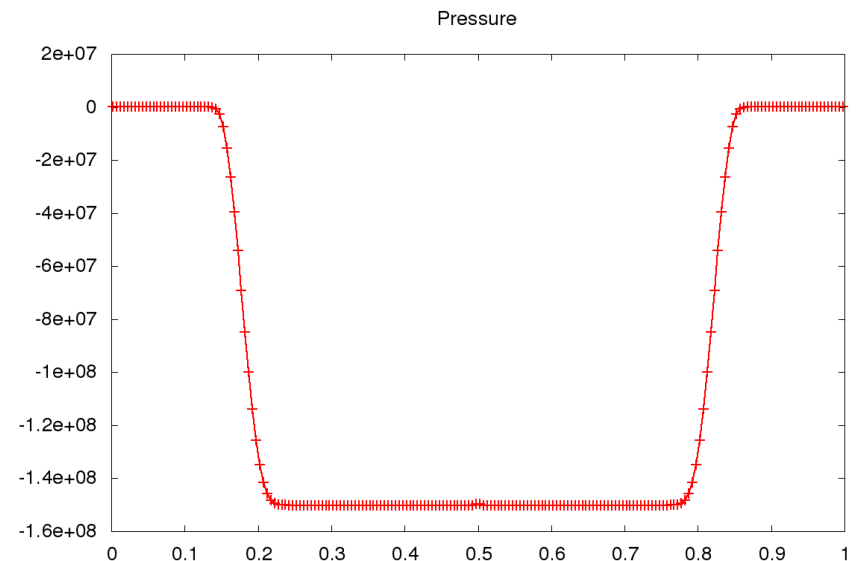
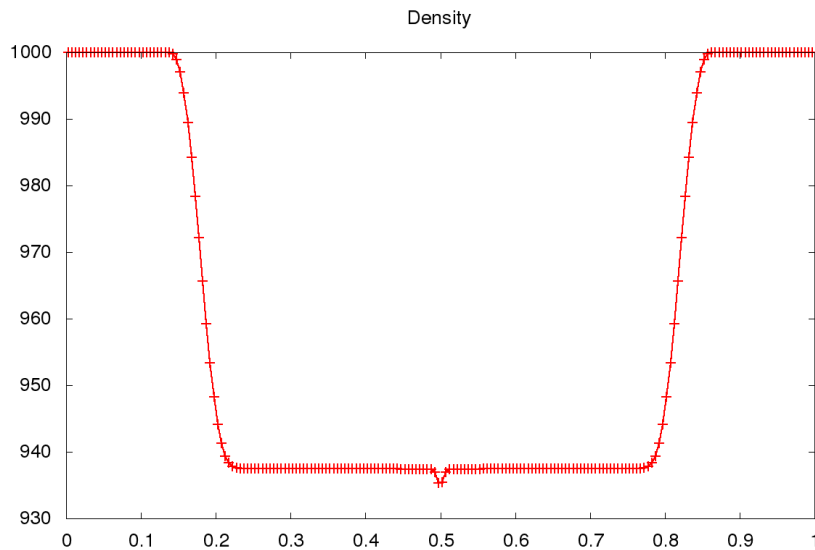
- Cavitation can be a very damaging profile, for example, in turbines



- Bubbles are formed, and when they burst, a shock wave is released
- This can cause erosion
- Additionally, the flow through the material changes in properties, this leads to inefficiency

Liquids in tension

- The stiffened gas EoS does not allow for cavitation to happen by itself
- We could consider a complex, more accurate EoS, and extra terms to model cavitation
- Alternatively, we can consider a multiphysics approach



Diffuse interface approach

- A multiphysics approach means we will treat water and water vapour as two different materials
- Because we need phase change, we have to use a diffuse interface formulation
- Additionally, we need to know when water has reached the saturation pressure, and will cavitate; we need **two pressures** in our model (or two energy equations)
- It is common to assume velocity equilibrium between water and vapour, so a six-equation model is used
- We also need a vapour EoS – it is standard to assume an ideal gas, $\gamma = 1.4$

Diffuse interface approach

- There are multiple six-equation approaches, here we consider the model of Saurel, Petitpas and Berry (2008)

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

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

- Here is the model without source terms

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

- Although written in a different form from our first six-equation formulation, it is equivalent

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

$$\frac{\partial \alpha_g \rho_g \varepsilon_g}{\partial t} + \frac{\partial \alpha_g \rho_g \varepsilon_g v_x}{\partial x} + \alpha_g p_g \frac{\partial v_x}{\partial x} = 0$$

$$\frac{\partial \alpha_l \rho_l \varepsilon_l}{\partial t} + \frac{\partial \alpha_l \rho_l \varepsilon_l v_x}{\partial x} + \alpha_l p_l \frac{\partial v_x}{\partial x} = 0$$

- No improvements in conservation, but nothing is worse, either

Cavitation terms

- The source terms for relaxation are as introduced before
- In this case, we only consider a single interfacial pressure – we drop the prime notation
- This model also provides a description for the interfacial pressure

$$p_I = \frac{Z_l p_g + Z_g p_l}{Z_l + Z_g}$$

- The weighting is based on **acoustic impedances**

$$Z_i = \rho_i c_{s,i}$$

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

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

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

$$\frac{\partial \alpha_g}{\partial t} + v_x \frac{\partial \alpha_g}{\partial x} = \mu (p_g - p_l)$$

$$\frac{\partial \alpha_g \rho_g \varepsilon_g}{\partial t} + \frac{\partial \alpha_g \rho_g \varepsilon_g}{\partial x} + \alpha_g p_g \frac{\partial v_x}{\partial x} = -p_I \mu (p_g - p_l)$$

$$\frac{\partial \alpha_l \rho_l \varepsilon_l}{\partial t} + \frac{\partial \alpha_l \rho_l \varepsilon_l}{\partial x} + \alpha_l p_l \frac{\partial v_x}{\partial x} = p_I \mu (p_g - p_l)$$

. Saurel, Gavriluk and Renaud (2003)

Conservation concerns

- It is clear that the non-conservative form will be an issue here
- We have already stated how shockwaves are an important consequence of cavitation
- Saurel et al. find that adding an additional equation helps here
- By additionally evolving the conserved quantity of total energy, conservation errors in specific internal energy can be "corrected"

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

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

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

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

$$\frac{\partial \alpha_g}{\partial t} + v_x \frac{\partial \alpha_g}{\partial x} = \mu (p_g - p_l)$$

$$\frac{\partial \alpha_g \rho_g \varepsilon_g}{\partial t} + \frac{\partial \alpha_g \rho_g \varepsilon_g}{\partial x} + \alpha_g p_g \frac{\partial v_x}{\partial x} = -p_l \mu (p_g - p_l)$$

$$\frac{\partial \alpha_l \rho_l \varepsilon_l}{\partial t} + \frac{\partial \alpha_l \rho_l \varepsilon_l}{\partial x} + \alpha_l p_l \frac{\partial v_x}{\partial x} = p_l \mu (p_g - p_l)$$

Pressure relaxation

- In order to achieve cavitation, we cannot avoid doing something to deal with these source terms, i.e. we need μ .
- The actual timescale over which cavitation occurs is still fast, we can still make the **instantaneous relaxation** assumption $\mu \rightarrow \infty$
- However, in this case, we don't reduce to the five-equation system since we are saying that this relaxation instantaneously causes **phase change**
- We deal with this in the normal manner for source terms – operator splitting
- The actual process, of relaxing to a known state, is similar to how plasticity is accounted for in elastoplastic solids
- And it is done through a technique we didn't actually consider when dealing with source terms – **analytically solving the ODE** (under a few assumptions)

Pressure relaxation

- This source term treatment requires the analytic treatment of three coupled source terms

$$\frac{d\mathbf{u}}{dt} = \mathbf{S}(\mathbf{u}) \begin{cases} \frac{\partial \alpha_g}{\partial t} = \mu (p_g - p_l) \\ \frac{\partial \alpha_g \rho_g \varepsilon_g}{\partial t} = -p_I \mu (p_g - p_l) \\ \frac{\partial \alpha_l \rho_l \varepsilon_l}{\partial t} = p_I \mu (p_g - p_l) \end{cases}$$

- The source term for all other conserved variables simply states that they are **constant during the relaxation procedure** (which is, itself, important)
- In order to solve this, we know that the solution **must** give $p_l = p_g$
- This is sufficient to close the system; we have four independent variables, the two densities, the volume fraction and the new pressure

Pressure relaxation

- The first step is to remove μ , since we don't want to deal with quantities tending to infinity

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

- We do this by combining these two equations, and using the fact that the conserved terms are constant during this source treatment

$$\frac{\partial \varepsilon_g}{\partial t} = \frac{p_I}{\alpha_g \rho_g} \frac{\partial}{\partial t} \left(\frac{\alpha_g \rho_g}{\rho_g} \right)$$

- The aim here is to be able to write the source term as a relationship between specific internal energy and density (and remove volume fraction) - then we can use the equation of state to equilibrate pressure

Pressure relaxation

- As with the other cases in which we have worked with equations of state, it works out neater (or, at least, follows the literature) if we use specific volume $\nu_g = 1/\rho_g$

- We obtain a direct relationship between specific internal energy and specific volume

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

- Following the same process of removing the relaxation parameter, but for the liquid, gives

$$\frac{\partial \varepsilon_l}{\partial t} = -p_I \frac{\partial \nu_l}{\partial t}$$

- Treating the source term analytically means we now have to integrate these two quantities

Pressure relaxation

- We use a subscript i for either the gas or the liquid states

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

- All quantities with superscript 0 are the initial states computed in the balance-law update part
- It is at this step, an approximation is necessary – we don't know how to compute a $\hat{p}_{I,i}$
- Saurel show that we can assume that $\hat{p}_{I,i} = p$ is sufficient, where pressure without any subscript is the **single relaxed pressure** that both liquid and gas reach through cavitation
- This assumption is consistent with instantaneous relaxation, the interfacial pressure immediately becomes the relaxed pressure

Pressure relaxation

- Using the equation of state, we now have two equations,

$$\varepsilon_i(p, \nu_i) - \varepsilon_i^0(p_i^0, \nu_i^0) + p(\nu_i - \nu_i^0) = 0$$

- Since we have three unknowns, p , ν_g and ν_l , we need to close the system – the volume fraction relationship is sufficient here:

$$\alpha_g + \alpha_l = (\alpha\rho)_g \nu_g + (\alpha\rho)_l \nu_l = 1$$

- Because $(\alpha\rho)_i$ quantities are conserved, we already know these in the relaxed state
- At this stage, the derivation has been quite general. If we stiffened gas (or ideal gas) equations of state, we can even solve this analytically

$$p_i = (\gamma_i - 1) \rho_i \varepsilon_i - \gamma_i p_{\infty, i}$$

- Other EoS may require a root-finding procedure

Pressure relaxation

- Using the equation of state, we get

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

- Our closure of this system came from the relationship between the two volume fractions – these can be obtained through

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

- This gives

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

- When rearranged, this is just a quadratic equation for the relaxed pressure

Pressure relaxation

- The negative root of this equation gives the relaxed pressure (one between the two initial values)
- Once this has been found, the two densities and new volume fractions can be found through

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

- The equation of state **could** now be used to compute the specific internal energy, but this is where Saurel et al. apply a correction term to help conservation
- This is done by obtaining a pressure directly from the conservative total energy

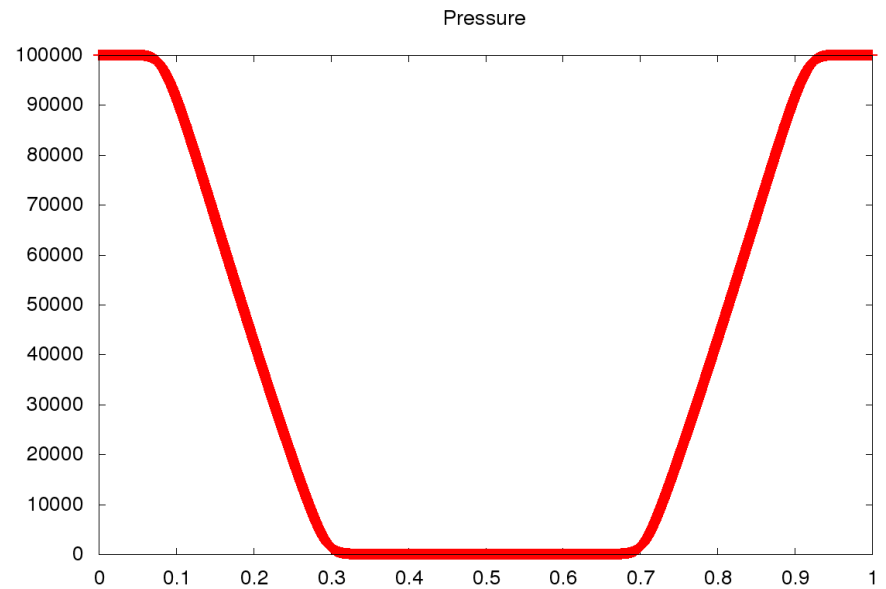
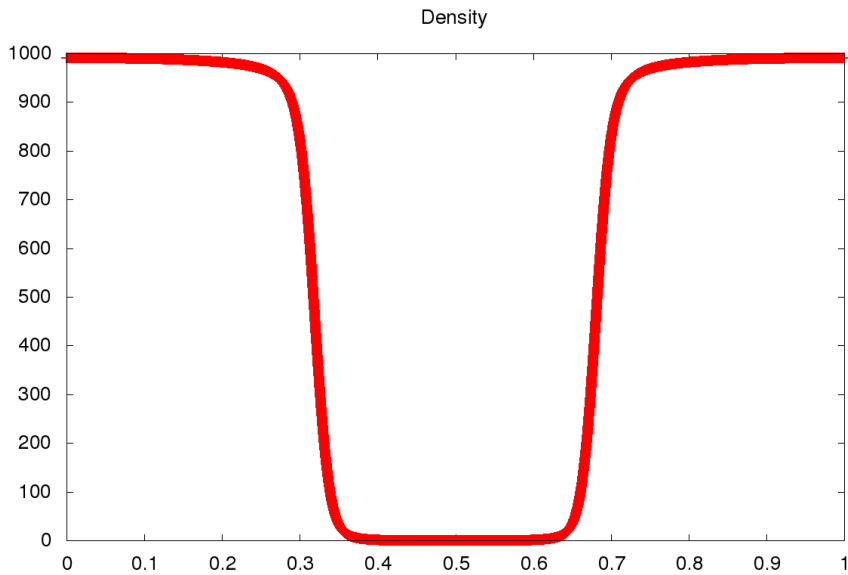
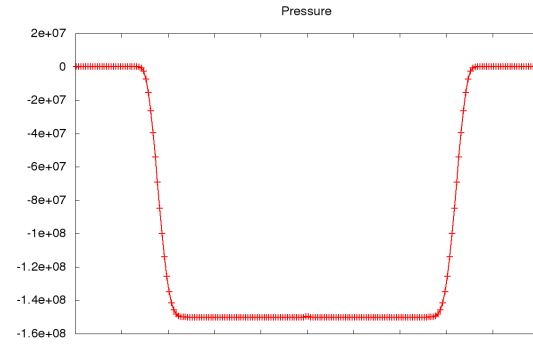
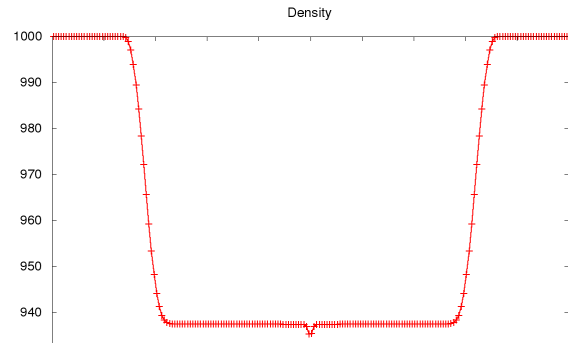
$$\varepsilon_i = \varepsilon_i \left(p_{\text{mix}}, \frac{(\alpha\rho)_i}{\alpha_i} \right), \quad p_{\text{mix}} = \frac{E - \frac{1}{2}\rho v^2 - \sum_i \frac{\alpha_i \gamma_i p_{\infty,i}}{\gamma_i - 1}}{\sum_i \frac{\alpha_i}{\gamma_i - 1}}$$

Total $\rho\varepsilon$
 Mixture γp_{∞}
 Mixture $(\gamma - 1)$

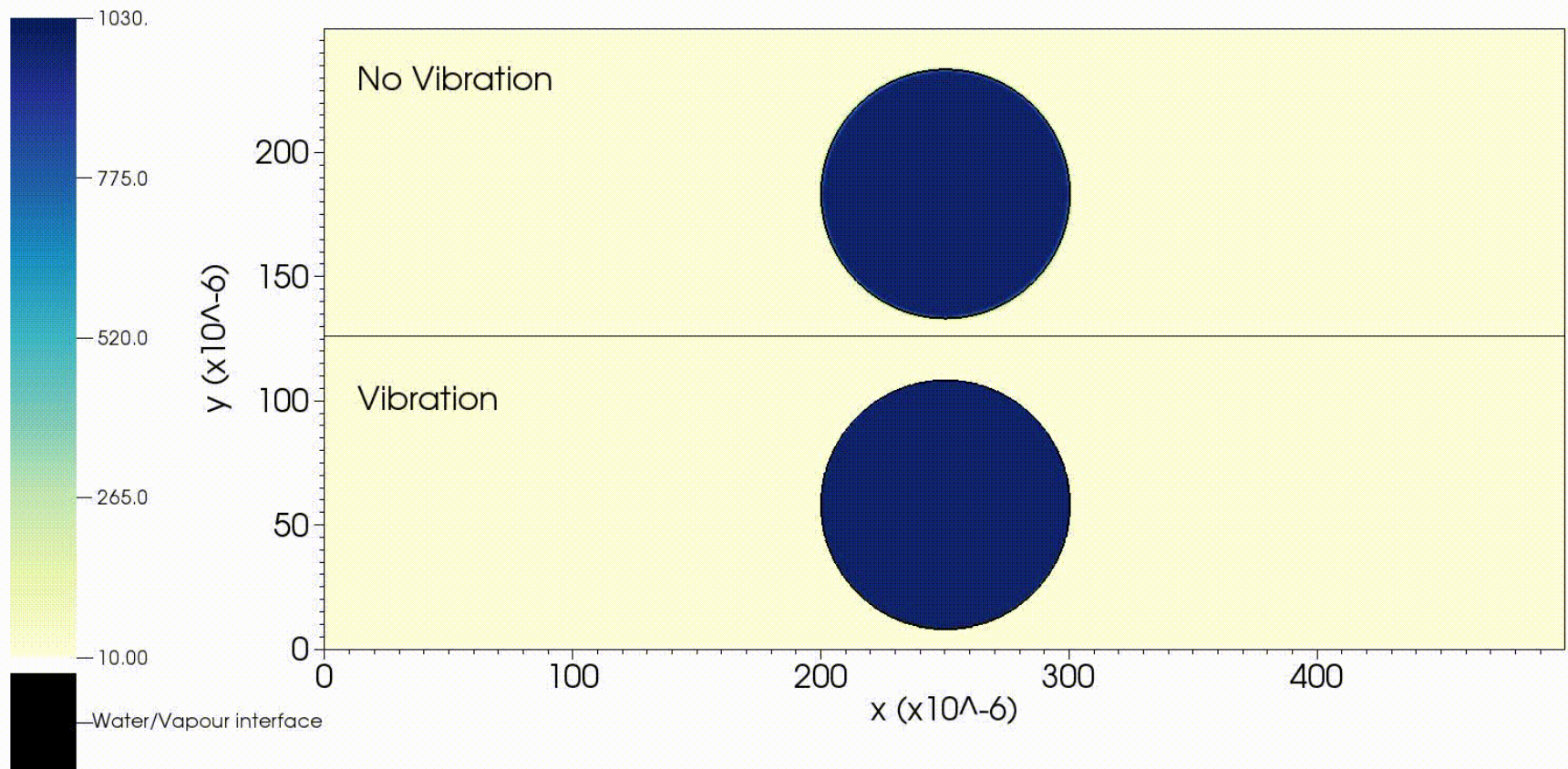
Notes on implementation

- Although standard numerical methods can be used (e.g. primitive variable MUSCL-Hancock with an HLLC approximate Riemann solver), they can be a bit unstable
- Typically, an unsplit version is required, and even then, a lower than expected CFL number (around 0.35)
- The complex nature of the equations makes it hard to identify stability criteria – such restrictions are often found for diffuse interface systems, and these are typically found by numerical experiment
- Additionally, care must be taken to ensure that all computed variables are physical, especially when an approximation is used to compute them
- A good example is p_{mix} , which could easily be negative, but physically, it should be within the bounds of both materials, which in this case, means it must be positive

Cavitation models in practice



Cavitation models in practice



Outline

- Cavitating flows
- Surface forces
- Fracture

Surface forces

- Surface forces are a **local** force caused by the interaction of two materials at an interface
- By their name, they automatically imply a sharp interface, though they could be considered a limit of drag effects between two different materials
- Surface tension and friction are two common examples
- If you know the force, they are mathematically easy to incorporate, for example, if they act on velocity

$$\frac{\partial}{\partial t} \begin{pmatrix} \rho \\ \rho v \\ E \end{pmatrix} + \frac{\partial}{\partial x} \begin{pmatrix} \rho v \\ \rho v^2 + p \\ (E + p) v \end{pmatrix} = \begin{pmatrix} 0 \\ \delta(\mathbf{x} - \mathbf{x}_S) \mathbf{f}_S \\ \delta(\mathbf{x} - \mathbf{x}_S) \mathbf{v} \cdot \mathbf{f}_S \end{pmatrix}$$

- In order for a surface force to exist in this specific set of equations, it would have to be part of a sharp interface multiphysics calculation (or there would be no surface), but the same general form can apply to diffuse interface methods

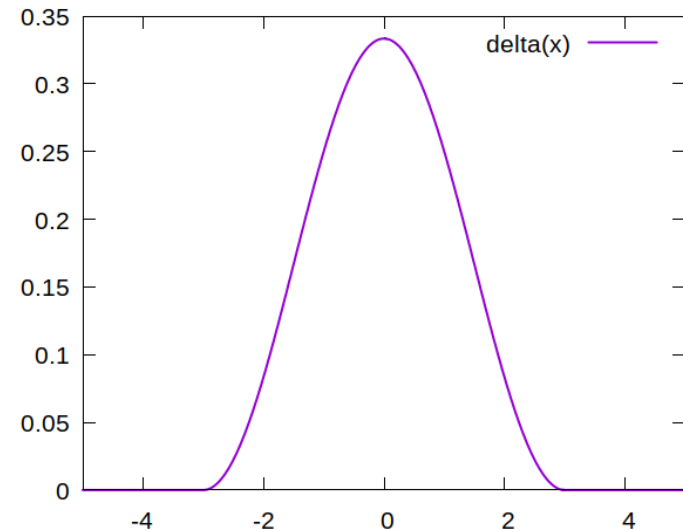
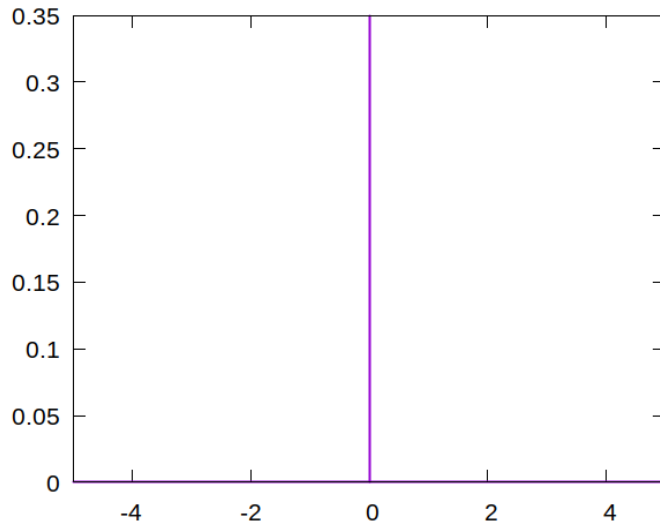
Surface quantities

$$\frac{\partial}{\partial t} \begin{pmatrix} \rho \\ \rho v \\ E \end{pmatrix} + \frac{\partial}{\partial x} \begin{pmatrix} \rho v \\ \rho v^2 + p \\ (E + p) v \end{pmatrix} = \begin{pmatrix} 0 \\ \delta(\mathbf{x} - \mathbf{x}_S) \mathbf{f}_S \\ \delta(\mathbf{x} - \mathbf{x}_S) \mathbf{v} \cdot \mathbf{f}_S \end{pmatrix}$$

- The delta function here is a result of our finite volume treatment – expressing a force which acts only along a surface as a volumetric quantity
- However, this is not great from a numerical method point of view – we compute \mathbf{x}_S from our interface representation, which may only be known at cell centres
- Almost all the time, this would evaluate as zero
- Whilst we could employ some form of interpolation, this could be expensive, and simple, accurate methods exist instead

Surface quantities

- One technique is to replace the delta function with a **smeared approximation**



- In order to make this approximation, the key feature is that the integral under the smeared delta function must be 1

Surface quantities

- One typical smeared delta function is

$$\bar{\delta}(\mathbf{x} - \mathbf{x}_S) = \begin{cases} 0 & |\mathbf{x} - \mathbf{x}_S| > \epsilon \\ \frac{1}{2\epsilon} + \frac{1}{2\epsilon} \cos\left(\frac{\pi(\mathbf{x} - \mathbf{x}_S)}{\epsilon}\right) & |\mathbf{x} - \mathbf{x}_S| \leq \epsilon \end{cases}$$

- Although it may seem like this should introduce a lot of error, smeared delta functions, with the correct choice of epsilon ($\epsilon \propto \Delta x^2$) are second-order accurate
- And they can deal with sharp corners in an interface without issue (which second-order accurate interpolation would struggle with)

Dealing with surface forces – diffuse interfaces

- Having a smeared delta function and a smeared interface is an appropriate combination
- The source term treatment is then based on what the surface force actually is
- Given that we haven't state what the force is, we are hoping that it also can be computed from quantities across a diffuse interface
- The challenge may then come from computing the distance $\mathbf{x} - \mathbf{x}_S$
- Diffuse interface methods obtain the location of the interface through the volume fraction, which does not have any distance information
- We **could** introduce a level set function too, but this is adding additional computational expense
- Alternatively, a smearing based on the volume fraction could be used, but this might be challenging to ensure it obeys the properties of the delta function

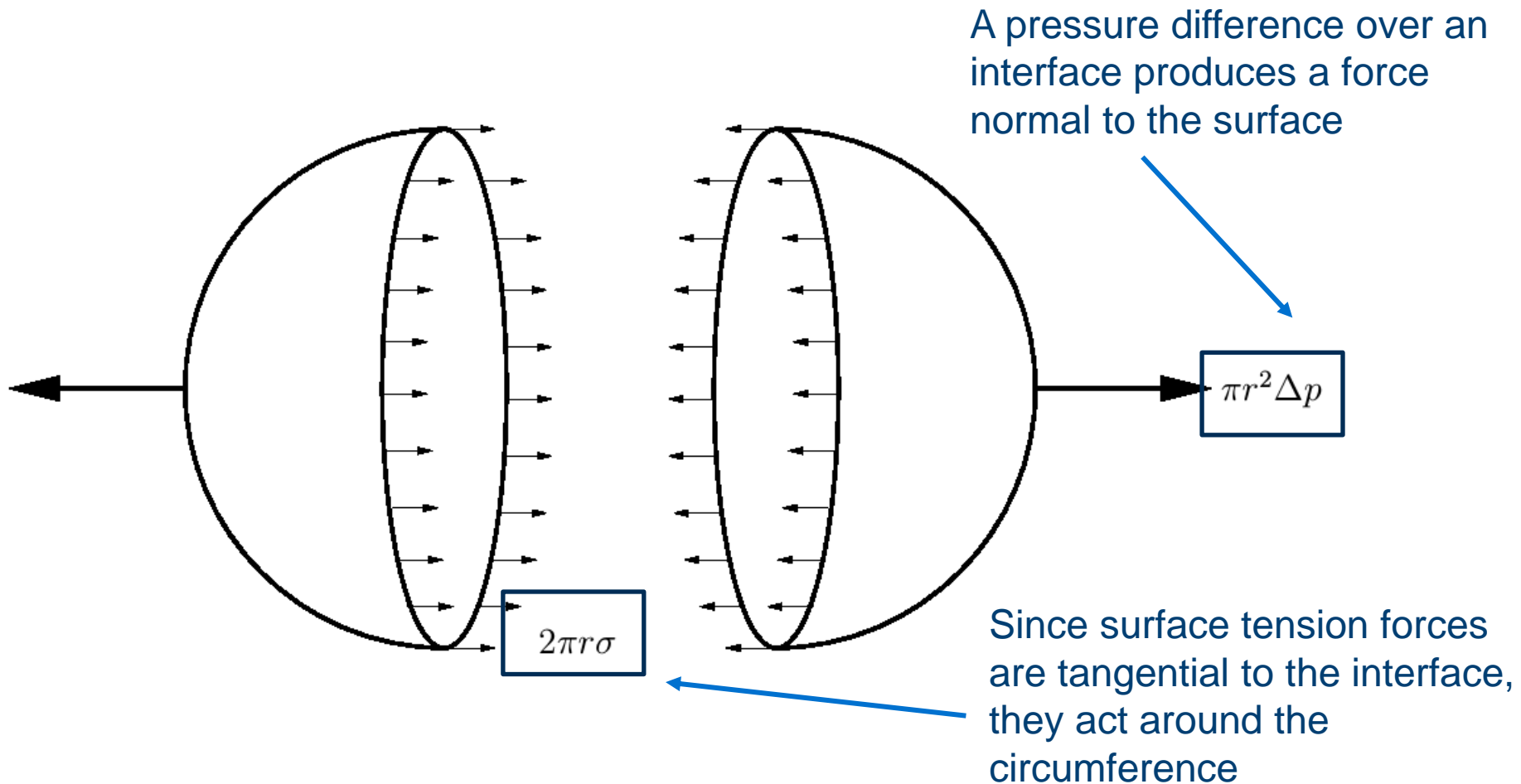
Dealing with surface forces – sharp interfaces

- Given that surface tension assumes a sharp interface, these methods are a natural choice to use
- Here, though, the smearing introduces different problems
- We would be combining smeared behaviour and zero-width behaviour at the same interface; this may lead to thermodynamic inconsistency
- However, an alternative approach is available – surface forces are effectively a condition on the boundary between the two materials
- This might mean we can incorporate them into our dynamic boundary conditions
- To see this, we consider a specific example; surface tension

Surface tension

- The physics of surface tension lies in molecular behaviour – at an interface, there is an asymmetry in the intermolecular forces due to the sudden change
- This creates a force which acts tangentially to the surface – typically represented by the force per unit length between two given materials, σ
- As with most other physical parameters, it needs to be computed either experimentally or from molecular simulations, and there is no reason for it to be constant for differing pressures or temperatures
- One key effect of surface tension for multiphysics is that an interface in thermodynamic equilibrium can now sustain a jump in pressure
- Effectively, the outwards force of pressure is balanced by the surface tension effects

Surface tension



Balancing forces

- For this example of a sphere, the balancing of the two forces gives what is sometimes known as the Young-Laplace law

$$\Delta p = \frac{2\sigma}{r}$$

- From this, we can start to consider what the surface tension source term should look like, considering the momentum equation

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

- Of course, since we have a discontinuity at the interface, we can't actually use this form, but use an integral form instead
- By considering a zero-velocity case, we can show that our surface force is given by

$$\mathbf{S} = \delta(\mathbf{x} - \mathbf{x}_S) \frac{2\sigma}{r} \hat{\mathbf{n}}$$

Surface tension

- We have a source term for a sphere in equilibrium, in general, we have neither spheres nor equilibria
- However, intuitively we can extend this – the surface force requires there to be some curvature of the interface, and a sphere has curvature $2/r$
- Generalising this (which could be done rigorously), we get

$$\mathbf{f}_S = \delta(\mathbf{x} - \mathbf{x}_S) \sigma \kappa \hat{\mathbf{n}}$$

- This adds an additional complication for diffuse interface methods – the curvature and normal vector are not trivial to recover, but techniques exist (e.g. Young's method)
- For sharp interface methods, these are straightforward to calculate from the level set function

Surface tension as a boundary condition

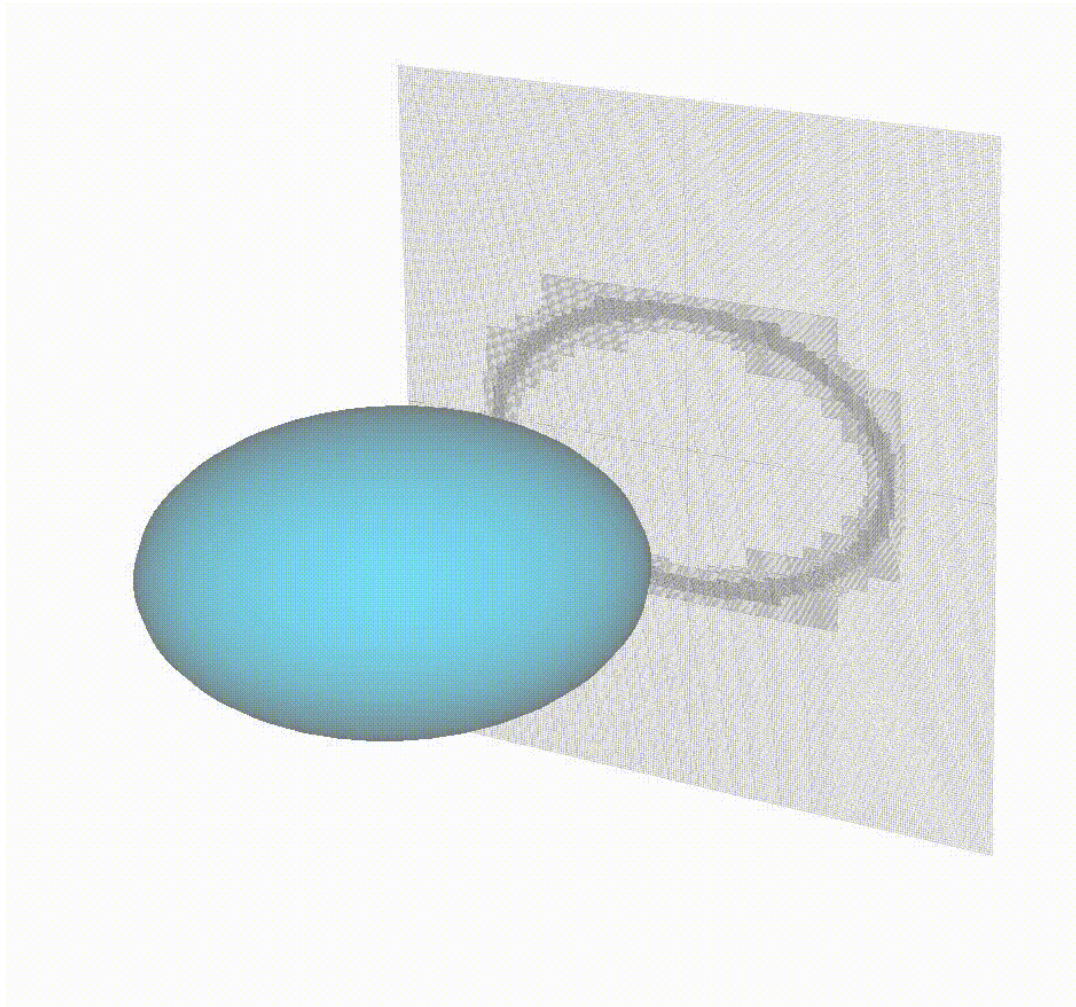
- When we derived dynamic boundary conditions, our first step, in all cases, has been to say we have pressure equilibrium across the interface
- This is no longer true, and, in fact, any method that attempts to use naive implementations of sharp interface methods which enforce this may introduce additional waves
- If we consider a Riemann-problem based GFM, then the first step is to find p^*
- We now have two intermediate pressures, fortunately, we know how they are related; the jump across the interface obeys $\Delta p = \sigma \kappa$
- This then closes the system for an exact Riemann problem solution

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

Surface tension as a boundary condition

- This method was first published by Fechter, Jaegle and Schleper (2013)
- Originally it was applied to Lagrangian material interfaces, but ultimately to the solution of a mixed-material Riemann problem
- The presence of the curvature term doesn't alter the fact that exact solvers (or linearised ones) can still be used, though iterative methods may find it easier to reach an unphysical negative pressure which prevents convergence
- One important note is that curvature contains second derivatives, and this **does** have a negative impact on time step
- It is obvious in diffuse interface methods, but still present in sharp interface methods
- Other surface forces may have similar treatments, but would require derivation of any variable jumps across the interface

Surface tension example



Outline

- Cavitating flows
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Fracture and multiphysics

- In many ways, fracture may seem to be a single material problem - one material is simply breaking and falling apart
- However, this process creates an interface; a feature along which the solid material stops - there must be a second material the other side of it
- This material depends on the solid you are modelling; is it in air? Underwater? Blowing up (i.e. surrounded by explosive)? In vacuum? (Note - many "conventional" codes always model solids in vacuum)
- The presence of the additional material(s) doesn't provide the largest challenge of modelling solids (we've already covered the techniques for this), but how we actually generate the fracture itself
- The challenges are how do we actually determine where this fracture is going to occur? And how do we model the creation of the new interfaces that arise

Damage

- Fracture is not simply a case of a material moving from being one piece to two pieces
- The actual process is complex; stress and strain can cause regions of a solid to separate at the atomistic level
- These are referred to as **micro-voids**, and further stress and strain can either cause these to grow, or additional micro-voids to appear
- Eventually, these become sufficiently large to be visible as a crack in the solid (fracture)
- From a continuum modelling perspective, these micro-voids cannot be individually modelled, instead we treat them as a continuum parameter, **damage**
- The behaviour of this damage is then governed by evolution equations, and requires a physical model to describe it (much like plasticity)

Damage modelling

- Unsurprisingly, modelling damage is very material specific, and even then, many damage models may exist for a given material
- One of the key challenges is that damage may be directionally dependent, either due to anisotropic materials, or the direction of stress and strain
- If we take a plane through a material, with area A_0 , then Bonora (1997) defines damage as the fractional area of this plane occupied by the micro-voids A_{eff}

$$D = 1 - \frac{A_{\text{eff}}}{A_0}$$

- Much like stress, this is a tensorial quantity, and will change depending on the plane
- However, for isotropic materials, we can often get away with using a **scalar damage model**, i.e. damage is a single scalar quantity

Approaches to fracture

- **Lagrangian:**

- Element removal – any element which exceeds some damage threshold is simply deleted – simple, and very non-conservative
- Fracture along element boundaries (cohesive zone method) - conservative, but your mesh can define your fracture pattern

- **Eulerian:**

- Level set-based – seemingly natural since fracture creates sharp interfaces, but defining where fracture happens is hard
- Diffuse interface-based – surprisingly straightforward and appropriate, or possibly unsurprising, since it simply scales up the micro-void-to-damage assumption

Level set-based fracture

- In many ways, it might seem like the sharp interfaces of level set methods are ideal for fracture, at least for metals, where the cracks are often clean
- Indeed, actually setting up the level set function for the fracture is not too difficult
- The challenges, though, are:
 1. When a crack appears, it will initially be very narrow, and would require **two interfaces in a single cell**
 2. When a crack appears, there is a new material within the crack which needs to be given a physical state; unless this state is vacuum, its properties are unclear
- Technically, a cell-deletion approach could also be used, but this is either extremely non-conservative, or requires a tricky mass, momentum and energy redistribution
- Techniques do exist, but are active research topics

Diffuse interface fracture

- To start with, we need a diffuse interface system where one of the materials is a solid

- We use the work of Wallis et al. (2021)

Volume fraction equation as before

$$\frac{\partial \alpha_1}{\partial t} + \frac{\partial}{\partial x_j} (\alpha_1 v_j) = \alpha_1 \frac{\partial v_j}{\partial x_j}$$

Each material still has its own density

$$\frac{\partial}{\partial t} (\alpha_m \rho_m) + \frac{\partial}{\partial x_j} (\alpha_m \rho_m v_j) = 0$$

$$\frac{\partial}{\partial t} (\rho v_i) + \frac{\partial}{\partial x_j} (\rho v_i v_j - \sigma_{ij}) = 0$$

Still a single momentum and total energy equation, i.e. velocity and pressure equilibrium

$$\frac{\partial E}{\partial t} + \frac{\partial}{\partial x_j} (v_j E - v_k \sigma_{kj}) = 0$$

A mixture rule exists for obtaining a mixture stress

$$\frac{\partial \bar{\mathbf{V}}_{ik}^e}{\partial t} + \frac{\partial}{\partial x_j} (\bar{\mathbf{V}}_{ik}^e v_j - \bar{\mathbf{V}}_{jk}^e v_i) = \frac{2}{3} \bar{\mathbf{V}}_{ik}^e \frac{\partial v_j}{\partial x_j} - v_i \frac{\partial \bar{\mathbf{V}}_{kj}^e}{\partial x_j} - \Psi_{ik}$$

$$\frac{\partial}{\partial t} (\alpha_m \rho_m \mathcal{H}_m) + \frac{\partial}{\partial x_j} (\alpha_m \rho_m \mathcal{H}_m v_j) = \alpha_m \rho_m \dot{\mathcal{H}}_m$$

Diffuse interface fracture

- To start with, we need a diffuse interface system where one of the materials is a solid
- We use the work of Wallis et al. (2021)

The deformation gradient has been replaced with the **unimodular left stretch tensor**

$$\mathbf{F}^e = \mathbf{V}^e \mathbf{R}^e$$

$$\bar{\mathbf{V}}^e = \det(\mathbf{V}^e)^{-1/3} \mathbf{V}^e$$

$$\frac{\partial \alpha_1}{\partial t} + \frac{\partial}{\partial x_j} (\alpha_1 v_j) = \alpha_1 \frac{\partial v_j}{\partial x_j}$$

$$\frac{\partial}{\partial t} (\alpha_m \rho_m) + \frac{\partial}{\partial x_j} (\alpha_m \rho_m v_j) = 0$$

$$\frac{\partial}{\partial t} (\rho v_i) + \frac{\partial}{\partial x_j} (\rho v_i v_j - \sigma_{ij}) = 0$$

$$\frac{\partial E}{\partial t} + \frac{\partial}{\partial x_j} (v_j E - v_k \sigma_{kj}) = 0$$

$$\frac{\partial \bar{V}_{ik}^e}{\partial t} + \frac{\partial}{\partial x_j} (\bar{V}_{ik}^e v_j - \bar{V}_{jk}^e v_i) = \frac{2}{3} \bar{V}_{ik}^e \frac{\partial v_j}{\partial x_j} - v_i \frac{\partial \bar{V}_{kj}^e}{\partial x_j} - \Psi_{ik}$$

$$\frac{\partial}{\partial t} (\alpha_m \rho_m \mathcal{H}_m) + \frac{\partial}{\partial x_j} (\alpha_m \rho_m \mathcal{H}_m v_j) = \alpha_m \rho_m \dot{\mathcal{H}}_m$$

Unimodular left stretch tensor

$$\mathbf{F}^e = \mathbf{V}^e \mathbf{R}^e$$

$$\bar{\mathbf{V}}^e = \det(\mathbf{V}^e)^{-1/3} \mathbf{V}^e$$

- This is a polar decomposition of the elastic components of the deformation gradient (and therefore isn't technically a tensor)
- Essentially, the deformation gradient is a rotation of the stretch tensor
- It was shown by Ortega, Lombardini, Pullin and Meiron (2014) that using this formulation avoided issues when one material splits, and then rejoins, but each side of the interface before rejoining has very different deformation gradient
- The stretch tensor itself is a measure of strain, related to the Hencky strain,

$$\mathbf{H}^e = \ln(\mathbf{V}^e)$$

Diffuse interface fracture

- To start with, we need a diffuse interface system where one of the materials is a solid
- We use the work of Wallis et al. (2021)

The evolution of plastic effects has been replaced with the evolution of a **history parameter**

This can then include damage, and can be used by the EoS

$$\frac{\partial \alpha_1}{\partial t} + \frac{\partial}{\partial x_j} (\alpha_1 v_j) = \alpha_1 \frac{\partial v_j}{\partial x_j}$$

$$\frac{\partial}{\partial t} (\alpha_m \rho_m) + \frac{\partial}{\partial x_j} (\alpha_m \rho_m v_j) = 0$$

$$\frac{\partial}{\partial t} (\rho v_i) + \frac{\partial}{\partial x_j} (\rho v_i v_j - \sigma_{ij}) = 0$$

$$\frac{\partial E}{\partial t} + \frac{\partial}{\partial x_j} (v_j E - v_k \sigma_{kj}) = 0$$

$$\frac{\partial \bar{\mathbf{V}}_{ik}^e}{\partial t} + \frac{\partial}{\partial x_j} (\bar{\mathbf{V}}_{ik}^e v_j - \bar{\mathbf{V}}_{jk}^e v_i) = \frac{2}{3} \bar{\mathbf{V}}_{ik}^e \frac{\partial v_j}{\partial x_j} - v_i \frac{\partial \bar{\mathbf{V}}_{kj}^e}{\partial x_j} - \Psi_{ik}$$

$$\frac{\partial}{\partial t} (\alpha_m \rho_m \mathcal{H}_m) + \frac{\partial}{\partial x_j} (\alpha_m \rho_m \mathcal{H}_m v_j) = \alpha_m \rho_m \dot{\mathcal{H}}_m$$

Damaging materials

- In order to achieve fracture in this model, we need to include damage as part of the material history

$$\frac{\partial}{\partial t} (\alpha_m \rho_m \mathcal{H}_m) + \frac{\partial}{\partial x_j} (\alpha_m \rho_m \mathcal{H}_m v_j) = \alpha_m \rho_m \dot{\mathcal{H}}_m$$

- The left hand side of this equation simply advects existing damage around, the right hand side is where we specify how the damage occurs
- We shall ignore plasticity for now, and assume the only history is the damage history

$$\frac{\partial}{\partial t} (\alpha_m \rho_m D_m) + \frac{\partial}{\partial x_j} (\alpha_m \rho_m D_m v_j) = \alpha_m \rho_m \dot{D}_m$$

- Whilst we allow a damage model for every material, for completeness, in some cases this equation can be ignored, e.g. $D_{\text{air}} = 0$

Damaging materials

- In order to provide some form of damage source term for the continuum damage approximation, we start with the effect damage has on stress
- If a damaged material is placed under a certain stress, σ , if it is damaged, it will behave as if it were under a higher stress, the **effective stress**

$$\sigma_{\text{eff}} = \frac{\sigma}{1 - D}$$

- The next step is to assume the **strain equivalence principle**, that the strain a damaged material experiences is given by evaluating strain under the effective stress
- A direct result of this is many material properties can be considered to be **linearly degraded** due to damage, e.g. the shear and bulk moduli, where a tilde quantity is the undamaged value

$$G = (1 - D)\tilde{G}, \quad K = (1 - D)\tilde{K}$$

A damage model

- Using this, it is possible to derive a damage evolution equation (see Wallis et al. for full details)

Material-dependent constants

Effective equivalent plastic strain

$$\dot{D} = \frac{1}{\mathcal{A}} \frac{(D_{\text{crit}} - D_0)^{1/\mathcal{A}}}{\ln(\epsilon_{\text{crit}}/\epsilon_{\text{thresh}})} R_t \left(\frac{p}{\sigma_{\text{eq}}} \right) (D_{\text{crit}} - D_0)^{(\mathcal{A}-1)/\mathcal{A}} \left(\frac{\dot{\epsilon}_p}{\epsilon_p} \right)$$

$$R_t \left(\frac{p}{\sigma_{\text{eq}}} \right) = \frac{2\tilde{E}(1-D)^2 \rho \tilde{\mathcal{E}}^c}{\sigma_{\text{eq}}^2} + \frac{\tilde{E}}{3\tilde{G}}$$

Young's modulus (degraded)

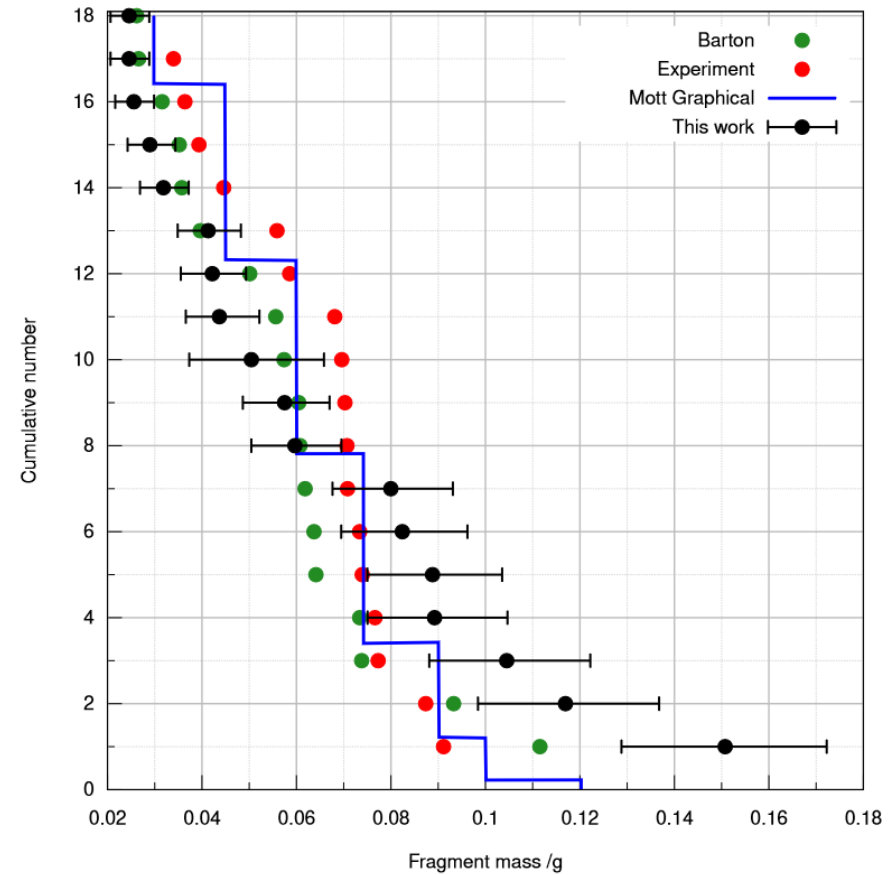
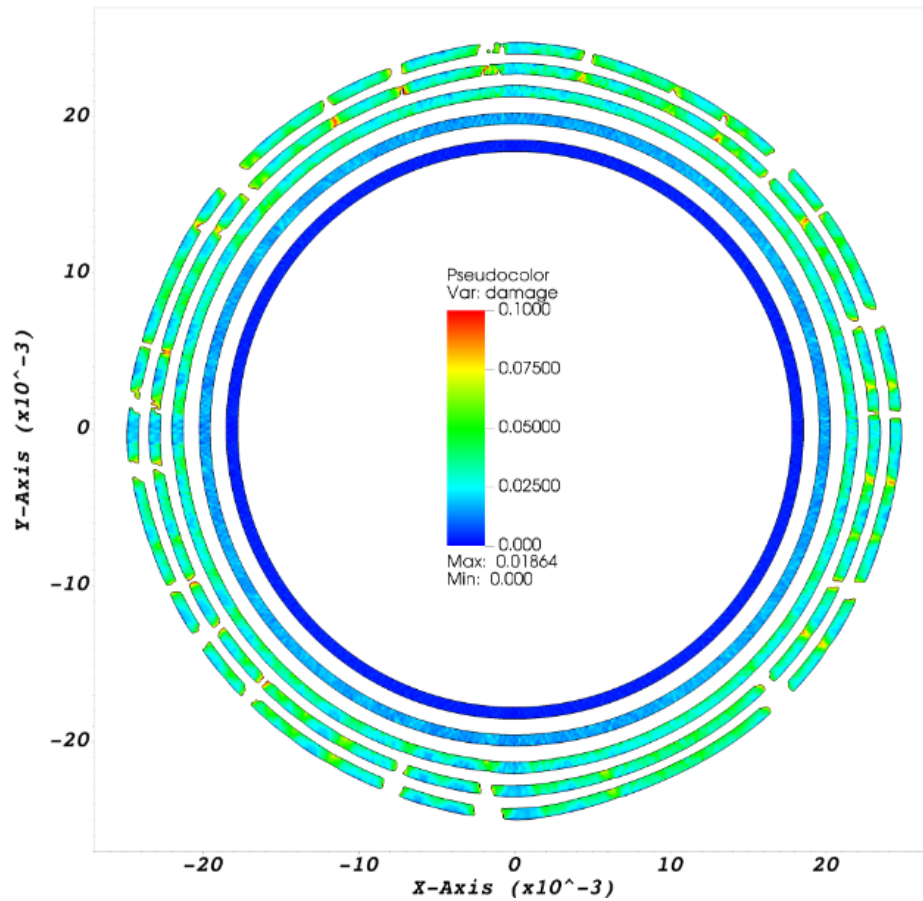
Volumetric shear strain (from EoS)

$\sigma_{\text{eq}} = (1 - D)\sqrt{6}\tilde{G}I_1$

Numerical approach

- The numerical technique for dealing with the damage source term is described, in detail, in Wallis, Barton and Nikiforakis (2021)
- Although the source term looks complex, almost everything required actually comes from the plasticity source term updates
- This includes the information for computing the time derivative of the effective equivalent plastic strain
- For more details on obtaining the plasticity source term update, see Barton (2019)

Fracture prediction



Large-scale fracture

