Advanced continuum modelling
Elastoplastic solids

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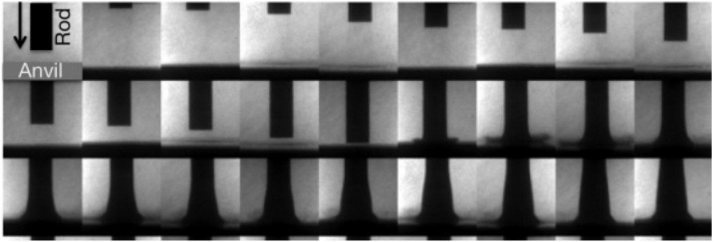
Outline

Numerical models for solids

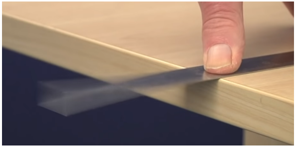
- So far in this course, we have covered models for gases, liquids and plasma
- The only mention to solids we have given so far is when they **behave hydrodynamically**
- Under very high-pressure impact scenarios, solid materials do effectively like a liquid



- This does not, however, provide a very general model

- Obviously, in general, solids behave very differently to the other states of matter
- In order to enable us to model this behaviour, we need to consider the physics behind some of these new properties
- In each case, we consider a situation where we have some initial solid structure, and we then apply force causing this structure to deform:

- **Elasticity**
  Can return to initial configuration
- **Plasticity**
  Permanently change in configuration
- **Fracture**
  Cracks form within the structure

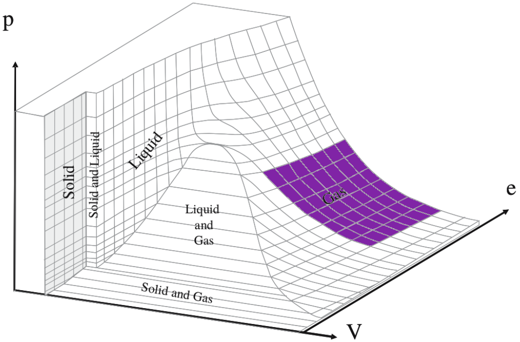


What will we cover?

- Solid mechanics is a large field, with enough material to fill several textbooks - we cannot cover all of it!
- So far, in this course, we have focused on compressible hyperbolic systems of conservation laws - this is not going to change
- It is possible to describe elasticity, plasticity and fracture within this framework - we shall give an overview of how evolution equations are obtained
- To do so, we shall introduce several concepts that were not required for modelling gas, liquid or plasma
- It may appear from the literature that this approach is unusual for modelling solid materials - we first consider why (and when) we want to apply this technique

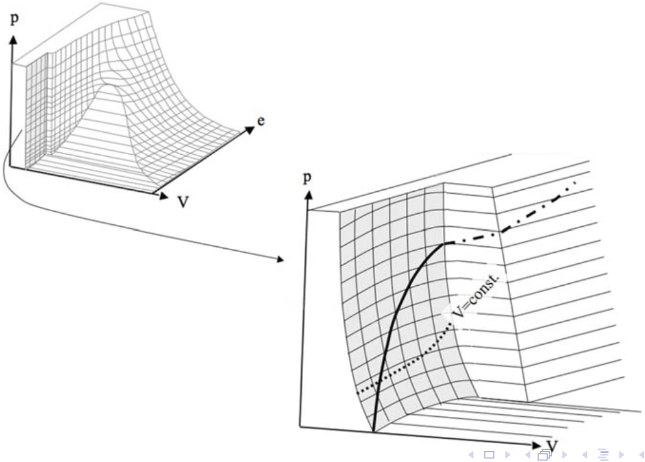
Revisiting the phase diagram

- The phase diagram can be used to visualise when compressible formulations are required
- We have highlighted a region representing the thermodynamic states which might be encountered by an application
- If this region is large, we need a thermodynamically coupled description, $p = p(\rho, \varepsilon)$
- Note that transition between states is not necessarily smooth (shock waves)
- This might be clear for a gas, but is the solid region constant in one variable?



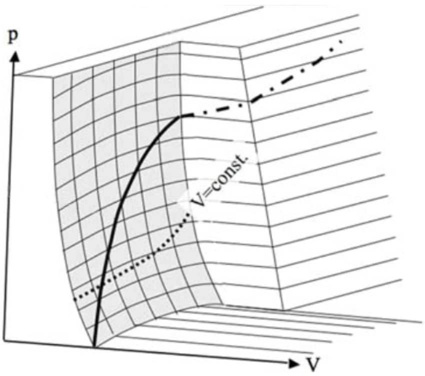
Revisiting the phase diagram

- We are trying to fit near-vacuum to dense solid on a single plot - let's look closer



Compressible effects in solids

- On this plot (adapted from Hiermaier "Structures Under Crash and Impact") a shock Hugoniot is plotted
- Recall this shows the possible states for a given shock speed and initial reference states
- We can see here that this is a true multivariate function, again we have something like $p = p(\rho, \varepsilon)$
- Note, pressure is not necessarily the natural quantity to work with in a solid - we shall consider this shortly



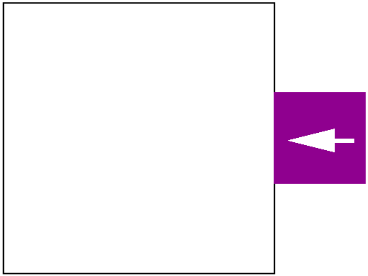
Outline

Stress, strain and strength

- Solids, like the other states of matter we have considered, have density, momentum and energy, and these must be conserved
- However, there are other quantities which are also introduced (or, at least, become more important)
- **Stress** - a measure of the force per unit area
- **Strain** - a measure of the deformation of a material
- These two quantities are not independent, the more force you apply to a material the more it deforms
- **Strength** - the phrase 'materials with strength' is often used in elastoplastic modelling, and does not seem to have such a clear definition
- One appropriate definition might be that a material with strength could support gradients in stress in an equilibrium configuration

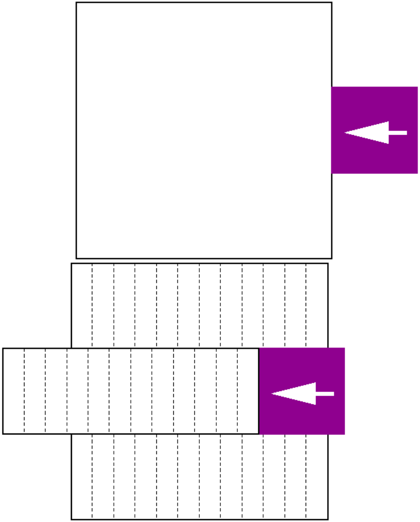
Stress

- We have been dealing with stress throughout the continuum lectures, though we have rarely called it that
- This is because, much like in the non-mechanical sense, e.g. when attempting to meet deadlines, 'stress' and 'pressure' describe similar things
- We shall now relate these concepts in a physically meaningful way
- We shall assume we have a volume of some material, and we are going to apply a force to this material - effectively we shall try to push some of it out of the way



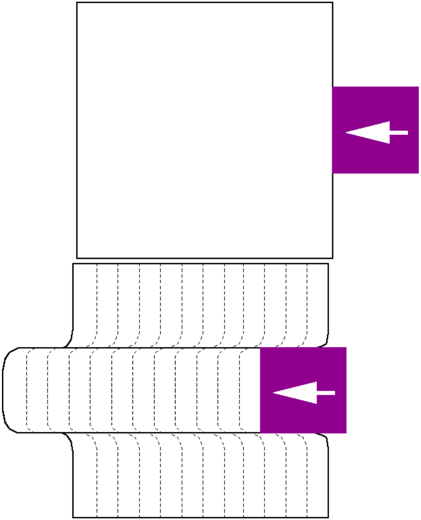
Stress - Inviscid materials

- If we have an inviscid material, we can effectively 'slide' material outwards as we push it
- Note - this is a simplification, ignoring waves which will start travelling through the material
- Here, the stress on this material acts in a single direction only, it could be parameterised with a scalar
- This is why we consider pressure, rather than stress in the Euler equations



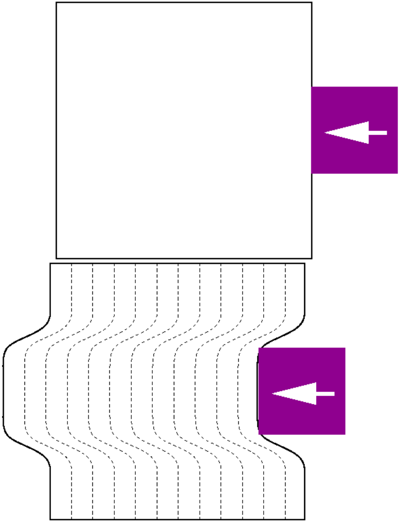
Stress - Viscous materials

- The intermolecular forces in viscous materials resist transverse motion between materials
- This means we see behaviour that is not in the normal direction - the force has acted in all directions
- We now consider the pressure (normal direction) to be a component of the overall stress
- Transverse motion of particles still occurs, and when the purple object stops moving, the material will settle to a zero-stress configuration



Stress - solids

- When we consider solids, atomic bonds prevent large-scale transverse motion
- The entire solid must deform under this applied force
- Again this no longer happens in a single direction - we consider an overall stress
- In this case, if the purple object stops moving, stress in the solid will remain, but will return to zero once the object is removed
- Note - if enough force is applied, bonds break and we see **fracture**
- Also note - the return to zero may not be the same as the return to the initial configuration



The stress tensor

- For solids (and viscous materials) the result of our purple block was stress in all directions - this may suggest that we need a vector quantity
- It is, in fact possible to define a stress vector, $\mathbf{t}$, for a force, $\mathbf{f}$ acting on a surface $\mathcal{S}$

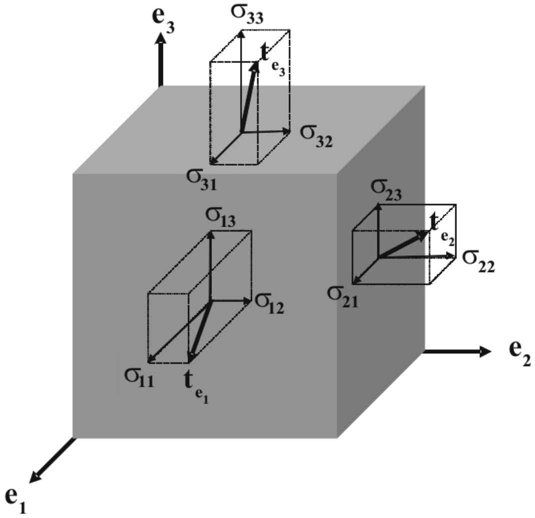
$$\mathbf{t}\left(\mathbf{x}, t, \mathbf{n}\right) = \frac{\mathrm{d}\mathbf{f}}{\mathrm{d}\mathcal{S}}$$

- However, this is dependent on the direction of the force; to fully describe the stress, we need to consider all directions
- This comes from a **stress tensor**

$$\sigma_{ij} = \begin{pmatrix} \mathbf{t}_1 \\ \mathbf{t}_2 \\ \mathbf{t}_3 \end{pmatrix} = \begin{pmatrix} \sigma_{11} & \sigma_{12} & \sigma_{13} \\ \sigma_{21} & \sigma_{22} & \sigma_{23} \\ \sigma_{31} & \sigma_{32} & \sigma_{33} \end{pmatrix}$$

- This quantity is also known as the **Cauchy stress tensor** - other stress tensors exist, they may be scaled by other variables, or only include some stress contributions

Visualising the stress tensor



Computing the stress tensor - non-solids

- Inviscid materials:

$$\sigma_{ij} = -p\delta_{ij} = \begin{pmatrix} -p & 0 & 0 \\ 0 & -p & 0 \\ 0 & 0 & -p \end{pmatrix}$$

- It is a convention that **compressive stress** is negative - solids can also display **tensile stress** (stretching)
- Viscous materials:

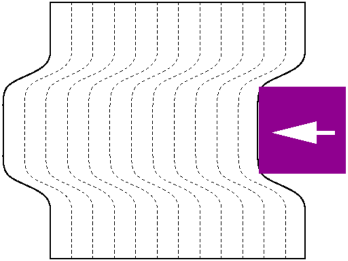
$$\sigma_{ij} = -p\delta_{ij} + \tau_{ij} = -p\delta_{ij} + \left(\lambda + \frac{2}{3}\mu\right)\nabla_k v_k \delta_{ij} + \mu\left(\nabla_i v_j + \nabla_j v_i - \frac{2}{3}\left(\nabla_k v_k\right)\delta_{ij}\right)$$

- μ is dynamic viscosity, λ is bulk viscosity and τ_{ij} is referred to as the **deviatoric stress**
- Note, for incompressible flow,

$$\tau_{ij} = \mu\left(\nabla_i v_j + \nabla_j v_i\right)$$

Computing the stress tensor - solids (part 1)

- Stress within a solid is more complicated that the other states of matter



- There is a relationship between the stress within the solid and the amount it has moved - its **deformation**
- If our object here was ten times longer (in the vertical direction), would the same distance of movement generate the same amount of stress?

Computing the stress tensor - solids (part 1)

- Stress within a solid is more complicated that the other states of matter
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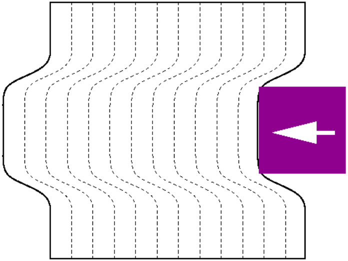

- We would expect a longer object to be under less stress than a shorter one for a given distance of motion
- In order to get more understanding about the stress tensor in solids, we need to consider deformation and strain in more detail

Reference configurations

- Solids have a **reference configuration** - if you leave them lying around undisturbed, they will form a certain shape
- As a solid deforms, we can describe this in a Lagrangian manner - if we consider a reference 'particle' at position $\mathbf{X}$, then at a future time, we can identify where this particle originated in the reference configuration
- Alternatively, we can describe the solid deformation in an Eulerian manner, where for a given point in space, $\mathbf{x}$, we identify 'particles' moving through it over time
- These quantities are related
$$\mathbf{x} = \mathbf{x}\left(\mathbf{X}_0, t\right)$$
- Deformation can be considered as being when two neighbouring Lagrangian particles separate (or come together) from an Eulerian point of view
- We can quantify this as a measure of deformation

Deformation gradient

$$F_{ij} = \frac{\mathrm{d}x_i}{\mathrm{d}X_i}$$

- The **deformation gradient** transforms an infinitesimal particle from its reference configuration $\mathrm{d}\mathbf{X}$ to its current Eulerian position $\mathrm{d}\mathbf{x}$
- Similarly, we have an **inverse deformation gradient**,

$$G_{ij} = F_{ij}^{-1} = \frac{\mathrm{d}X_i}{\mathrm{d}x_i}$$

- Why is the deformation gradient a good way to quantify deformation?

Deformation gradient

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- Why is the deformation gradient a good way to quantify deformation?
  1. It is not affected by translation or rotation - movement of $\mathbf{X}$ but not with respect to local ‘particles’
  2. Length scales are accounted for - a 1 cm motion of the centre of a 1 m rod has lower deformation gradient than of a 10 cm rod

Deformation gradient and strain

- We have said that strain is a measure of the deformation of the material, however, it is not a unique quantity:
- **Engineering strain** and **True strain** are one-dimensional strain measurements
- **Infinitesimal strain** (Lagrangian or Eulerian) tensors are measures of strain under small deformation assumptions (such as material density change is negligible)
- **Finite strain** tensors allow for more severe deformation, here we have Green-Lagrange, Euler-Almansi, Hencky, Biot, Piola and Finger Strain tensors (at least)
- Since we are working with compressible models, in more than 1D, finite strain tensors are most useful
- These can all be defined in terms of the deformation gradient
- For example, the Green-Lagrange Strain tensor is

$$\epsilon_{ij} = \frac{1}{2}\left(F^T_{ik}F_{kj} - \delta_{ij}\right) = \frac{1}{2}\left(F_{ki}F_{kj} - \delta_{ij}\right)$$

- See Hiermaier's book for more detail

Deformation gradient and density

- As long as we know what measure of strain we are using, we can relate it to deformation gradient, though we have not yet said why we want to do this
- The short answer is; stress is related to strain, strain to deformation gradient and deformation gradient to density, and a relationship between strain and conserved variables is going to be essential for closing our solid system of equations
- So far we have considered the central regions of this chain, now to the edges...
- To start with, we would like to consider how to map a volume of material from an initial configuration, $V_0\left(\mathbf{X}\right)$ to its deformed configuration $V\left(\mathbf{x}\right)$
- This is effectively a coordinate transformation

$$V(x_i) = \det\left(\frac{\partial x_i}{\partial X_j}\right) V_0(X_j) = \det\left(F_{ij}\right) V_0(X_j)$$

- Effectively, the deformation gradient acts as the Jacobian for converting between these two frames of reference

Deformation gradient and density

$$V(x_i) = \det\left(\frac{\partial x_i}{\partial X_j}\right) V_0(X_j) = \det\left(F_{ij}\right) V_0(X_j)$$

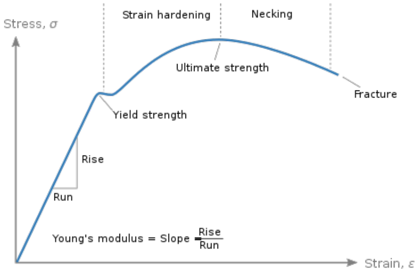
- Now in our transformed volume of material, mass has not changed
- Density will have, however

$$\rho = \frac{m}{V} = \frac{m}{\det(F_{ij})V_0} = \frac{\rho_0}{\det(F_{ij})}$$

- Note that the initial density is $\rho_0 = m/V_0$
- Therefore, we can express density in terms of the deformation gradient
- Clearly, we cannot obtain the deformation gradient, a matrix quantity, from the density, a scalar - the implications of this on what quantities our evolution equations will evolve, will be considered shortly

Stress-strain relationships

- To complete the picture, we now consider how stress and strain are related
- It is common to hear of a stress-strain curve in solid applications
- Here we show an example for a low-carbon steel, which, as strain increases, demonstrates several different features
- These are directly related to the behaviours in a solid we showed at the start of the lecture



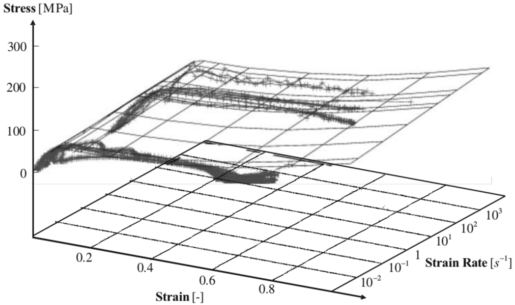
- Stress-strain relationships are experimentally measured and exist for a huge number of materials
- These curves suggest $\boldsymbol{\sigma} = \boldsymbol{\sigma}(\mathbf{F})$, since strain and deformation gradient are related - is this all the information we need?

Measuring stress-strain curves

- Recall that the concepts of stress and pressure are related, and that deformation gradient is directly related to density
- $\boldsymbol{\sigma} = \boldsymbol{\sigma}(\mathbf{F})$ could be considered an analogous statement to $p = p(\rho)$ - what is missing?
- It is worth considering how stress-strain curves are derived
- A load is gradually applied to a test material and the deformation is measured
- For many engineering purposes, this is sufficient, for example, we need to know that the ground floor of a building will support the load of the floors above it
- But what if the upper floors weren't built gradually, but were put in place already completed
- We might see the same overall deformation of the support structures, but it would happen more quickly - could this cause problems?

Strain rate

- **Strain rate** is a measure of how quickly deformation occurs
- Stress-strain curves can be computed at different strain rates



- This example (from Hiermaier's book) shows a curve fitted to stress-strain measurements at different strain rates

High strain rate models

- Rapid deformation can lead to higher stress levels than gradual deformation, and thus will alter the overall evolution of the system
- Many of the problems for which we have applied non-linear compressible models are highly energetic - these are likely to cause rapid deformation when interacting with a solid material
- The models we are working towards are therefore often called **high strain rate models** - they can deal with different behaviours associated with different strain rate
- They are also, less helpfully, referred to as high-deformation models - if something deforms a lot, but at a low strain rate, the standard stress-strain curves can be used
- There may appear similarities between the stress-strain-strain rate curve and the $p - V - \varepsilon$ phase diagram we have seen previously
- Much as strain is related to deformation gradient (and hence density), strain rate is related to changes in the internal energy of the solid

Back to an equation of state

- It is hopefully now clear that we are arriving at an equation of state for a solid material

$$\boldsymbol{\sigma} = \boldsymbol{\sigma}\left(\mathbf{F}, \varepsilon\right)$$

- Specifying this equation of state requires even more work than those that we have considered so far
- A full equation of state needs to consider elastic behaviour, plastic behaviour and fracture
- These can be complicated, especially if a material is **anisotropic**
- However, many equations of state do exist, based on high strain rate experimental measurements
- We will outline a few, but first we should consider what equations we are actually going to solve

Outline

Conservation equations for a solid

- So far, we have used conservation equations for mass, momentum and energy
- These quantities are still conserved, therefore the familiar form of the equations remains valid

Hydrodynamic equations:

$$\frac{\partial \rho}{\partial t} + \nabla_j \left(\rho v_j\right) = 0$$

$$\frac{\partial \rho v_i}{\partial t} + \nabla_j \left(\rho v_i v_j + p\delta_{ij}\right) = 0$$

$$\frac{\partial E}{\partial t} + \nabla_j \left[v_j \left(E + p\right)\right] = 0$$

$\rightarrow$

Elastoplastic equations:

$$\frac{\partial \rho}{\partial t} + \nabla_j \left(\rho v_j\right) = 0$$

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

$$\frac{\partial E}{\partial t} + \nabla_j \left[v_j E - v_k \sigma_{kj}\right] = 0$$

- The hydrodynamic description of stress, $\sigma_{ij} = -p\delta_{ij}$, has been replaced with the full stress tensor

Conservation equations for a solid

$$\frac{\partial \rho}{\partial t} + \nabla_j \left(\rho v_j \right) = 0$$

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

$$\frac{\partial E}{\partial t} + \nabla_j \left[v_j E - v_k \sigma_{kj} \right] = 0$$

- For elastoplastic solids, we still have

$$E = \rho \varepsilon \left(\mathbf{F}, \boldsymbol{\sigma} \right) + \frac{1}{2} \rho v^2$$

- As we have mentioned previously, knowledge of the deformation gradient, rather than the density, is needed for the equation of state
- Can we introduce a conservation law for the deformation gradient?

Conservation law for deformation gradient

- Initial definitions:

$$\frac{\partial \rho}{\partial t} + \nabla_j (\rho v_j) = 0, \qquad F_{ij} = \frac{\partial x_i}{\partial X_j}, \qquad v_i = \frac{\mathrm{d} x_i}{\mathrm{d} t}$$

- We now consider the **material derivative** of the deformation gradient, which can be written

$$\frac{\mathrm{D}}{\mathrm{D}t} F_{ij} = \frac{\partial v_i}{\partial X_j}$$

- We don't really want to consider derivatives with respect to $\mathbf{X}$, we use the chain rule

$$\frac{\mathrm{D}}{\mathrm{D}t} F_{ij} = \frac{\partial v_i}{\partial X_j} = \frac{\partial v_i}{\partial x_k} \frac{\partial x_k}{\partial X_j} = (\nabla_k v_i) F_{kj}$$

- We have a relationship between the time derivative of the deformation gradient to spatial derivatives, though not yet in conservation law form

Conservation law for deformation gradient

$$\frac{\mathrm{D}}{\mathrm{D}t} F_{ij} - \left(\nabla_k v_i\right) F_{kj} = 0$$

- We now consider a manipulation of this equation, including writing out the material derivative in an Eulerian manner

$$\rho \left(\frac{\partial}{\partial t} F_{ij} + v_k \nabla_k F_{kj} - \left(\nabla_k v_i\right) F_{kj} \right) + F_{ij} \left(\frac{\partial \rho}{\partial t} + \nabla_k \left(\rho v_k\right) \right) = 0$$

- We now note that

$$\nabla_k \left(\rho v_k F_{ij}\right) = \rho v_k \nabla_k F_{ij} + F_{ij} \nabla_k \left(\rho v_k\right), \quad \nabla_k \left(\rho v_i F_{kj}\right) = \left(\nabla_k v_i\right) \rho F_{kj} + v_i \nabla_k \left(\rho F_{kj}\right)$$

- This gives us a conservation law (with source term) for the quantity ρF_{ij}

$$\frac{\partial}{\partial t} \left(\rho F_{ij}\right) + \nabla_k \left(\rho v_k F_{ij} - \rho v_i F_{kj}\right) = -v_i \nabla_k \left(\rho F_{kj}\right)$$

The elastoplastic evolution equations

$$\frac{\partial \rho v_i}{\partial t} + \nabla_j \left(\rho v_i v_j - \sigma_{ij} \right) = 0$$
$$\frac{\partial E}{\partial t} + \nabla_j \left[v_j E - v_k \sigma_{kj} \right] = 0$$
$$\frac{\partial}{\partial t} \left(\rho F_{ij} \right) + \nabla_k \left(v_k \rho F_{ij} - v_i \rho F_{kj} \right) = -v_i \nabla_k \left(\rho F_{kj} \right)$$

- We have a system of evolution equations, an as yet unspecified equation of state, and a relationship between density and deformation gradient

$$\rho = \frac{\rho_0}{\det F_{ij}}$$

- So seemingly now what we need is an EoS, of the form $\varepsilon \left(\mathbf{F}, \boldsymbol{\sigma} \right)$, though looking at the literature, this is not often seen

Stress, specific internal energy and the EoS

- It is far more common, for elastoplastic solids, to see an equation of state of the form

$$\varepsilon = \varepsilon(\mathbf{F}, s)$$

- Although previously, we said that we did not like using entropy as a variable, this was only because for other states of matter, we don't have a suitable definition
- Since this doesn't involve stress directly, we also need another relationship

$$\sigma_{ij} = \rho F_{ik} \frac{\partial \varepsilon}{\partial F_{kj}}$$

- Getting into the full details of this relationship is beyond what we have time for, see, Godunov and Romenskii, "Nonstationary equations of nonlinear elasticity theory in Eulerian coordinates" (1972) - originally published in Russian, but fortunately (for me, at least) it has been translated

Stress, specific internal energy and the EoS

$$\varepsilon = \varepsilon(\mathbf{F}, s), \qquad \sigma_{ij} = \rho F_{ik} \frac{\partial \varepsilon}{\partial F_{kj}}$$

- Unfortunately, this is still not quite enough - it cannot be guaranteed that an equation of state using $\mathbf{F}$ and s will give a symmetric stress tensor
- However, ways to express the EoS are available, for example, using a strain tensor, and using a symmetric one to start with
- It is common to use the **Finger tensor**,

$$\mathbf{C} = \mathbf{F}^{-T}\mathbf{F}^{-1}$$

- If we have this, then we can write

$$\sigma_{ij} = -2\rho C_{ik} \frac{\partial \varepsilon}{\partial C_{kj}}$$

Stress, specific internal energy and the EoS

$$\varepsilon = \varepsilon(\mathbf{C}, s), \qquad \sigma_{ij} = -2\rho C_{ik} \frac{\partial \varepsilon}{\partial C_{kj}}$$

- Whilst using the Finger tensor does not, in general, confirm that the stress tensor is symmetric, in practice it works out for many isotropic materials, including most metals
- This is because for these materials, we can actually write the equation of state as

  $$\varepsilon = \varepsilon(I_1, I_2, I_3, s)$$

  where I_1, I_2 and I_3 are the invariants of the Finger tensor
- See Barton et al. "Exact and approximate solutions of Riemann problems in non-linear elasticity" (2009) and references within for more detail

Back to the full system

$$\frac{\partial}{\partial t}\left(\rho F_{ij}\right) + \nabla_k\left(v_k \rho F_{ij} - v_i \rho F_{kj}\right) = -v_i \nabla_k\left(\rho F_{kj}\right)$$

- When we introduced the "conservation" equation for the deformation gradient, we had a source term on the right hand side
- Because this has first derivatives of the quantity we are trying to conserve, it is technically not a conservation equation
- Fortunately, we can use an additional constraint on the system (see Barton et al. again for details)
- If

  $$\nabla_k\left(\rho F_{kj}\right) = 0$$

  for the initial data, then this relationship holds true for all time
- So for appropriately chosen initial data, we have a system of conservation laws

Hyperbolicity of the system

- It is possible to write the elastoplastic solid system in hyperbolic form

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

- It is not a short calculation though, fortunately someone has done it for us, the matrix B is given by (for our coordinates, $\hat{F} = F$, $\bar{u} = v$)

$$\begin{pmatrix}
\overline{u}_k & 0 & 0 & -A^{k1}_{11} & -A^{k1}_{12} & -A^{k1}_{13} & -A^{k2}_{11} & -A^{k2}_{12} & -A^{k2}_{13} & -A^{k3}_{11} & -A^{k3}_{12} & -A^{k3}_{13} & -b^k_1 \\
0 & \overline{u}_k & 0 & -A^{k1}_{21} & -A^{k1}_{22} & -A^{k1}_{23} & -A^{k2}_{21} & -A^{k2}_{22} & -A^{k2}_{23} & -A^{k3}_{21} & -A^{k3}_{22} & -A^{k3}_{23} & -b^k_2 \\
0 & 0 & \overline{u}_k & -A^{k1}_{31} & -A^{k1}_{32} & -A^{k1}_{33} & -A^{k2}_{31} & -A^{k2}_{32} & -A^{k2}_{33} & -A^{k3}_{31} & -A^{k3}_{32} & -A^{k3}_{33} & -b^k_3 \\
-\widehat{F}_{k1} & 0 & 0 & \overline{u}_k & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\
-\widehat{F}_{k2} & 0 & 0 & 0 & \overline{u}_k & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\
-\widehat{F}_{k3} & 0 & 0 & 0 & 0 & \overline{u}_k & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\
0 & -\widehat{F}_{k1} & 0 & 0 & 0 & 0 & \overline{u}_k & 0 & 0 & 0 & 0 & 0 & 0 \\
0 & -\widehat{F}_{k2} & 0 & 0 & 0 & 0 & 0 & \overline{u}_k & 0 & 0 & 0 & 0 & 0 \\
0 & -\widehat{F}_{k3} & 0 & 0 & 0 & 0 & 0 & 0 & \overline{u}_k & 0 & 0 & 0 & 0 \\
0 & 0 & -\widehat{F}_{k1} & 0 & 0 & 0 & 0 & 0 & 0 & \overline{u}_k & 0 & 0 & 0 \\
0 & 0 & -\widehat{F}_{k2} & 0 & 0 & 0 & 0 & 0 & 0 & 0 & \overline{u}_k & 0 & 0 \\
0 & 0 & -\widehat{F}_{k3} & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & \overline{u}_k & 0 \\
0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & \overline{u}_k
\end{pmatrix}$$

Hyperbolicity of the system

- For this model your primitive variables are $\mathbf{w} = \left(\mathbf{v}, F^T, s\right)^T$
- This requires several additional definitions

$$A_{ijkl} = \frac{1}{\rho}\frac{\partial \sigma_{ki}}{\partial F_{lj}}, \quad b_{ik} = \frac{1}{\rho}\frac{\partial \sigma_{ki}}{\partial s}$$

- It is not straightforward, but you can get eigenvalues from the equation

$$(v-\lambda)^7 \det\left|\Omega - (v-\lambda)^2 I\right|$$

$$\Omega_{ij} = \left(\mathbf{e}_i^T A_{kj}\right) \cdot \left(F^T \mathbf{e}_k\right)$$

- The quantity Ω contains derivatives of the stress tensor with respect to density - it is known as the **acoustic tensor** and is related to sound speeds
- This equation does provide real eigenvalues; not easy to write down ones, but real ones

Elasticity, plasticity and fracture

- We have three distinct behaviours within a solid, and unsurprisingly (but unfortunately) these need separate treatments
- Typically, models for solving these start with a purely elastic description of the material
- Plasticity effects can then be incorporated
- There are two advantages to this strategy
  1. The solid displays elastic behaviour across the entire stress-strain-strain rate surface, whilst plasticity (mostly) requires sufficiently high strain
  2. Plasticity can (largely) be incorporated through source terms to an elastic system
- Fracture is yet another addition to the system of equations - however, it is also very much a current research topic how this happens, we will not attempt to go into details in this lecture

Elasticity models

- If a solid displays only elastic behaviour, then any deformation that occurs due to the applied stress will disappear again once the solid is left to relax - the solid will return to its initial configuration
- There is no single model to describe elastic behaviour
- **Linear elasticity** assumes that a linear relationship exists between stress and strain
- **Hyperelastic** materials relax this assumption, allowing for non-linear stress-strain relationships
- Hyperelastic models are commonly used for high strain rate simulations of solid materials
- Even more general is a **Cauchy-elastic** material, in which the work done by the stress may be dependent on the path - on how the deformation occurred
- Going beyond this, the stress itself may differ based on the path

Isotropic hyperelasticity

- Your choice of elasticity model (roughly equivalent to your choice of material) determines the form of the equation of state
- Many metals and plastics can be modelled as **isotropic** at continuum level, and as **hyperelastic**
- In this case, an equation of state can be given by

$$\varepsilon = \varepsilon\left(I_1, I_2, I_3, s\right)$$

- This is the form we introduced previously, with the invariants of the Finger tensor
- We consider a few common equations of state

Hyperelastic equations of state

Mie-Grüneisen:

$$\epsilon = \begin{cases} \left(\frac{c_0}{\hat{s}}\right)^2 \left[\left(\frac{1}{r} - 1\right) + \ln r\right] + \frac{G}{2\rho_0}\left(\frac{I_2}{I_3} - \frac{3}{(I_3)^{1/3}}\right) & I_3 \geq 1 \\ c_0^2 \left(\frac{1}{2}\ln I_3 + I_3^{-1/2} - 1\right) + \frac{G}{2\rho_0}\left(\frac{I_2}{I_3} - \frac{3}{(I_3)^{1/3}}\right) & I_3 \leq 1 \end{cases}$$

$$r = 1 - \hat{s}(1 - I_3^{-1/2})$$

- c_0: sound speed
- G: Young's modulus
- $\hat{s}$: Ratio between shock and particle velocity (as before)
- Note that the conditions $I_3 \geq 1$ or $I_3 \leq 1$ are directly related to the conditions for compression or expansion when we introduced the hydrodynamic Mie-Grüneisen equation of state

Hyperelastic equations of state

Romenskii:

$$\varepsilon = \frac{K_0}{2\alpha_R^2}\left(I_3^{\alpha_R/2} - 1\right)^2 + c_V T_0 I_3^{\gamma_R/2}\left(e^{s/c_v} - 1\right) + \frac{b_0^2}{2} I_3^{\beta_R/2}\left(\frac{I_1^2}{3} - I_2\right)$$

$$K_0 = c_0^2 - \frac{4}{3} b_0^2$$

- c_0: sound speed
- b_0: reference shear wave speed
- T_0: reference temperature
- α_R, β_R and γ_R - experimentally derived constants to determine the nonlinear dependence of sound speed, shear wave speed and temperature on density

Notes on the system so far

- We have introduced several reference quantities as part of these models - these are all computed for a single reference state (generally the zero stress, zero strain state)
- The formulation we have presented is not the only one available, it is also possible to evolve the **inverse deformation gradient**
- Initial data for deformation gradient can be assumed to be $F_{ij} = \delta_{ij}$ - this will not normally be stated in a reference (though should be if it is known and non-zero)
- Ideally, references will give you full information about the equation of state - unfortunately, in the real world, this is not always the case

Numerical methods

- We have talked a lot about formulation of the equations, and not a lot about the numerical methods required
- Fortunately, our FORCE and SLIC methods will still work (all we need is a hyperbolic system)
- Going beyond these methods gets complicated very fast, these methods are widely used
- Approximate Riemann solvers do exist, however, for example an **HLLD** (Harten-Lax-van Leer-discontinuities) solver can be used
- This is a reasonably straightforward extension (give the complexities of the system) of the HLL and HLLC-type methods we have seen

Plasticity models

- Plastic deformation is **irreversible** - once the system relaxes, it will not recover its initial configuration
- A plastically deformed material will have non-zero strain at zero stress
- Underlying the plastic behaviour of the system is **flow plasticity theory** - the amount of plastic deformation can be described by a **flow rule**
- A direct result of this is that the total deformation can be decomposed into **elastic deformation** and **plastic deformation**

$$F_{ij} = F^e_{ik} F^p_{kj}$$

- We shall give a brief overview of how this fits into the general conservation system - full details are beyond the scope (and time limit) of the course

Effects of the decomposition

- Recall we derived an equation for the total derivative of deformation gradient

$$\frac{\mathrm{D}}{\mathrm{D}t} F_{ij} - \left(\nabla_k v_i\right) F_{kj} = 0 \quad \rightarrow \quad \frac{\mathrm{D}}{\mathrm{D}t}\left(F^e_{ik} F^p_{kj}\right) - \left(\nabla_k v_i\right)\left(F^e_{kl} F^p_{lj}\right) = 0$$

- Based on the decomposition, we can use the chain rule on this derivatives

$$\frac{\mathrm{D}F^e_{ik}}{\mathrm{D}t} F^p_{kj} + F^e_{ik} \frac{\mathrm{D}F^p_{kj}}{\mathrm{D}t} - \left(\nabla_k v_i\right)\left(F^e_{kl} F^p_{lj}\right) = 0$$

- A multiplication through by $\left(F^p\right)^{-1}$ gives

$$\frac{\mathrm{D}F^e_{ij}}{\mathrm{D}t} + F^e_{ik} \frac{\mathrm{D}F^p_{kl}}{\mathrm{D}t} \left(F^p_{lj}\right)^{-1} - \left(\nabla_k v_i\right) F^e_{kj} = 0$$

- Effectively, we recover the original expression, but for the elastic deformation only, and include an additional 'source term'

The full system (again)

- Using this, we can follow previous mathematical arguments to produce a system which evolves only elastic deformation gradient

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

$$\frac{\partial E}{\partial t} + \nabla_j \left[v_j E + v_k \sigma_{kj}\right] = 0$$

$$\frac{\partial}{\partial t}\left(\rho F^e_{ij}\right) + \nabla_k \left(v_k \rho F^e_{ij} - v_i \rho F^e_{kj}\right) = -v_i \nabla_k \left(\rho F_{kj}\right) - \rho F^e_{ik} L^p_{kj}$$

$$L^p_{kj} = F^e_{kl} \frac{\mathrm{D} F^p_{lm}}{\mathrm{D}t} \left(F^p_{mn}\right)^{-1} \left(F^e_{nj}\right)^{-1}$$

- This final source term is often written as P_{ij} for ‘neatness’
- The idea behind this is that it is possible to compute F^p_{ij} from the evolution of this system and knowledge about the plasticity of the material - at this point, computing P_{ij} is messy, but simple

The yield surface

- In a simple stress-strain curve, the **yield strength** of a solid is the point at which the material stops behaving elastically
- However, given that stress and strain are tensor quantities, this is not actually a single point
- Because the stress tensor, $\boldsymbol{\sigma}$, is symmetric, it therefore contains six independent quantities
- The **yield surface** is a surface in this six-dimensional space (or using any equivalent independent quantities), inside of which the material behaves elastically
- Stressed states outside of this surface are not physically permitted (in the models of plasticity we apply) - from the point of view of our equations, there is nothing to prevent this though
- Any attempt to push the material states into this region must instead appear as **plastic deformation**

Remapping stressed states

- If our evolution equation results in stresses outside of the yield surface, these can be **remapped** back to the yield surface
- Effectively we decrease the stress by increasing the plastic deformation
- The standard procedure to achieve this is described by Miller and Colella, "A high-order eulerian godunov method for elasticplastic flow in solids" (2001)
- The idea behind this is that deviations beyond the yield surface are small, hence can be recovered by taking the steepest (six-dimensional) path back to this surface
- Doing so **relaxes** the stress, and introduces additional plastic deformation, recorded in F_{ij}^{p}

Example yield surface

- As with elasticity, there is no single plasticity model, and no single way to define a yield surface
- **Ideal plasticity** is the case in which plastic behaviour can **only** happen beyond the yield surface
- A common definition for **ductile materials** is the **von Mises** criterion

$$\left|\left|\boldsymbol{\sigma} - \frac{1}{3}\left(\mathrm{tr}\boldsymbol{\sigma}\right) I\right|\right| - \sqrt{\frac{2}{3}}\sigma_Y = 0$$

- Here, $||\boldsymbol{a}|| = \mathrm{tr}\left(\boldsymbol{a}^T\boldsymbol{a}\right)$
- The quantity σ_Y is the yield stress
- Other models (e.g. Johnson-Cook) can introduce an additional advected quantity, **work hardening**, which alters the properties of plastically deformed materials
- This also allows small plastic deformations to occur within the yield surface

A brief note on fracture

- We have now covered, at least in passing, the techniques for modelling a compressible elastoplastic solid
- However, beyond a certain strain, this model will still break down - the solid can take no more deformation and fractures
- This can be incorporated into the system of equations, we need to introduce the concept of **damage**
- Once a region of solid has reached sufficient damage, it **fails** and some part of this material is no longer connected to some other part
- The challenge is: how do we introduce this fracture into our model?
- How do we let our model know that two seemingly neighbouring grid cells are not connected?
- We shall consider this in a little more detail in “Multiphysics Modelling for Four States of Matter”