Advanced continuum modelling Equations of state (part 2) and magnetohydrodynamics (part 1)

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### Outline

- Beyond ideal gases some examples
- 2 Beyond equations
- Magnetohydrodynamics
- 4 Equations of magnetohydrodynamics
- Conservation form

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## Stiffened gas equation of state

- The stiffened gas equation of state is an attempt to modify the ideal gas EoS such that it can be used for liquids, including water
- We know that water is resistant to compression (stiff), and that it has a high sound speed under atmospheric conditions
- We can approximate this in the equation of state through

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

- $oldsymbol{p}_{\infty}$  is a constant quantity it can be considered to represent the attraction between water molecules
- $\bullet$   $\gamma$  is also a constant, much like it was for the ideal gas EoS is this also the adiabatic index?

## Stiffened gas equation of state

Recall that the adiabatic index was given by

$$\gamma_{\rm adiab.} = -\frac{\nu}{p} \left. \frac{\partial p}{\partial \nu} \right|_s = \frac{\rho}{p} \left. \frac{\partial p}{\partial \rho} \right|_s$$

Also recall that

$$c_s = \sqrt{\frac{\partial p}{\partial \rho}}\Big|_s = \sqrt{\frac{p}{\rho^2 \frac{\partial \varepsilon}{\partial p}} - \frac{\frac{\partial \varepsilon}{\partial \rho}}{\frac{\partial \varepsilon}{\partial p}}}$$

• For the stiffened gas, we have

$$c_s^2 = \frac{\gamma \left( p + p_\infty \right)}{\rho}$$

Therefore the adiabatic index is

$$\gamma_{\text{adiab.}} = \frac{\rho}{p}c_s^2 = \gamma \left(1 + \frac{p_{\infty}}{p}\right)$$

• This is **not constant** and  $\gamma$  is **not the adiabatic index** 



## Stiffened gas equation of state

- $\bullet$  Beyond the ideal gas EoS, many equation of state parameters do not have a clear physical origin, but are empirical fits to measured behaviour for a stiffened gas,  $\gamma$  is one such parameter
- ullet This does then provide a definition for  $p_{\infty}$  as a function of a known state,  ${f u}_0$

$$p_{\infty} = \frac{\rho_0 c_{s,0}^2}{\gamma} - p_0$$

 In general, you will need to find a suitable reference state, it is far more common to take values from the literature, for example, water might take

$$\gamma = 2.35, \qquad p_{\infty} = 1 \times 10^9 \, \text{Pa}$$

One thing to consider as we move to more complex equations of state - density
has to be positive, as does sound speed (otherwise things don't make sense), what
about pressure?

Computing

# Negative pressure and tension

$$c_s^2 = \frac{\gamma \left( p + p_\infty \right)}{\rho}$$

- In order to have a real (and positive) sound speed, we need  $p>-p_{\infty}$  there is nothing to stop pressure being negative
- What does this mean?
- Negative pressure is, in general, valid, and is described as a material being in tension
- In solids this makes sense positive pressure leads to something wanting to expand, negative pressure is the opposite effect, to contract towards an initial configuration
- Under short time scales, liquids can also experience tension, though this is quickly equilibrated
- In practice, if your pressure goes negative for a stiffened gas, you probably no longer have an accurate representation of material properties

4 D > 4 A > 4 B > 4 B > B

## When is a stiffened gas used?

- A stiffened gas is one of the simplest methods to model water, but has limited accuracy
- It is based on high-pressure behaviour of water though, so one of the areas it can be used is when dealing with shock waves
- Note that even for water, there is **no consistent parameterisation** used in the literature (nor notation, sometimes the constant  $\gamma p_{\infty}$  is given a single variable name, sometimes it is called  $p^*$ )
- Other liquids can also be modelled using this EoS, including some explosive products, however, a slight change is needed here:

$$p = (\gamma - 1) \rho \left(\varepsilon - \varepsilon_{\infty}\right) - \gamma p_{\infty}$$

- We have introduced a reference energy which can include a contribution from the heat of formation of a material
- For inert materials (such as water and air),  $\varepsilon_{\infty} = 0$



# A complete stiffened gas EoS

- To complete the stiffened gas EoS, we need information about specific heat
- The simplifications of this EoS mean that deriving these from thermodynamic properties may not be as accurate as we would hope, but fortunately, for many materials, these can be measured experimentally and treated as constant
- It is then possible to complete the EoS, the Helmholtz free energy is a simple modification of that of an ideal gas

$$F(\nu, T) = F_{\text{ideal}}(\nu, T) + \nu p_{\infty} + \varepsilon_{\infty}$$

We then get

$$T(\nu, \varepsilon) = \frac{\varepsilon + \varepsilon_{\infty} - \nu p_{\infty}}{c_{v}}$$
$$s(\nu, p) = c_{v} \ln \left( \frac{(p + p_{\infty}) \nu^{\gamma}}{(p_{0} + p_{\infty}) \nu_{0}^{\gamma}} + s_{0} \right)$$

# Mie-Grüneisen equation of state

- Much like the stiffened gas EoS is designed for high-pressure liquids, the Mie-Grüneisen EoS is designed for high-pressure solids
- At high enough pressure (e.g. following ballistic impact), a solid behaves **hydrodynamically**, i.e. as a fluid elastic and plastic behaviour is now negligible
- Despite this original aim, rather than being a single EoS, we can think of a family
  of Mie-Grüneisen equations of state
- These can then cover a wide range of material, including (hydrodynamic) solids, liquids and gases

# Mie-Grüneisen equation of state

$$p(\rho, \varepsilon) = p_{\text{ref}}(\rho) + \Gamma(\rho)\rho \left(\varepsilon - \varepsilon_{\text{ref}}(\rho)\right)$$

- The constant parameters in the previous equations of state have been replaced, they are now functions of density (or specific volume in some literature)
- ullet However, the quantity  $\Gamma(
  ho)$  is still the Grüneisen coefficient described earlier

$$\Gamma = -\left. \frac{\nu}{T} \frac{\partial T}{\partial \nu} \right|_{s} = \nu \left. \frac{\partial p}{\partial \varepsilon} \right|_{\nu}$$

- We also need a **reference curve**, some measurement of p and  $\varepsilon$  along a known curve as density changes how do we do this?
  - Along an isentrope
  - Along an isotherm
  - Along a shock locus



#### What are these references?

- We have covered curves of constant entropy in the EoS (isentropes), and isotherms are a similar concept - a curve of constant temperature
- The shock locus is another reference curve, derived from the Rankine-Hugoniot conditions across a discontinuity

$$S\left(\mathbf{u}_{2}-\mathbf{u}_{1}\right)=\mathbf{f}\left(\mathbf{u}_{2}\right)-\mathbf{f}\left(\mathbf{u}_{1}\right)$$

- For the Euler equations, this is a system of three equations for five unknowns (the four independent variables and the shock speed)
- Eliminating the shock speed and the velocity components gives the Hugoniot equation

$$\varepsilon_2 - \varepsilon_1 = \frac{1}{2} (p_2 + p_1) (\nu_1 - \nu_2)$$

 Through the EoS, and a reference state, u<sub>1</sub>, this gives a curve (the shock locus) with all possible states behind the discontinuity which satisfy the Rankine-Hugoniot conditions

## Mie-Grüneisen equation of state

- So far we have introduced a lot of parameters for the Mie-Grüneisen equation of state, and we've described how some of them are related - is this enough information yet?
- We do still need to provide one of the reference states, and the Grüneisen coefficient - this will be derived empirically
- ullet It is common to be given the reference pressure,  $p_{\rm ref}(
  u)$  note that it is a function of specific volume
- Depending on what reference state we have specified, we can then compute the reference energy:

$$\begin{aligned} \text{Hugoniot}: \quad \varepsilon_{\text{ref}}(\nu) &= \varepsilon_0 + \frac{1}{2} \left( p_{\text{ref}}(\nu) + p_0 \right) \left( \nu_0 - \nu \right) \\ \text{Isentrope}: \quad \varepsilon_{\text{ref}}(\nu) &= \varepsilon_0 - \int_{\nu_0}^{\nu} p_{\text{ref}} \left( \nu' \right) \text{d}\nu' \\ \text{Isotherm}: \quad \varepsilon_{\text{ref}}(\nu) &= \varepsilon_0 - \int_{\nu_0}^{\nu} \left( p_{\text{ref}} \left( \nu' \right) - \frac{\Gamma \left( \nu' \right)}{\nu'} c_V \left( \nu', T_{\text{ref}} \right) T_{\text{ref}} \right) \text{d}\nu' \end{aligned}$$

# Examples of Mie-Grüneisen equations of state

$$p(\rho, \varepsilon) = p_{\text{ref}}(\rho) + \Gamma(\rho)\rho \left(\varepsilon - \varepsilon_{\text{ref}}(\rho)\right)$$

- Since the Mie-Grüneisen EoS represents a family of models, which can model a wide range of materials, it is worth considering a few examples
- Have we seen any already?
- Ideal gas:

$$\Gamma = \gamma - 1, \qquad p_{\text{ref}} = 0, \qquad \varepsilon_{\text{ref}} = 0$$

Stiffened gas:

$$\Gamma = \gamma - 1, \qquad p_{\text{ref}} = -\gamma p_{\infty}, \qquad \varepsilon_{\text{ref}} = \varepsilon_{\infty}$$

These are very simple examples, with constant coefficients



### JWL equation of state

- The Jones-Wilkins-Lee (JWL) EoS is used in modelling explosives
- It is commonly used for the products of a detonation, and occasionally for the reactants too
- It is a Mie-Grüneisen type EoS, and uses an isentrope reference

$$p(\rho, \varepsilon) = p_{\text{ref}}(\rho) + \Gamma(\rho)\rho \left(\varepsilon - \varepsilon_{\text{ref}}(\rho)\right)$$

- The Grüneisen coefficient is constant
- The reference quantities are given (in terms of specific volume) by

$$p_{\text{ref}}(\nu) = A \exp\left(-\frac{R_1 \nu}{\nu_0}\right) + B \exp\left(-\frac{R_2 \nu}{\nu_0}\right) + C\left(\frac{\nu}{\nu_0}\right)^{-\Gamma - 1}$$

$$\varepsilon_{\rm ref}(\nu) = -\Delta\varepsilon + \nu_0 \left[ \frac{A}{R_1} \exp\left(-\frac{R_1\nu}{\nu_0}\right) + \frac{B}{R_2} \exp\left(-\frac{R_2\nu}{\nu_0}\right) + \frac{C}{\Gamma} \left(\frac{\nu}{\nu_0}\right)^{-\Gamma} \right]$$

## JWL equation of state

 It might be clear that as you go beyond the ideal and stiffened gas EoS, things get complicated rapidly!

$$p_{\rm ref}(\nu) = A \exp\left(-\frac{R_1 \nu}{\nu_0}\right) + B \exp\left(-\frac{R_2 \nu}{\nu_0}\right) + C \left(\frac{\nu}{\nu_0}\right)^{-\Gamma - 1}$$
$$\varepsilon_{\rm ref}(\nu) = -\Delta \varepsilon + \nu_0 \left[\frac{A}{R_1} \exp\left(-\frac{R_1 \nu}{\nu_0}\right) + \frac{B}{R_2} \exp\left(-\frac{R_2 \nu}{\nu_0}\right) + \frac{C}{\Gamma} \left(\frac{\nu}{\nu_0}\right)^{-\Gamma}\right]$$

- A, B,  $R_1$  and  $R_2$  are parameters that must be empirically determined (in addition to  $\Gamma$ )
- ullet  $u_0$  is the initial density of the explosive (again empirical, but easy to measure)
- $\Delta \varepsilon$  is an offset to specific internal energy, also empirically determined; for explosive products this can be the **heat of detonation** (a measure of energy generated by the detonation)
- $\bullet$   $\,C$  is a constant of integration based on the isentrope you take C=0 is common



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## Complexities of the EoS

- The JWL equation of state requires a lot of parameters, all of which are material-specific
- This is driven by the requirement for accuracy in detonation simulations if you're blowing something up, you need to get it right first time!
- Even with all these parameters (or, perhaps, because of all these parameters), there is still a region of validity for the EoS
- Menikoff (2015) has produced an excellent derivation and overview of the JWL EoS
- For a lot of materials (even commonly encountered ones), such a detailed EoS is not available
- However, sometimes you don't need this, you just need to make sure bulk behaviour is correct



- In general, the Hugoniot EoS could be any EoS that uses the shock locus as the reference curve for pressure (also referred to as the Hugoniot locus)
- The reference energy then comes from the Rankine-Hugoniot conditions,

$$\varepsilon_2 - \varepsilon_1 = \frac{1}{2} (p_2 - p_1) (\nu_1 - \nu_2)$$

- ullet In this case,  ${f u}_1$  is some known reference state, and  ${f u}_2$  is a state on the shock locus
- However, we note that this technique to obtain an equation of state is based entirely on shock behaviour - its validity is limited to compression from the reference state

$$\nu_2 \le \nu_1$$
 or  $\rho_2 \ge \rho_1$ 

 Generally, references to the Hugoniot EoS often have something a bit more specific in mind - we shall come to this shortly

## Hugoniot reference pressure

 Our starting point is the Rankine-Hugoniot conditions for density and momentum (the energy condition is used later, to obtain the reference energy)

$$\rho_2 v_2 - \rho_1 v_1 = S (\rho_2 - \rho_1)$$
  
$$\rho_2 v_2^2 + p_2 - \rho_1 v_1^2 - p_1 = S (\rho_2 v_2 - \rho_1 v_1)$$

- ullet Our goal is to provide the pressure  $p_2$  as a function of  $ho_2$  and the known state,  ${f u}_1$ , only
- $\bullet$  We need to eliminate two variables,  $v_2$  and S at some point we are going to need another equation
- We first consider a few conventions for the reference state

#### Reference state for solids

- Whilst any reference state could produce an EoS, the range of the validity of the EoS might end up being very limited
- However, for solids, there is an obvious choice of reference state which allows for the Hugoniot EoS to be used in many practical applications
- That is, our reference state is (in primitive variables):

$$\mathbf{w}_1 = (\rho_1, v_1, p_1)^T = (\rho_1, 0, 0)^T$$

- The choice of zero velocity is reasonably obvious as a reference state
- However, for solids, the concept of zero pressure is useful (more accurately, zero stress)
- Under atmospheric conditions, a solid material is close to zero-stress conditions as a result, this reference state removes several variables from the Rankine-Hugoniot conditions and is easy to measure experimentally
- ullet Note, it is common to see  $ho_0$  as a reference density in the literature



# Linear shock relationship

- Part of the reason for the popularity of the Hugoniot EoS is that for many solid materials, there is a linear relationship between shock velocity and particle velocity
- In other words:  $S \propto v_2$
- Additionally, this linear relationship is relatively easy to obtain experimentally,

$$S = c_0 + \hat{s}v_2$$

- ullet  $c_0$  is (usually) the sound speed of the reference state (the **bulk sound speed**) though for some materials, it needs empirically modifying to produce the linear fit
- ullet  $\hat{s}$  is a dimensionless, empirically-derived parameter
- ullet We can now use this to obtain a reference pressure,  $p_{
  m ref}\left(
  ho
  ight)$

- For consistency with other literature, we shall denote the reference density  $\rho_0$  and drop subscripts elsewhere in the Rankine-Hugoniot conditions (we are obtaining a function, not a relationship between two pre-existing states)
- Additionally, we shall introduce a new variable

$$\eta = 1 - \frac{\rho_0}{\rho}$$

- Aside from making the equations we shall derive neater, this is also a physical quantity - the volumetric strain
- We shall discuss strain a bit more later, but we can see that it is directly related to a change in volume from the reference state

$$\eta = \frac{\nu_0 - \nu}{\nu_0}$$



 To derive our reference pressure, we start with the Rankine-Hugoniot condition for density:

$$\rho v = S\left(\rho - \rho_0\right)$$

• We then divide through by  $\rho$ , and use the linear shock relationship to get

$$v = (c_0 + \hat{s}v)\left(1 - \frac{\rho_0}{\rho}\right) = (c_0 + \hat{s}v)\eta$$

Rearranging this to obtain the (post shock) velocity gives

$$v = \frac{c_0 \eta}{1 - \hat{s} \eta}$$

• We can now use this in the Rankine-Hugoniot condition for momentum

$$\rho v^2 + p = S\rho v$$



We start (again) by using the linear shock relationship

$$p = S\rho v - \rho v^2 = \rho v (S - v) = \rho v (c_0 + \hat{s}v - v)$$

ullet Substituting in our relationship for v gives

$$p = \frac{\rho c_0 \eta}{1 - \hat{s} \eta} \left[ c_0 + \frac{c_0 \eta}{1 - \hat{s} \eta} \left( \hat{s} - 1 \right) \right]$$

• This can then be rearranged to give

$$p = \frac{c_0^2 (1 - \eta) \rho \eta}{(1 - \hat{s}\eta)^2}$$

• We then note that  $(1 - \eta) \rho = \rho_0$ , giving the standard form for the Hugoniot EoS reference pressure,

$$p = p_{\text{ref}}(\rho) = \frac{\rho_0 c_0^2 \eta}{(1 - \hat{s}\eta)^2}$$



## Hugoniot equation of state - summary

The Hugoniot EoS has the standard Mie-Grüneisen form

$$p(\rho,\varepsilon) = p_{\rm ref}(\rho) + \Gamma(\rho)\rho\left(\varepsilon - \varepsilon_{\rm ref}(\rho)\right)$$

Reference pressure is given by

$$p_{\text{ref}}(\rho) = \frac{\rho_0 c_0^2 \eta}{(1 - \hat{s}\eta)^2}$$

Reference energy by

$$\varepsilon_{\text{ref}}(\rho) = \varepsilon_0 + \frac{1}{2} p_{\text{ref}}(\rho) \left( \frac{1}{\rho_0} - \frac{1}{\rho} \right)$$

- We haven't given any information about the Grüneisen coefficient yet, but once again, we have  $\Gamma = \Gamma_0$  (constant)
- This is enough information to use this as an (incomplete) EoS but what happens if your solid expands?



### Extending the Hugoniot equation of state

- It can be easy to determine when the Hugoniot equation of state is outside its range of validity:  $\rho < \rho_0$  (note this is not the only constraint on validity)
- ullet However, if we consider our reference state,  $\mathbf{u}_0$ , we can also derive an isentrope at this point
- This isentrope is tangential to the shock locus to second order (i.e. first and second derivatives are the same for both curves)
- As a result, the isentrope is a natural extension for these regions
- This gives (see e.g. the useful report by Robinson (2019), and references)

$$p_{\mathrm{ref}} = K_0 \eta, \qquad arepsilon_{\mathrm{ref}} = rac{K_0 \eta^2}{2 
ho_0} + arepsilon_0$$

ullet Just one more constant is needed,  $K_0$ 



## Equations of state so far

- So far, we have described equations of state for:
  - 1 Ambient air, fully ionised plasma, astrophysical materials: ideal gas
  - 4 High-pressure water: stiffened gas
  - Some explosives (in the reactive regime): JWL and Mie-Grüneisen
  - Some solids (behaving hydrodynamically): Hugoniot and Mie-Grüneisen
- Does this cover everything we want to model?
- We have not covered every possible equation of state, and nor is every equation of state given above unique to the material described
- With enough experimental measurements, curve fitting exercises and, possibly, loose handling of error bars, all sorts of equations of state could be created
- So why have we focused on these ones?



Computing

# Equations of state so far

- We have focused on generality so far:
  - The ideal gas EoS covers some of the most commonly simulated materials with a wide range of physical validity
  - The Mie-Grüneisen EoS is a formulation from which many equations of state are derived
- One other feature of all the equations of state we have shown so far is that they
  are invertible
- We tend to write  $p=p(\rho,\varepsilon)$ , but in a numerical simulation, it is important to have  $\varepsilon=\varepsilon(p,\rho)$ , when converting between primitive and conserved variables
- Do we also need  $\rho(p,\varepsilon)$ ?



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# Things get more complicated still...

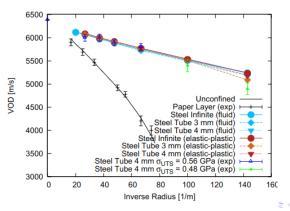
- Equations of state are a continuum description approximating a wide range of molecular behaviour and thermodynamics
- On top of this, materials undergo phase change, which could be thermally-induced (e.g. boiling) or pressure-induced (e.g. cavitation)
- The thermal behaviour is particularly awkward since as materials undergo phase change, latent heat effects are necessary; energy input without rise in temperature
- This is necessary to overcome attraction e.g. between liquid molecules which are about to boil
- Worse still, materials can also exist in superheated or supercooled states, where they lack nucleation sites to allow energy release for phase change

## Coping with equations of state

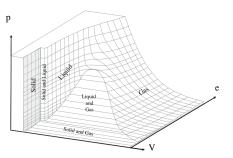
- All equations of state we have considered are valid only for a single phase
- It is hard work to fit an equation to the full range of physically reasonable behaviour for most materials, and possibly even harder work to invert it
- In many cases, your equation of state needs to be correct enough to capture the behaviour across the majority of the domain - you can still reproduce experimental results and make useful predictions
- But what do you do when an accurate equation of state is essential to your results?

## Using the 'wrong' EoS

- In this work (Schoch, Nikiforakis and Lee, 2013), a detonation inside a steel tube was simulated and compared to experiments
- Something wasn't quite right about the final two results for the 4 mm thick steel



# Tabulated equations of state



- An equation of state is effectively fitting a multivariate function (or combination of functions) to cover this surface
- Instead, we could lay down a grid on this surface, and store a series of values within a table
- In this example, a grid has been laid in  $\varepsilon-p$  space, i.e. we have  $\nu=\nu(\varepsilon,p)$ , or  $\rho=\rho(\varepsilon,p)$  is this a sensible choice?
- $\bullet$  For an arbitrary given parameter pair,  $(\varepsilon,p),$  how do we get density (or specific volume)?
- If we have a table of data, is this really an **equation** of state?

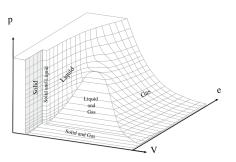
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## Interpolation of values

- There are three general requirements for a tabulated equation of state:
  - There are enough data points such that accuracy is comparable to a close functional fit
  - There aren't so many data points that using the table would lead to computational memory issues
  - Any look-up procedure in the table should be fast certainly faster than a root-finding inversion procedure
- Fortunately, many fast algorithms exist for this, depending on your tabulated structure
- For example, if you have a rectangular structure in internal energy and pressure, and need the density for a specific pair  $(\varepsilon, p)$ :
  - ① Use a search algorithm to identify neighbouring indices in the table such that  $\varepsilon_i \leq \varepsilon \leq \varepsilon_{i+1}$  and  $p_j \leq p \leq p_{j+1}$
  - 2 Use a bisection algorithm to compute density



# Tabulating your data



- It is clear that the  $\varepsilon-p$  tabulation might have some issues here
- There are no points in the 'Liquid and Gas' or 'Solid and Gas' Regions
- Note this region is not necessarily discontinuous, just might change very sharply
- Discontinuities in derivatives do exist at phase boundaries though
- Your choice of discretisation will ultimately depend on what you need to capture, and what your underlying material is
- Any pair of independent variables  $(\rho, \varepsilon, p \text{ and } T)$  could be used some of these might produce better tables than others
- If you need to model phase change, there is an advantage to using density as one of your parameters - why?

#### Phase boundaries

- At phase boundaries, the equation of state changes sharply (nearly discontinuously)
- $\bullet$  For example, the density of water at atmospheric pressure drops from 1000 kg/m  $^3$  to  $1\,\mathrm{kg/m}^3$
- Sharp changes in gradient can cause errors and oscillations in interpolation techniques (much like they can in numerical methods...)
- $\bullet$  For example, you may end up with an interpolated density of  $500 \, \text{kg/m}^3$ , which is neither a sensible liquid or vapour value
- If you know density, you know which side of the phase transition you are on you can ignore certain data points, or use advanced techniques (cut cells for equations of state)

## Populating tables

- When populating your table of data, for general equations of state, it is likely that
  a uniform grid structure is not ideal, either too much memory is wasted on smooth
  areas, or there is not enough detail on sharp areas
- However, there is no need to do this, and advanced meshing techniques can be used here for optimal searching
- See, e.g. Föll *et al.* "On the use of tabulated equations of state for multi-phase simulations in the homogeneous equilibrium limit" (2019)

### Where do you get tabulated data from?

#### Experiments:

- Theoretically the most accurate way to get data, providing your equipment provides small error bars
- Can be challenging what do you use to measure pressure in a pool of molten steel?
- Actual data tends to be sparse interpolation may be inaccurate
- From complicated multivariate functions:
  - These might come from fits to experimental data, or from underlying molecular theory and energy calculation
  - We have previously stated that inverting and manipulating functions was too
    expensive
  - When doing this for a table of data, though, we only need to do this once
  - Can combine multiple functions to cover all appropriate regions



### Examples of tabulated data

- Water (and ice and steam) displays very complex behaviour, especially close to phase change - stiffened gas models are only appropriate for high-pressure waves
- From a thermodynamic perspective, water at room temperature is close to phase change
- Unsurprisingly, water simulation and properties are required in many industrial applications - not only do these applications need an accurate equation of state, they need a standardised one too
- This is compiled (and distributed) by the International Association for the Properties of Water and Steam (IAPWS)
- ullet For other materials, Los Alamos National Laboratory has compiled the **SESAME** database a series of tabulated equations of state including metals and polymers, giving p=p(
  ho,T) and covering melting and vaporisation
- A final example, which we shall look at in a bit more detail later, is plasma for use in lightning models



## Notes on practical use

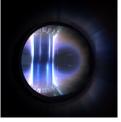
- It is unlikely that you will be creating your own equation of state (though you may end up tabulating data)
- When working from papers, hopefully there will be information about the equation
  of state used and the parameters selected (though it may be in a reference, or a
  reference in a reference...)
- It is worth being aware of the limits of validity of the equation of state you are using, but...
- Even if you do go beyond these theoretical limits, results are not necessarily
  useless, qualitative correlations can be valuable, as could a correct shock speed
  (even if a subsequent rarefaction isn't quite right)

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## Magnetohydrodynamics and plasma





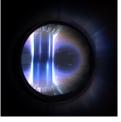


- At high temperatures, a gas becomes ionised, forming a plasma, the 'fourth state of matter'
- Although similar to a gas in many ways, the motion of a plasma is dominated by electric and magnetic fields, and not pressure changes
- As a result, the equations of motion for such a state of matter are referred to as magnetohydrodynamics (MHD)

Computing

### Modelling a plasma







- Over 90% of the 'regular' matter in the universe is plasma, therefore there are many applications involving modelling plasma flow
- Obviously, astrophysical applications dominate (stellar evolution, jets, neutron stars, etc.) but also terrestrial examples include fusion technology and lightning
- In this lecture, we consider the starting point for all these models, the general equations of MHD - specific applications may need additional treatment

Computing

### Implications of a magnetic field

- MHD adds complexity over standard hydrodynamics since:
  - 1 The motion of a plasma generates a magnetic field
  - The magnetic field can affect how a charged particle moves, thus the magnetic field effects the motion of a plasma
- In other words, the magnetic field is **coupled** to the hydrodynamic behaviour, we cannot simply add a source term to the equations to deal with this behaviour
- Fortunately, for our numerical methods, this behaviour can be described through a hyperbolic system of conservation equations
- Starting from the Euler equations and Maxwell's equations, we shall derive a complete conservation system for MHD (under certain assumptions)

#### Outline

- Beyond ideal gases some examples
- 2 Beyond equations
- Magnetohydrodynamics
- 4 Equations of magnetohydrodynamics
- Conservation form

Computing

#### Outline

- Beyond ideal gases some examples
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- Magnetohydrodynamics
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### Maxwell's equations

 By now we have seen the Euler equations many times, we begin instead with Maxwell's equations, four equations governing electrodynamics

$$\frac{\partial \mathbf{B}}{\partial t} + \nabla \times \mathbf{E} = 0$$

$$\frac{1}{c^2}\frac{\partial \mathbf{E}}{\partial t} + \mu_0 \mathbf{J} - \nabla \times \mathbf{B} = 0$$

$$\nabla \cdot \mathbf{B} = 0$$
$$\nabla \cdot \mathbf{E} = \frac{\tau}{-}$$

- Gauss's law
- ullet Maxwell's equations describe the evolution magnetic field,  ${f B}$  and electric field  ${f E}$
- ullet  ${f J}$  is the current density, au the charge density
- Constants are: c, the speed of light,  $\mu_0=4\pi\times 10^{-7}\, {\rm H/m}$  the magnetic constant, or vacuum permeability and  $\epsilon_0$  the vacuum permittivity, where  $c^2=1/\mu_0\epsilon_0$

### Euler and Maxwell's equations

 In order to describe the flow of a plasma, we need to combine the Euler equations with Maxwell's equations

$$\frac{\partial \rho}{\partial t} + \nabla \cdot (\rho \mathbf{v}) = 0 \qquad \qquad \frac{\partial \mathbf{B}}{\partial t} + \nabla \times \mathbf{E} = 0$$

$$\rho \left[ \frac{\partial \mathbf{v}}{\partial t} + (\mathbf{v} \cdot \nabla) \mathbf{v} \right] - \nabla \cdot \boldsymbol{\sigma} = 0 \qquad \qquad \frac{1}{c^2} \frac{\partial \mathbf{E}}{\partial t} + \mu_0 \mathbf{J} - \nabla \times \mathbf{B} = 0$$

$$\nabla \cdot \mathbf{B} = 0$$

$$\nabla \cdot \mathbf{E} = \frac{\tau}{\epsilon_0}$$

- ullet Note the Euler equations have been written in a non-conservative form, and for a general stress tensor,  $\sigma$
- Also note if the material has resistivity (resists the flow of electrons), this adds internal energy to the system through **Joule heating**,  $\eta \mathbf{J} \cdot \mathbf{J}$
- This is because magnetic and electric fields contribute to the total energy and overall forcing (stress) on a plasma



#### Stress tensor

$$\frac{\partial \rho}{\partial t} + \nabla \cdot (\rho \mathbf{v}) = 0 \qquad \qquad \frac{\partial \mathbf{B}}{\partial t} + \nabla \times \mathbf{E} = 0$$

$$\rho \left[ \frac{\partial \mathbf{v}}{\partial t} + (\mathbf{v} \cdot \nabla) \mathbf{v} \right] - \nabla \cdot \boldsymbol{\sigma} = 0 \qquad \qquad \frac{1}{c^2} \frac{\partial \mathbf{E}}{\partial t} + \mu_0 \mathbf{J} - \nabla \times \mathbf{B} = 0$$

$$\nabla \cdot \mathbf{B} = 0$$

$$\nabla \cdot \mathbf{E} = \frac{\tau}{\epsilon_0}$$

- We have written the equations in this form (for now) since this is a general representation of the non-conservative Euler equations which looks the same for both ionised and unionised flow
- For the standard Euler equations, the stress is described through internal pressure forces,  $\sigma = -p\mathbf{I}$ , hence we can write this term as the standard  $\nabla p$  term
- In a plasma, magnetic fields also exert a force, the Lorentz force, in this case we have

$$\nabla \cdot \boldsymbol{\sigma} = -\nabla p + \tau \mathbf{E} + \mathbf{J} \times \mathbf{B}$$



#### A full set of equations

$$\begin{split} \frac{\partial \rho}{\partial t} + \nabla \cdot (\rho \mathbf{v}) &= 0 \\ \rho \left[ \frac{\partial \mathbf{v}}{\partial t} + (\mathbf{v} \cdot \nabla) \mathbf{v} \right] + \nabla p - \tau \mathbf{E} - \mathbf{J} \times \mathbf{B} &= 0 \\ \frac{\partial \rho \varepsilon}{\partial t} + \nabla \cdot (\rho \varepsilon \mathbf{v}) + p \nabla \cdot \mathbf{v} &= \eta \mathbf{J} \cdot \mathbf{J} \end{split} \qquad \begin{aligned} \frac{\partial \mathbf{B}}{\partial t} + \nabla \times \mathbf{E} &= 0 \\ \frac{\partial \mathbf{E}}{\partial t} + \mu_0 \mathbf{J} - \nabla \times \mathbf{B} &= 0 \\ \nabla \cdot \mathbf{B} &= 0 \\ \nabla \cdot \mathbf{E} &= \frac{\tau}{\epsilon_0} \end{aligned}$$

- Assuming we know an equation of state, we have five equations, and two constraint equations (required for initial conditions), for six independent variables, e.g.  $\rho$ ,  $\mathbf{v}$ , p,  $\mathbf{B}$ ,  $\mathbf{E}$  and  $\tau$
- Ohm's law relates the current density to known quantities

$$\eta \mathbf{J} = \mathbf{E} + \mathbf{v} \times \mathbf{B}$$

Charge conservation is a physical requirement that allows closure of the system

$$\frac{\partial \tau}{\partial t} + \nabla \cdot \mathbf{J} = 0$$



### Simplifying the system

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

$$\rho \left[ \frac{\partial \mathbf{v}}{\partial t} + (\mathbf{v} \cdot \nabla) \mathbf{v} \right] + \nabla p - \tau \mathbf{E} - \mathbf{J} \times \mathbf{B} = 0$$

$$\frac{1}{c^2} \frac{\partial \mathbf{E}}{\partial t}$$

$$\frac{\partial \rho \varepsilon}{\partial t} + \nabla \cdot (\rho \varepsilon \mathbf{v}) + p \nabla \cdot \mathbf{v} = \eta \mathbf{J} \cdot \mathbf{J}$$

$$\frac{\partial \mathbf{B}}{\partial t} + \nabla \times \mathbf{E} = 0$$

$$\frac{1}{c^2} \frac{\partial \mathbf{E}}{\partial t} + \mu_0 \mathbf{J} - \nabla \times \mathbf{B} = 0$$

$$\nabla \cdot \mathbf{B} = 0$$

$$\nabla \cdot \mathbf{E} = \frac{\tau}{\epsilon_0}$$

$$\frac{\partial \tau}{\partial t} + \nabla \cdot \mathbf{J} = 0, \qquad \eta \mathbf{J} = \mathbf{E} + \mathbf{v} \times \mathbf{B}$$

- Although we have a complete description of the plasma evolution, this is not necessarily the best form for numerical applications
- Firstly, it is not in conservation form
- Secondly, the presence of the speed of light within the system governs information travel timescales, and thus can add a severe time step restriction
- We restrict ourselves to a non-relativistic assumption ( $|\mathbf{v}| \ll c$ ), for which we can greatly simplify the system



## Simplifying the system - charge density

$$\begin{split} \frac{\partial \rho}{\partial t} + \nabla \cdot (\rho \mathbf{v}) &= 0 \\ \rho \left[ \frac{\partial \mathbf{v}}{\partial t} + (\mathbf{v} \cdot \nabla) \, \mathbf{v} \right] + \nabla p - \tau \mathbf{E} - \mathbf{J} \times \mathbf{B} &= 0 \\ \frac{\partial \rho \varepsilon}{\partial t} + \nabla \cdot (\rho \varepsilon \mathbf{v}) + p \nabla \cdot \mathbf{v} &= \eta \mathbf{J} \cdot \mathbf{J} \end{split}$$

$$\frac{\partial \mathbf{B}}{\partial t} + \nabla \times \mathbf{E} = 0$$

$$\frac{1}{c^2} \frac{\partial \mathbf{E}}{\partial t} + \mu_0 \mathbf{J} - \nabla \times \mathbf{B} = 0$$

$$\nabla \cdot \mathbf{B} = 0$$

$$\nabla \cdot \mathbf{E} = \frac{\tau}{60}$$

$$\frac{\partial \tau}{\partial t} + \nabla \cdot \mathbf{J} = 0$$
  $\eta \mathbf{J} = \mathbf{E} + \mathbf{v} \times \mathbf{B}$ 

- Given that we compute the electric field, and this must obey the Poisson's
  equation for electrostatics, we can use this to compute the charge density directly
- As a result, we don't need the charge continuity equation, reducing the number of
  equations we need to solve
- This is true, even for relativistic flow, further simplifications require relative magnitudes of the various terms to be considered

# Simplifying the system - scaling

$$\frac{\partial \rho}{\partial t} + \nabla \cdot (\rho \mathbf{v}) = 0 \qquad \qquad \frac{\partial \mathbf{B}}{\partial t} + \nabla \times \mathbf{E} = 0$$

$$\rho \left[ \frac{\partial \mathbf{v}}{\partial t} + (\mathbf{v} \cdot \nabla) \mathbf{v} \right] + \nabla p - \tau \mathbf{E} - \mathbf{J} \times \mathbf{B} = 0 \qquad \qquad \frac{1}{c^2} \frac{\partial \mathbf{E}}{\partial t} + \mu_0 \mathbf{J} - \nabla \times \mathbf{B} = 0$$

$$\nabla \cdot \mathbf{B} = 0$$

$$\nabla \cdot \mathbf{E} = \frac{\tau}{\epsilon_0}$$

$$\eta \mathbf{J} = \mathbf{E} + \mathbf{v} \times \mathbf{B}$$

- In order to make further simplifications, we need to understand how variables are related
- The first assumption is that magnetic field and velocity are non negligible (or else we would reduce to regular fluid flow, or no flow), we consider magnitudes  $|\mathbf{B}| \sim B$ ,  $|\mathbf{v}| \sim v$
- ullet Secondly, derivatives operate over a length scale a,  $|
  abla|\sim rac{1}{a}$
- ullet This gives a time step relationship as  $\left|\frac{\partial}{\partial t}\right|\sim \frac{v}{a}$



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## Simplifying the system - electric field scaling

$$\frac{\partial \rho}{\partial t} + \nabla \cdot (\rho \mathbf{v}) = 0 \qquad \qquad \frac{\partial \mathbf{B}}{\partial t} + \nabla \times \mathbf{E} = 0$$

$$\rho \left[ \frac{\partial \mathbf{v}}{\partial t} + (\mathbf{v} \cdot \nabla) \mathbf{v} \right] + \nabla p - \tau \mathbf{E} - \mathbf{J} \times \mathbf{B} = 0 \qquad \qquad \frac{1}{c^2} \frac{\partial \mathbf{E}}{\partial t} + \mu_0 \mathbf{J} - \nabla \times \mathbf{B} = 0$$

$$\nabla \cdot \mathbf{B} = 0$$

$$\nabla \cdot \mathbf{B} = 0$$

$$\nabla \cdot \mathbf{E} = \frac{\tau}{60}$$

$$\eta \mathbf{J} = \mathbf{E} + \mathbf{v} \times \mathbf{B}$$

 $\bullet$  Starting from Faraday's law, and scaling  $|\mathbf{E}|\sim E$  can relate the magnitude to other quantities

$$\frac{v}{a}B \sim -\frac{1}{a}E$$

- Therefore (since magnitudes ignore sign) we have  $E \sim vB$
- We can then use this to compare the electric field and magnetic field contributions within the electric field evolution equation



## Simplifying the system - electric field scaling

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

$$\frac{\partial \mathbf{B}}{\partial t} + \nabla \times \mathbf{E} = 0$$

$$\rho \left[ \frac{\partial \mathbf{v}}{\partial t} + (\mathbf{v} \cdot \nabla) \mathbf{v} \right] + \nabla p - \tau \mathbf{E} - \mathbf{J} \times \mathbf{B} = 0$$

$$\frac{\partial \rho \varepsilon}{\partial t} + \nabla \cdot (\rho \varepsilon \mathbf{v}) + p \nabla \cdot \mathbf{v} = \eta \mathbf{J} \cdot \mathbf{J}$$

$$\nabla \cdot \mathbf{B} = 0$$

$$\nabla \cdot \mathbf{E} = \frac{\tau}{\epsilon_0}$$

$$\eta \mathbf{J} = \mathbf{E} + \mathbf{v} \times \mathbf{B}$$

• The magnitudes for these two quantities are

$$\frac{1}{c^2} \frac{\partial \mathbf{E}}{\partial t} \sim \frac{v^2 B}{c^2 a}, \qquad \nabla \times \mathbf{B} \sim \frac{B}{a}$$

- Under the non-relativistic consideration, the time derivative of electric field can be considered negligible
- As a result, this equation simply becomes becomes Ampere's law

$$\mathbf{J} = \mu_0^{-1} 
abla imes \mathbf{B}$$



## Simplifying the system - current and charge scaling

$$\begin{split} \frac{\partial \rho}{\partial t} + \nabla \cdot (\rho \mathbf{v}) &= 0 \\ \rho \left[ \frac{\partial \mathbf{v}}{\partial t} + (\mathbf{v} \cdot \nabla) \mathbf{v} \right] + \nabla p - \tau \mathbf{E} - \mathbf{J} \times \mathbf{B} &= 0 \\ \frac{\partial \rho \varepsilon}{\partial t} + \nabla \cdot (\rho \varepsilon \mathbf{v}) + p \nabla \cdot \mathbf{v} &= \eta \mathbf{J} \cdot \mathbf{J} \end{split} \qquad \begin{aligned} \frac{\partial \mathbf{B}}{\partial t} + \nabla \times \mathbf{E} &= 0 \\ \mathbf{J} &= \mu_0^{-1} \nabla \times \mathbf{B} \\ \nabla \cdot \mathbf{B} &= 0 \\ \nabla \cdot \mathbf{E} &= \frac{\tau}{\epsilon_0} \end{aligned}$$

$$\eta \mathbf{J} = \mathbf{E} + \mathbf{v} \times \mathbf{B}$$

- ullet We now apply scaling to current density through Ampere's law,  $J\sim rac{B}{\mu_0 a}$
- $\bullet$  Similarly, we scale the charge density,  $\tau \sim \frac{\epsilon_0 E}{a} = \frac{vB}{c^2 \mu_0 a}$
- Comparing magnitudes of the two components of the Lorentz force, we have

$$au \mathbf{E} \sim \frac{v^2 B^2}{c^2 \mu_0 a}, \quad \mathbf{J} \times \mathbf{B} \sim \frac{B^2}{\mu_0 a}$$

• As a result, we can neglect the  $\tau {\bf E}$  component, and, since charge density no longer appears in any of the evolution equations, we can also ignore the initial condition for  $\tau$  from Poisson's equation for electrostatics

## Magnetohydrodynamics equations

$$\begin{split} \frac{\partial \rho}{\partial t} + \nabla \cdot (\rho \mathbf{v}) &= 0 \\ \rho \left[ \frac{\partial \mathbf{v}}{\partial t} + (\mathbf{v} \cdot \nabla) \, \mathbf{v} \right] + \nabla p - \mathbf{J} \times \mathbf{B} &= 0 \\ \frac{\partial \rho \varepsilon}{\partial t} + \nabla \cdot (\rho \varepsilon \mathbf{v}) + p \nabla \cdot \mathbf{v} &= \eta \mathbf{J} \cdot \mathbf{J} \end{split} \qquad \begin{aligned} \frac{\partial \mathbf{B}}{\partial t} + \nabla \times \mathbf{E} &= 0 \\ \mathbf{J} &= \mu_0^{-1} \nabla \times \mathbf{B} \\ \mathbf{E} &= \eta \mathbf{J} - \mathbf{v} \times \mathbf{B} \\ \nabla \cdot \mathbf{B} &= 0 \end{aligned}$$

- For non-relativistic plasma, we can describe a system of four evolution equations, one constraint equation and relationships for additional electromagnetic quantities
- It is this set of equations that are referred to as the equations of magnetohydrodynamics (MHD)
- We now wish to describe these equations in conservation form, such that we can
  use the finite volume methods to provide numerical solutions

#### Outline

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#### Ideal MHD

$$\begin{split} \frac{\partial \rho}{\partial t} + \nabla \cdot (\rho \mathbf{v}) &= 0 \\ \rho \left[ \frac{\partial \mathbf{v}}{\partial t} + (\mathbf{v} \cdot \nabla) \, \mathbf{v} \right] + \nabla p - \mathbf{J} \times \mathbf{B} &= 0 \\ \frac{\partial \rho \varepsilon}{\partial t} + \nabla \cdot (\rho \varepsilon \mathbf{v}) + p \nabla \cdot \mathbf{v} &= \eta \mathbf{J} \cdot \mathbf{J} \end{split} \qquad \begin{aligned} & \frac{\partial \mathbf{B}}{\partial t} + \nabla \times \mathbf{E} &= 0 \\ & \mathbf{J} = \mu_0^{-1} \nabla \times \mathbf{B} \\ & \mathbf{E} = \eta \mathbf{J} - \mathbf{v} \times \mathbf{B} \\ & \nabla \cdot \mathbf{B} &= 0 \end{aligned}$$

- $\bullet$  For many applications, we can use  $\mathit{ideal}$  MHD, which makes the assumption that  $\eta=0$
- This corresponds to a plasma which is perfectly conductive this is a valid assumption for many astrophysical plasma applications, where length scales are large, and the material is fully ionised
- As a result, the source term in the energy equation vanishes, and electric field is no longer (directly) related to current density



#### Ideal MHD

$$\begin{split} \frac{\partial \rho}{\partial t} + \nabla \cdot (\rho \mathbf{v}) &= 0 \\ \rho \left[ \frac{\partial \mathbf{v}}{\partial t} + (\mathbf{v} \cdot \nabla) \, \mathbf{v} \right] + \nabla p - \mathbf{J} \times \mathbf{B} &= 0 \\ \frac{\partial \rho \varepsilon}{\partial t} + \nabla \cdot (\rho \varepsilon \mathbf{v}) + p \nabla \cdot \mathbf{v} &= 0 \end{split} \qquad \begin{aligned} \frac{\partial \mathbf{B}}{\partial t} + \nabla \times \mathbf{E} &= 0 \\ \mathbf{J} &= \nabla \times \mathbf{B} \\ \mathbf{E} &= -\mathbf{v} \times \mathbf{B} \\ \nabla \cdot \mathbf{B} &= 0 \end{aligned}$$

- It is also standard in MHD literature to apply scalings to the electromagnetic quantities,  $\mathbf{B} \to \mathbf{B}/\sqrt{\mu_0}$ ,  $\mathbf{E} \to \mathbf{E}/\sqrt{\mu_0}$  and  $\mathbf{J} \to \sqrt{\mu_0}\mathbf{J}$
- ullet This removes  $\mu_0$  from the equations entirely; care must be taken when recovering physical quantities
- Similar in principle to atmospheric pressure being scaled to unity in e.g. Toro's tests

#### MHD in conservation form: momentum

- We now consider the four evolution equations
- The mass conservation equation is already in the correct form
- We can rewrite the non-magnetic terms of the momentum (velocity) equation in the standard conservation form

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

$$\frac{\partial \rho \mathbf{v}}{\partial t} + \nabla \cdot (\rho \mathbf{v} \otimes \mathbf{v} + p\mathbf{I}) - \mathbf{J} \times \mathbf{B} = 0$$

$$\frac{\partial \rho \varepsilon}{\partial t} + \nabla \cdot (\rho \varepsilon \mathbf{v}) + p\nabla \cdot \mathbf{v} = 0$$

$$\frac{\partial \mathbf{B}}{\partial t} + \nabla \times \mathbf{E} = 0$$

- We can write the Lorentz force term in terms of magnetic field only through Ampere's law  ${f J}=\nabla\times{f B}$
- Standard vector calculus identities, and the divergence constraint, can be used to show

$$-\mathbf{J} \times \mathbf{B} = \mathbf{B} \times (\nabla \times \mathbf{B}) = \nabla \cdot \left(\frac{1}{2}B^2\mathbf{I} - \mathbf{B} \otimes \mathbf{B}\right)$$

## MHD in conservation form: magnetic field

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

$$\frac{\partial \rho \mathbf{v}}{\partial t} + \nabla \cdot \left[ \rho \mathbf{v} \otimes \mathbf{v} + \left( p + \frac{1}{2} B^2 \right) \mathbf{I} - \mathbf{B} \otimes \mathbf{B} \right] = 0$$

$$\frac{\partial \rho \varepsilon}{\partial t} + \nabla \cdot (\rho \varepsilon \mathbf{v}) + p \nabla \cdot \mathbf{v} = 0$$

$$\frac{\partial \mathbf{B}}{\partial t} + \nabla \times \mathbf{E} = 0$$

- $\begin{tabular}{ll} \bullet & \mbox{We can use Ohm's law to remove} \\ & \mbox{electric field dependence,} \\ & \mbox{$\mathbf{E}=-\mathbf{v}\times\mathbf{B}$} \\ \end{tabular}$
- Therefore, in this case, electric field is not an independent variable
   this is not true for all applications
- As seen previously, the magnetic field evolution equation can be written in conservation form

$$-\nabla \times (\mathbf{v} \times \mathbf{B}) = \nabla \cdot (\mathbf{B} \otimes \mathbf{v} - \mathbf{v} \otimes \mathbf{B})$$

 The evolution of the magnetic field is coupled to the hydrodynamic evolution through the velocity

## MHD in conservation form: magnetic field

$$\begin{split} \frac{\partial \rho}{\partial t} + \nabla \cdot (\rho \mathbf{v}) &= 0 \\ \frac{\partial \rho \mathbf{v}}{\partial t} + \nabla \cdot \left[ \rho \mathbf{v} \otimes \mathbf{v} + \left( p + \frac{1}{2} B^2 \right) \mathbf{I} - \mathbf{B} \otimes \mathbf{B} \right] &= 0 \\ \frac{\partial \rho \varepsilon}{\partial t} + \nabla \cdot (\rho \varepsilon \mathbf{v}) + p \nabla \cdot \mathbf{v} &= 0 \\ \frac{\partial \mathbf{B}}{\partial t} + \nabla \cdot (\mathbf{B} \otimes \mathbf{v} - \mathbf{v} \otimes \mathbf{B}) &= 0 \end{split}$$

- The momentum and magnetic field equations are straightforward to bring into conservation form
- The energy equation requires a bit more work
- As expected, only total energy is conserved; in the presence of a magnetic field, this contains contributions from the internal energy and kinetic energy and also from the internal magnetic energy
- Internal magnetic energy is given by  $\varepsilon_B=\frac{1}{2}B^2$ , hence the total conserved quantity is

$$U=\rho\varepsilon+\frac{1}{2}\rho v^2+\frac{1}{2}B^2$$

ullet U is often used as total energy for MHD systems to avoid confusion with electric field



## MHD in conservation form: energy (1)

 In order to obtain the conservation form for total energy, we need to obtain 'evolution equations' for each component (we have the internal energy already)

$$U=\rho\varepsilon+\frac{1}{2}\rho v^2+\frac{1}{2}B^2$$

First, note that

$$\mathbf{v} \cdot \frac{\partial \rho \mathbf{v}}{\partial t} = \frac{\partial}{\partial t} \left( \frac{1}{2} \rho v^2 \right) + \frac{1}{2} v^2 \frac{\partial \rho}{\partial t}$$

• This means that we can obtain the kinetic energy term through the momentum equation by considering the dot product with velocity

$$\mathbf{v} \cdot \left\{ \frac{\partial \rho \mathbf{v}}{\partial t} + \nabla \cdot \left[ \rho \mathbf{v} \otimes \mathbf{v} + \left( p + \frac{1}{2} B^2 \right) \mathbf{I} - \mathbf{B} \otimes \mathbf{B} \right] \right\} = 0$$

## MHD in conservation form: energy (2)

$$\mathbf{v} \cdot \left\{ \frac{\partial \rho \mathbf{v}}{\partial t} + \nabla \cdot \left[ \rho \mathbf{v} \otimes \mathbf{v} + \left( p + \frac{1}{2} B^2 \right) \mathbf{I} - \mathbf{B} \otimes \mathbf{B} \right] \right\} = 0$$

Considering the first term in the spatial derivative component

$$\mathbf{v} \cdot [\nabla \cdot (\rho \mathbf{v} \otimes \mathbf{v})] = \nabla \cdot \left(\frac{1}{2}\rho v^2 \mathbf{v}\right) + \frac{1}{2}v^2 \nabla \cdot \rho \mathbf{v}$$

 Combining the first two terms, we see some cancel through the conservation of mass

$$\mathbf{v} \cdot \left[ \frac{\partial \rho \mathbf{v}}{\partial t} + \nabla \cdot (\rho \mathbf{v} \otimes \mathbf{v}) \right] = \frac{\partial}{\partial t} \left( \frac{1}{2} \rho v^2 \right) + \frac{1}{2} v^2 \frac{\partial \rho}{\partial t} + \nabla \cdot \left( \frac{1}{2} \rho v^2 \mathbf{v} \right) + \frac{1}{2} v^2 \nabla \cdot \rho \mathbf{v}$$

• So far, this derivation is no different to the standard Euler equations



## MHD in conservation form: energy (3)

$$\mathbf{v} \cdot \left\{ \frac{\partial \rho \mathbf{v}}{\partial t} + \nabla \cdot \left[ \rho \mathbf{v} \otimes \mathbf{v} + \left( p + \frac{1}{2} B^2 \right) \mathbf{I} - \mathbf{B} \otimes \mathbf{B} \right] \right\} = 0$$

Considering the second term in the spatial derivative component, we have

$$\mathbf{v} \cdot \left\{ \nabla \cdot \left[ \left( p + \frac{1}{2} B^2 \right) \mathbf{I} \right] \right\} = \nabla \cdot \left[ \left( p + \frac{1}{2} B^2 \right) \mathbf{v} \right] - \left( p + \frac{1}{2} B^2 \right) \nabla \cdot \mathbf{v}$$

Considering the third term, we have

$$\mathbf{v} \cdot [\nabla \cdot (\mathbf{B} \otimes \mathbf{B})] = \mathbf{v} \cdot [(\mathbf{B} \cdot \nabla) \, \mathbf{B}]$$



## MHD in conservation form: energy (4)

• Finally, we consider the internal magnetic energy contribution, noting that

$$\mathbf{B} \cdot \frac{\partial \mathbf{B}}{\partial t} = \frac{\partial}{\partial t} \left( \frac{1}{2} B^2 \right)$$

As before, this suggests we consider

$$\mathbf{B} \cdot \left[ \frac{\partial \mathbf{B}}{\partial t} + \nabla \cdot (\mathbf{B} \otimes \mathbf{v} - \mathbf{v} \otimes \mathbf{B}) \right] = 0$$

The spatial derivative term gives

$$\mathbf{B} \cdot [\nabla \cdot (\mathbf{B} \otimes \mathbf{v} - \mathbf{v} \otimes \mathbf{B})] = \frac{1}{2} \nabla \cdot (B^2 \mathbf{v}) + \frac{1}{2} B^2 \nabla \cdot \mathbf{v} - \mathbf{B} \cdot [(\mathbf{B} \cdot \nabla) \mathbf{v}]$$

## MHD in conservation form: energy (5)

 If we now combine the results for the internal energy, the momentum and the magnetic field equations, we have

$$\frac{\partial}{\partial t} \left( \rho \varepsilon + \frac{1}{2} \rho v^2 + \frac{1}{2} B^2 \right) + \nabla \cdot (\rho \varepsilon \mathbf{v}) + p \nabla \cdot \mathbf{v} + \nabla \cdot \left( \frac{1}{2} \rho v^2 \mathbf{v} \right) + \nabla \cdot \left[ \left( p + \frac{1}{2} B^2 \right) \mathbf{v} \right]$$

$$-\left(p + \frac{1}{2}B^2\right)\nabla \cdot \mathbf{v} - \mathbf{v} \cdot \left[\left(\mathbf{B} \cdot \nabla\right)\mathbf{B}\right] + \nabla \cdot \left(\frac{1}{2}B^2\mathbf{v}\right) + \frac{1}{2}B^2\nabla \cdot \mathbf{v} - \mathbf{B} \cdot \left[\left(\mathbf{B} \cdot \nabla\right)\mathbf{v}\right] = 0$$

• Noting that the  $\nabla \cdot \mathbf{v}$  terms cancel, and using the definition of total energy for the time derivative, we have

$$\frac{\partial U}{\partial t} + \nabla \cdot \left[ \left( \rho \varepsilon + \frac{1}{2} \rho v^2 + p + \frac{1}{2} B^2 + \frac{1}{2} B^2 \right) \mathbf{v} \right] - \mathbf{v} \cdot \left[ (\mathbf{B} \cdot \nabla) \mathbf{B} \right] - \mathbf{B} \cdot \left[ (\mathbf{B} \cdot \nabla) \mathbf{v} \right] = 0$$

• Finally, we note that

$$-\mathbf{v}\cdot\left[\left(\mathbf{B}\cdot\nabla\right)\mathbf{B}\right]-\mathbf{B}\cdot\left[\left(\mathbf{B}\cdot\nabla\right)\mathbf{v}\right]=-\nabla\cdot\left[\left(\mathbf{v}\cdot\mathbf{B}\right)\mathbf{B}\right]$$



Computing

#### Conservation law form

• These equations give us the conservation law form of the ideal MHD equations

$$\begin{split} \frac{\partial \rho}{\partial t} + \nabla \cdot \left( \rho \mathbf{v} \right) &= 0 \\ \frac{\partial \rho \mathbf{v}}{\partial t} + \nabla \cdot \left[ \rho \mathbf{v} \otimes \mathbf{v} + \left( p + \frac{1}{2} B^2 \right) \mathbf{I} - \mathbf{B} \otimes \mathbf{B} \right] &= 0 \\ \frac{\partial U}{\partial t} + \nabla \cdot \left[ \left( U + p + \frac{1}{2} B^2 \right) \mathbf{v} - \left( \mathbf{v} \cdot \mathbf{B} \right) \mathbf{B} \right] &= 0 \\ \frac{\partial \mathbf{B}}{\partial t} + \nabla \cdot \left( \mathbf{B} \otimes \mathbf{v} - \mathbf{v} \otimes \mathbf{B} \right) &= 0 \end{split}$$

 As with the standard Euler equations, we need an equation of state to link pressure, density and specific internal energy

## Plasma equation of state

- Much like other materials, there is no single equation of state for a plasma
- Typically, two 'types' of plasma can be distinguished; fully ionised and partially ionised plasma
- The equation of state for partially ionised plasma is complex we shall consider this in a bit more detail when we consider the plasma model for lightning
- When we made the decision to work with ideal MHD, we implicitly also made the decision to work with a fully ionised plasma
- Zero resistivity is the same as infinite conductivity, which would require all electrons to be able to move freely
- This cannot be the case in non-ionised or partially-ionised material, hence for these materials, resistivity must always be modelled

## Plasma equation of state

An ideal plasma is well described by an ideal gas law

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

- ullet In this case, we can take  $\gamma=5/3$  for almost all ideal MHD applications resulting from the thermodynamics of non-interacting monatomic mixtures
- In many papers (and even textbooks), this is implicitly assumed when using ideal MHD
- Not all fully ionised plasma is an ideal plasma, it depends on the **plasma** parameter,  $\Lambda$ ,

$$\Lambda = 4\pi n_e \lambda_D$$

- ullet  $n_e$  is the electron number density and  $\lambda_D$  the Debye length, a length scale over which a charge carrier's electrostatic field extends
- For  $\Lambda\gg 1$ , the interaction with the electrostatic field dominates over particle collisions, and we have an ideal plasma



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