

Simulation of Matter under Extreme Conditions

Source terms and equations of state (part 1)

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Outline

- 1 Source terms
- 2 Equation of state
- 3 Ideal gas equation of state
- 4 Beyond ideal gases

Why do we need source terms?

- So far, we have assumed that the only reason for evolution within our system of equations comes from gradients of our three conserved variables

$$\frac{\partial \mathbf{u}}{\partial t} + \nabla \cdot \mathbf{f}(\mathbf{u}) = \mathbf{0}$$

- These gradients result in a force applied to the conserved quantities, causing the evolution
- When solving this type of system of equations, we've repeatedly ignored 'negligible' quantities such as gravity, thermal diffusion, viscosity
- These, along with other effects, such as chemical reaction, result in additional forces which are 'dealt with' through **source terms**

Why do we need source terms?

- Additional terms are used to deal with forces that arise from things other than gradients of the conserved quantities
- For example, we may consider
 - Body forces - an external force acting throughout the control volume, e.g. gravity
 - Surface forces - a force arising from molecular behaviour at an interface between two materials, e.g. surface tension
 - Frictional forces - a force arising from molecular behaviour within a material, e.g. viscosity
- All of these can be described through modifying our system of evolution equations to include source terms (though sometimes these terms can also be brought within the conservation system)

How do source terms act?

$$\frac{\partial \mathbf{u}}{\partial t} + \nabla \cdot \mathbf{f}(\mathbf{u}) = \mathbf{s}(\mathbf{u})$$

- If a system has source terms, these are normally placed on the right hand side of the conservation law form
- This is technically not a conservation law now, but a **balance law**
- Since these are a function of the conserved variables, they will evolve in time, i.e. something needs to be applied every time step
- The most common approach to solving a hyperbolic system with source terms is similar the approach for multidimensional equations
- We use **operator splitting** to separate the conservation law update and the source term update

- A simple splitting technique is to first solve the balance law **ignoring** source terms (i.e. as a conservation law):

$$\left. \begin{array}{lcl} \text{PDE} & : & \frac{\partial \mathbf{u}}{\partial t} + \nabla \cdot \mathbf{f}(\mathbf{u}) = 0 \\ \text{IC} & : & \mathbf{u}^n \end{array} \right\} \Rightarrow \bar{\mathbf{u}}^{n+1}$$

- This gives the solution $\bar{\mathbf{u}}^{n+1}$, which is a state evolved to t^{n+1} , just not the correct one
- This can then be used as the initial condition for solving the balance law **ignoring** the divergence operator:

$$\left. \begin{array}{lcl} \text{ODE} & : & \frac{d\mathbf{u}}{dt} = \mathbf{s}(\mathbf{q}) \\ \text{IC} & : & \bar{\mathbf{u}}^{n+1} \end{array} \right\} \Rightarrow \mathbf{u}^{n+1}$$

- At the end of this process, all physical behaviour has been accounted for and the solution \mathbf{u}^{n+1} has been obtained

Operator splitting

- Toro's book contains a proof that this operator splitting approach is equivalent to solving the underlying system of equations
- This is not the only approach to solving source terms, for example, we could reverse the order of ODE and PDE
- Much like dimensional splitting, this can be written in terms of operators on the original data, \mathbf{u}^n

$$\mathbf{u}^{n+1} = \mathcal{S}^{(\Delta t)} \mathcal{C}^{(\Delta t)} (\mathbf{u}^n)$$

- Here, \mathcal{S} is the source term operator, and \mathcal{C} the conservation law operator
- If we are solving multidimensional equations, then the conservation law operator, \mathcal{C} , **can include dimensional splitting** with any of the approaches we considered

Higher-order operator splitting

$$\mathbf{u}^{n+1} = \mathcal{S}^{(\Delta t)} \mathcal{C}^{(\Delta t)} (\mathbf{u}^n)$$

- This update scheme is first-order accurate in time - a second-order accurate scheme is perhaps now obvious

$$\mathbf{u}^{n+1} = \mathcal{S}^{(\frac{1}{2}\Delta t)} \mathcal{C}^{(\Delta t)} \mathcal{S}^{(\frac{1}{2}\Delta t)} (\mathbf{u}^n)$$

- Unlike unsplit techniques for multi-dimensional systems, there is not a **general method** for solving a conservation law and source terms in a 'single step', analogous to a dimensionally unsplit method
- As a result, operator splitting is the most widely used approach to solving hyperbolic PDEs with source terms

Solving the ODE

- As part of the operator splitting process, we need to solve the ODE

$$\frac{d\mathbf{u}}{dt} = \mathbf{s}(\mathbf{q})$$

- Whilst any ODE solving technique could be used, Runge-Kutta methods are ideal for this
- This can be done through any standard ODE solver
- For example the first-order accurate (in time) Euler Method

$$\mathbf{u}^{n+1} = \bar{\mathbf{u}}^{n+1} + \Delta t \mathbf{s}(\bar{\mathbf{u}}^{n+1})$$

- Or, if the source term is updated before the conservation law part,

$$\bar{\mathbf{u}}^{n+1} = \mathbf{u}^n + \Delta t \mathbf{s}(\mathbf{u}^n)$$

Common Runge-Kutta choices

- There are a few common RK methods for systems conservation laws, chosen for a combination of stability, accuracy and efficiency
- Heun's method is popular for second order accuracy:

$$\mathbf{K}_1 = \Delta t s(\bar{\mathbf{u}}^{n+1}), \quad \mathbf{K}_2 = \Delta t s(\bar{\mathbf{u}}^{n+1} + \mathbf{K}_1)$$

$$\mathbf{u}^{n+1} = \bar{\mathbf{u}}^{n+1} + \frac{1}{2}(\mathbf{K}_1 + \mathbf{K}_2)$$

- The original method is popular for fourth order accuracy:

$$\mathbf{K}_1 = \Delta t s(\bar{\mathbf{u}}^{n+1}), \quad \mathbf{K}_2 = \Delta t s\left(\bar{\mathbf{u}}^{n+1} + \frac{1}{2}\mathbf{K}_1\right), \quad \mathbf{K}_3 = \Delta t s\left(\bar{\mathbf{u}}^{n+1} + \frac{1}{2}\mathbf{K}_2\right)$$

$$\mathbf{K}_4 = \Delta t s(\bar{\mathbf{u}}^{n+1} + \mathbf{K}_3), \quad \mathbf{u}^{n+1} = \bar{\mathbf{u}}^{n+1} + \frac{1}{6}(\mathbf{K}_1 + 2\mathbf{K}_2 + 2\mathbf{K}_3 + \mathbf{K}_4)$$

- Both have been written here assuming the conservation law is solved first, then the source term

Source terms and time steps

$$\mathbf{u}^{n+1} = \mathcal{S}^{(\Delta t)} \mathcal{C}^{(\Delta t)} (\mathbf{u}^n)$$

- It is probably obvious that the time step for both parts of the update must be the same
- Is this always going to be governed by the CFL condition?
- Source terms are modelling physical behaviour not included in the conservation law, and this will have its own time scale
- This may be smaller than the Δt obtained through the CFL condition
- Just like numerical methods for PDEs, those for ODEs can cause instabilities if the time step taken is too large
- Note - there is not a general method for calculating the time step of a source term - it depends on the physical and mathematical behaviour being modelled

Dealing with restrictive time steps

- Running the code with the minimum stable time step

$$\Delta t = \min(\Delta t_{\text{CFL}}, \Delta t_s)$$

is possible, and is a sensible choice when first implementing a new algorithm

- However, using a lower time step than necessary on a numerical method results in an **unnecessary accumulation of error**
- There is additionally greater **computational expense** when running at a lower time step
- Two options for avoiding this (we assume the source term has the lower time step):
 - 1 Use a stable **implicit** scheme to evolve the source term, ignoring (or greatly relaxing) the source term time step
 - 2 Run the ODE solver several times for each single time step in the conservation law - **subcycling**

Implicit schemes for source terms

- It may be that our 'hyperbolic system with source terms' is actually a mixed hyperbolic-parabolic system
- For example, the advection-diffusion equation

$$\frac{\partial u}{\partial t} + \frac{\partial}{\partial x} (au) = D_c \frac{\partial^2 u}{\partial x^2}$$

- The diffusion part can be treated as a source term, with time step restriction

$$\Delta t_s = \frac{(\Delta x)^2}{2D_c}$$

- The infinite propagation speed and lack of discontinuities of the parabolic term makes it an ideal candidate for an implicit solution (see Numerical Methods for Incompressible Fluid Dynamics for details)

Subcycling for source terms

- When dealing with parabolic source terms, the time step restriction came from algorithmic stability of explicit schemes
- The actual behaviour did not need to be evolved at this time step for an accurate solution
- However, it may be that there is genuine behaviour in the source term that needs to be captured at a small time step
- **If** this behaviour depends only on the material within a grid cell, then we can use subcycling
- Chemistry is often an ideal case here - the speed with which something converts reactants into products is often much faster than the speed with which the material moves

Subcycling for source terms

- Chemical reactions and kinetics are commonly required for detonations and explosives modelling
- We shall consider an actual example shortly, for now we focus on the implementation

```
updateConservative(u, dtCFL);  
  
double subTime = 0.0;  
do {  
    double dtS = computeSourceTimeStep();  
    //TODO - Manually reduce dts if subTime  
    // would overshoot dtCFL  
    subTime += dtS;  
    updateSource(u, dtS);  
} while (subTime < dtCFL);
```

Body forces - gravity

- Gravity is the classic example of a body force - it affects the entire computational domain, and is (technically) present in **every** application
- Generally, we consider the effects of gravity as acceleration through the vector \mathbf{g}
- This is naturally placed in the primitive form of the Euler equations

$$\frac{\partial \mathbf{v}}{\partial t} + (\mathbf{v} \cdot \nabla) \mathbf{v} + \frac{1}{\rho} \nabla p = \mathbf{g}$$

- In the conserved form of the equations, this results in a source term contribution to both the momentum equation and the total energy equation (through the kinetic energy contribution)

$$\frac{\partial}{\partial t} \begin{pmatrix} \rho \\ \rho \mathbf{v} \\ E \end{pmatrix} + \nabla \cdot \begin{pmatrix} \rho \mathbf{v} \\ \rho \mathbf{v} \otimes \mathbf{v} + \mathbf{I} p \\ (E + p) \mathbf{v} \end{pmatrix} = \begin{pmatrix} 0 \\ \rho \mathbf{g} \\ \rho \mathbf{v} \cdot \mathbf{g} \end{pmatrix}$$

- The source term itself for gravity is the solution to the gravitational potential, Φ , for example

$$\nabla^2 \Phi(\mathbf{r}) = 4\pi G \rho(\mathbf{r}), \quad \mathbf{g} = -\nabla \Phi$$

- Whilst essential for astrophysical applications (where it might need to be solved once, or already known if you are lucky), it is rarely worth worrying about solving this Poisson's equation for applications on Earth
- Here, it is better to use $\mathbf{g} = (0, 0, -9.8)^T \text{ ms}^{-2}$
- For terrestrial hyperbolic problems, generally the time scale of the behaviour of interest is much faster than the scales over which gravitational acceleration acts
- It is for this reason, we did not consider in in our initial Euler equation models, and we will often neglect it from many of the systems we consider

Body forces - not gravity

- One definition of a body force is a force which **does not require contact** to transfer energy
- Depending on how you model a system, electric and magnetic fields can produce body forces
- We shall consider these in more detail later
- Radiative heat emission or absorption is another body force, unlike other heat transfer behaviour, e.g. convection and conduction
- Some of these body forces act on energy, rather than velocity/momentum
- For example, radiative emission is given by

$$\frac{\partial E}{\partial t} + \nabla \cdot [(E + p) \mathbf{v}] = -S_r$$

Frictional forces - viscosity

- So far we have only considered **inviscid** equations, those with zero viscosity
- For many high-speed applications this is reasonable - for high speed flow for both air and water, viscosity tends to be negligible (high Reynolds number)
- This is not always true, and, additionally, the concepts behind viscosity also apply to elastoplastic solid modelling
- In both these cases, we have a **stress tensor** which can allow for shear stresses in the material in question
- This can (seemingly) be incorporated into our numerical model

$$\frac{\partial}{\partial t} \begin{pmatrix} \rho \\ \rho \mathbf{v} \\ E \end{pmatrix} + \nabla \cdot \begin{pmatrix} \rho \mathbf{v} \\ \rho \mathbf{v} \otimes \mathbf{v} - \boldsymbol{\sigma} \\ E \mathbf{v} - \boldsymbol{\sigma} \cdot \mathbf{v} \end{pmatrix} = 0$$

- But, the stress tensor, $\boldsymbol{\sigma}$, may contain derivatives itself

Viscosity and the stress tensor

- We shall consider the stress tensor in more detail when we cover elastoplastic equations
- For a viscous material, the stress tensor is given by

$$\boldsymbol{\sigma} = -p\mathbf{I} + \boldsymbol{\sigma}'$$

- If the material is **Newtonian** (constant viscosity), then the viscous stress, $\boldsymbol{\sigma}'$, is given by

$$\boldsymbol{\sigma}' = 2\eta \left[\mathbf{D} - \frac{1}{3} \text{Tr}(\mathbf{D}) \mathbf{I} \right] + \xi \text{Tr}(\mathbf{D}) \mathbf{I}, \quad \mathbf{D} = \frac{1}{2} \left(\nabla \mathbf{v} + (\nabla \mathbf{v})^T \right)$$

- η is **shear viscosity**, ξ is **bulk viscosity**
- Note that this definition already contains derivatives of velocity

Back to balance law form

$$\frac{\partial}{\partial t} \begin{pmatrix} \rho \\ \rho \mathbf{v} \\ E \end{pmatrix} + \nabla \cdot \begin{pmatrix} \rho \mathbf{v} \\ \rho \mathbf{v} \otimes \mathbf{v} + \mathbf{I} p \\ (E + p) \mathbf{v} \end{pmatrix} = \begin{pmatrix} 0 \\ \nabla \cdot \boldsymbol{\sigma}' \\ \nabla \cdot (\boldsymbol{\sigma}' \cdot \mathbf{v}) \end{pmatrix}$$

- We can write $\nabla \cdot \boldsymbol{\sigma}'$ as

$$\nabla \cdot \boldsymbol{\sigma}' = \eta \nabla^2 \mathbf{v} + \left(\xi + \frac{1}{3} \eta \right) \nabla (\nabla \cdot \mathbf{v})$$

- This introduces a diffusive term (second derivative) into our source term
- It is common to deal with viscosity in incompressible flow, where $\nabla \cdot \mathbf{v} = 0$
- In this case, we recover the more familiar

$$\nabla \cdot \boldsymbol{\sigma}' = \eta \nabla^2 \mathbf{v}$$

$$\frac{\partial}{\partial t} \begin{pmatrix} \rho \\ \rho \mathbf{v} \\ E \end{pmatrix} + \nabla \cdot \begin{pmatrix} \rho \mathbf{v} \\ \rho \mathbf{v} \otimes \mathbf{v} + \mathbf{I} p \\ (E + p) \mathbf{v} \end{pmatrix} = \begin{pmatrix} 0 \\ \nabla \cdot \boldsymbol{\sigma}' \\ \nabla \cdot (\boldsymbol{\sigma}' \cdot \mathbf{v}) \end{pmatrix}$$

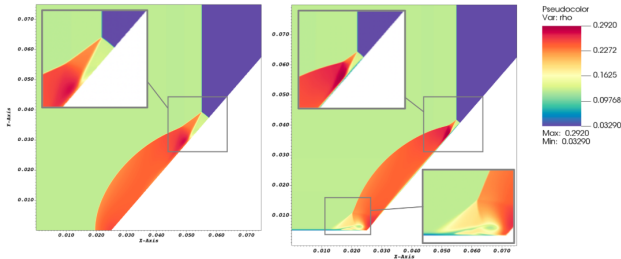
- We can write $\nabla \cdot \boldsymbol{\sigma}'$ as

$$\nabla \cdot \boldsymbol{\sigma}' = \eta \nabla^2 \mathbf{v} + \left(\xi + \frac{1}{3} \eta \right) \nabla (\nabla \cdot \mathbf{v})$$

- As with the advection-diffusion equation, this introduces a Δx^2 dependence on the time step - solving this system requires careful treatment of the viscous terms
- If viscous effects dominate, it will typically be the case that an incompressible model is appropriate, but not always

Viscosity dominated solutions

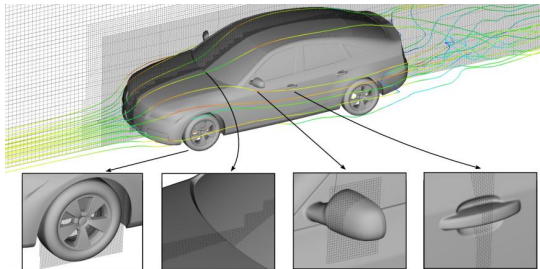
- Hypersonic re-entry vehicles are certainly in the high-speed regime, and viscosity is important
- Here, A shock passes over a body at around 3,000 m/s (from Heather Muir's thesis)



- The extreme speed here means that the hyperbolic time step is already very small

Viscosity dominated solutions

- For earth-based vehicles being driven reasonably fast, both compressible effects and viscosity can be important (though much work is done assuming incompressibility)
- Here, we return to Nandan's cut cell simulation



- Here, the length scales are such that the viscous time step is not actually an issue

- Modelling reactive materials and detonations is a big topic, here we consider a very simple case
- When modelling detonations, the system is inherently multiphysics; we have **reactants** which are chemically converted into **products**
- However, because we haven't covered multiphysics yet, we'll consider just one of these materials
- Before we even get this far, though, we first need to be able to deal with the fact that we need to know where our detonation is taking place

$$\frac{\partial}{\partial t} \begin{pmatrix} \rho \\ \rho \mathbf{v} \\ E \\ \rho \lambda \end{pmatrix} + \nabla \cdot \begin{pmatrix} \rho \mathbf{v} \\ \rho \mathbf{v} \otimes \mathbf{v} + \mathbf{I} p \\ (E + p) \mathbf{v} \\ \rho \lambda \mathbf{v} \end{pmatrix} = \begin{pmatrix} 0 \\ 0 \\ 0 \\ 0 \end{pmatrix}$$

- This is the **augmented Euler** equations, augmented with the additional variable λ

Augmented Euler equations and tracers

$$\frac{\partial}{\partial t} \begin{pmatrix} \rho \\ \rho \mathbf{v} \\ E \\ \rho \lambda \end{pmatrix} + \nabla \cdot \begin{pmatrix} \rho \mathbf{v} \\ \rho \mathbf{v} \otimes \mathbf{v} + \mathbf{I} p \\ (E + p) \mathbf{v} \\ \rho \lambda \mathbf{v} \end{pmatrix} = \begin{pmatrix} 0 \\ 0 \\ 0 \\ 0 \end{pmatrix}$$

- Without any other source terms, this new system of equations can also be described as being the Euler equations with and **advected tracer**
- That is, if we have a variable, which is sufficiently similar in properties to the underlying material, and also low enough mass to be negligible in material effects, it will simply move with the flow
- For example, adding food colouring to water; the two are effectively the same material, but this way we can see how the colour spreads
- In the case of reactions, λ is the **reaction progress variable** - for a given point in the domain, it tells us how much of the reactant has turned to product

Including the reaction

$$\frac{\partial}{\partial t} \begin{pmatrix} \rho \\ \rho \mathbf{v} \\ E \\ \rho \lambda \end{pmatrix} + \nabla \cdot \begin{pmatrix} \rho \mathbf{v} \\ \rho \mathbf{v} \otimes \mathbf{v} + \mathbf{I} p \\ (E + p) \mathbf{v} \\ \rho \lambda \mathbf{v} \end{pmatrix} = \begin{pmatrix} 0 \\ 0 \\ \pm \rho K Q \\ \rho K \end{pmatrix}$$

- Two new variables, $K(\mathbf{q})$ is the reaction rate law, and determines when the material starts reacting and Q is the heat of detonation, a quantity which describes the exothermic nature of the reaction
- Note the \pm - this deals with the fact that energy moves **from** products **to** reactants
- Sometimes you won't see the source term in the energy equation, it can, instead, be incorporated into the total energy, effectively incorporating **chemical energy** into the definition
- In this case, λ is directly used by the material's equation of state (we have $p = p(\rho, \varepsilon, \lambda)$)

Including the reaction

$$\frac{\partial}{\partial t} \begin{pmatrix} \rho \\ \rho \mathbf{v} \\ E \\ \rho \lambda \end{pmatrix} + \nabla \cdot \begin{pmatrix} \rho \mathbf{v} \\ \rho \mathbf{v} \otimes \mathbf{v} + \mathbf{I} p \\ (E + p) \mathbf{v} \\ \rho \lambda \mathbf{v} \end{pmatrix} = \begin{pmatrix} 0 \\ 0 \\ \pm \rho K Q \\ \rho K \end{pmatrix}$$

- The reaction rate law is material dependent, common examples are the single-step Arrhenius and the simple pressure-based laws

$$K = -\lambda C \exp(-T_A/T), \quad K = -\sigma(1 - \lambda)^\nu p^n$$

- Here, T_A , C , σ , ν , n and also Q are constants given for the material you are interested in
- However, more complex rules exist, depending on how well someone has studied the material in question
- In many cases, the time scale over which the reaction takes place is short, and can have an adverse effect on the simulation; the subcycling approach is common

Other physical source terms

- Source terms are very much dependent on the problem you are trying to solve - we cannot create an exhaustive list!
- However, it is worth listing a few more...
- **Temperature diffusion** - another diffusive term, this time on the Energy equation - diffusion is typically a slower-time scale problem
- **Surface tension** - requires an **interface** between two materials - see Multiphysics Modelling for Four States of Matter
- **Chemical reactions** - we touched on these, but other chemistry occurs than just detonations, including mixing fluids and burning, very problem dependent
- The key feature is that source terms will be a given equation, which act upon your conserved variables \mathbf{u} (before and/or after a conservative update)
- It is also possible to introduce mathematical source terms to your system of equations...

Non-Cartesian coordinates

- All equations we have considered have been written using Cartesian coordinates
- However, the conservation laws are **invariant under coordinate transformation**
- It may be that Cartesian coordinates are not the most suitable for your problem at hand
- Cylindrical and spherical coordinates are often useful for behaviour around a fixed axis or point
- Problems with cylindrical or spherical **symmetry** can be reduced from three-dimensions to one or two by an appropriate choice of coordinates
- However, we must describe our derivative operators appropriately for this coordinate system

Cylindrical coordinates

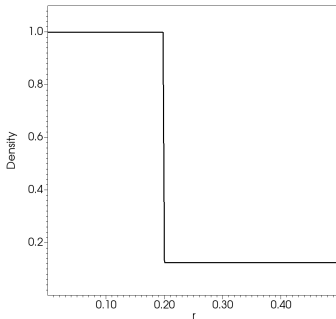
$$\nabla f = \frac{\partial f}{\partial r} \mathbf{e}_r + \frac{1}{r} \frac{\partial f}{\partial \theta} \mathbf{e}_\theta + \frac{\partial f}{\partial z} \mathbf{e}_z$$
$$\nabla \cdot \mathbf{f} = \frac{\partial f_r}{\partial r} + \frac{f_r}{r} + \frac{1}{r} \frac{\partial f_\theta}{\partial \theta} + \frac{\partial f_z}{\partial z}$$

- In cylindrical symmetry, we can ignore all θ terms
- This gives an Euler equation system:

$$\frac{\partial}{\partial t} \begin{pmatrix} \rho \\ \rho v_r \\ \rho v_z \\ E \end{pmatrix} + \frac{\partial}{\partial r} \begin{pmatrix} \rho v_r \\ \rho v_r^2 + p \\ \rho v_r v_z \\ (E + p) v_r \end{pmatrix} + \frac{\partial}{\partial z} \begin{pmatrix} \rho v_z \\ \rho v_r v_z \\ \rho v_z^2 + p \\ (E + p) v_z \end{pmatrix} = - \begin{pmatrix} \frac{\rho v_r}{r} \\ \frac{\rho v_r^2}{r} \\ \frac{\rho v_r v_z}{r} \\ \frac{(E + p) v_r}{r} \end{pmatrix}$$

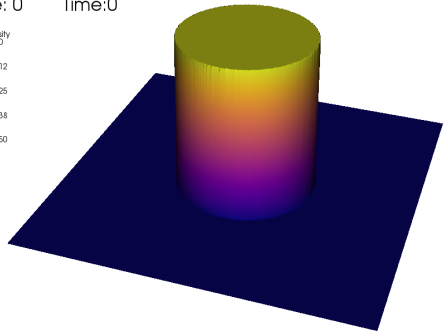
- Note - the pressure term is a gradient, not a divergence, hence this does not appear in the source term

Cylindrical Sod test

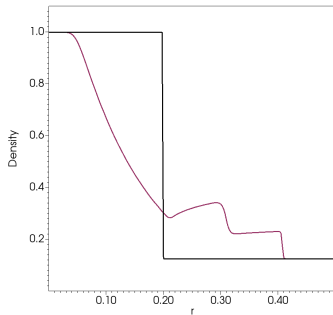


DB: Header
Cycle: 0 Time:0

Pseudocolor
Var: Air_density
1.000
0.7812
0.5625
0.3438
0.1250
Max: 1.000
Min: 0.1250

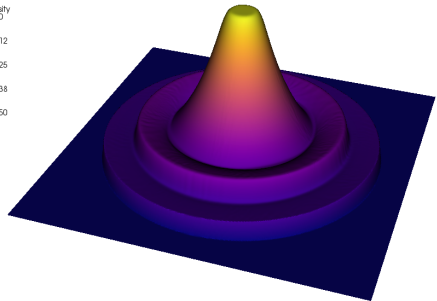


Cylindrical Sod test



DB: Header
Cycle: 115 Time: 0.126103

Pseudocolor
Var: Air_density
Max: 1.000
Min: 0.1250



$$\nabla f = \frac{\partial f}{\partial r} \mathbf{e}_r + \frac{1}{r} \frac{\partial f}{\partial \theta} \mathbf{e}_\theta + \frac{1}{r \sin \theta} \frac{\partial f}{\partial \phi} \mathbf{e}_\phi$$
$$\nabla \cdot \mathbf{f} = \frac{\partial f_r}{\partial r} + \frac{2f_r}{r} + \frac{1}{r \sin \theta} \frac{\partial (f_\theta \sin \theta)}{\partial \theta} + \frac{1}{r \sin \theta} \frac{\partial f_\phi}{\partial \phi}$$

- In spherical symmetry, we can ignore all θ and ϕ terms
- This gives an Euler equation system:

$$\frac{\partial}{\partial t} \begin{pmatrix} \rho \\ \rho v_r \\ E \end{pmatrix} + \frac{\partial}{\partial r} \begin{pmatrix} \rho v_r \\ \rho v_r^2 + p \\ (E + p) v_r \end{pmatrix} = - \begin{pmatrix} \frac{2\rho v_r}{r} \\ \frac{2\rho v_r^2}{r} \\ \frac{2(E+p)v_r}{r} \end{pmatrix}$$

General 1D coordinate systems

- It is possible to write the one-dimensional Euler equations generally for Cartesian, cylindrical or spherical coordinates

$$\frac{\partial}{\partial t} \begin{pmatrix} \rho \\ \rho v \\ E \end{pmatrix} + \frac{\partial}{\partial r} \begin{pmatrix} \rho v \\ \rho v^2 + p \\ (E + p) v \end{pmatrix} = -\frac{\alpha}{r} \begin{pmatrix} \rho v \\ \rho v^2 \\ (E + p) v \end{pmatrix}$$

- For Cartesian coordinates, $\alpha = 0$, for cylindrical, $\alpha = 1$, for spherical, $\alpha = 2$
- Note - this assumes a single velocity (v_x or v_r)
- The advantage to this expression (and those on the last two slides) is that the numerical methods **do not need to change** - we still have “Cartesian-looking” flux vectors
- The coordinate effects are then applied through source terms
- In this case, your source term time step is the same as the CFL time step - this is an ideal case to simply use RK methods for the source terms

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The equation of state

- None of the systems of equations we consider in this course are **closed systems**

$$\frac{\partial}{\partial t} \begin{pmatrix} \rho \\ \rho \mathbf{v} \\ E \end{pmatrix} + \nabla \cdot \begin{pmatrix} \rho \mathbf{v} \\ \rho \mathbf{v} \otimes \mathbf{v} + \mathbf{I} p \\ (E + p) \mathbf{v} \end{pmatrix} = 0$$

- For example, the Euler equations are three equations for four independent variables, e.g. density, momentum, energy and pressure
- In Continuum Computational Methods, we stated that an equation of state was used to close the system
- We also gave an equation of state suitable for air,

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

with $\gamma = 1.4$

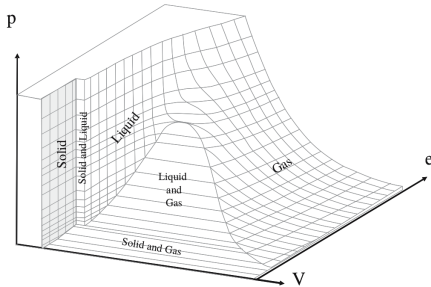
- Where does this come from?

Assumptions behind the continuum model

- The equation of state can be used to provide a continuum description of molecular thermodynamic behaviour
- It is worth considering when (or why) the continuum approach is suitable for modelling a material which is composed of discrete molecules
- The continuum approach requires that then **length scale of the flow** is greater than the **mean free path** of a constituent molecule
- At this scale, behaviour is the result of bulk motions of particles, and statistical deviations of a single particle are negligible
- For air under atmospheric conditions, the mean free path is around 100 nm
- The continuum approach is valid providing we are not looking at very small scales, or too close to vacuum (where the mean free path becomes large)

The phase diagram

- The equation of state provides closure between pressure, density and specific internal energy
- For a given material, this forms a **state surface**, represented on a phase diagram



- It is common when considering equations of state to work with specific volume (ν or sometimes V) where $\nu = 1/\rho$
- Ideally, an equation of state should cover this entire surface - is that ever possible?

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- The ideal gas equation of state arises by considering a gas as comprising **non-interacting point particles**
- These approximations are valid providing the intermolecular forces result in a potential energy that is much lower than the kinetic energy of the particles
- One of the key advantages of the ideal gas model is that the equation of state behaviour can be derived from the laws of thermodynamics, both at a microscopic scale, and also at the continuum scale
- Additionally, there are a wide range of gases (and plasma) that can be modelled with this equation of state (and over a wide range of conditions)
- This includes air (mostly nitrogen and oxygen) and noble gases at atmospheric conditions, plasma for astrophysical or fusion models and also the interior of a neutron star

Derivation of the ideal gas EoS

- We begin with some of the underlying physical laws we will need, and use these to get to $p = (\gamma - 1) \rho \varepsilon$
- The ideal gas law itself was originally empirically derived, but can be obtained through kinetic theory

$$pV = nRT$$

- This relates pressure and volume, V , to temperature through the number of moles of the substance, n , and the ideal gas constant, R
- We can move from using temperature in the EoS to using (specific internal) energy through the first law of thermodynamics
- This relates heat, Q , to internal energy, U , pressure and volume

$$dQ = dU + pdV$$

Derivation of the ideal gas EoS

- As we have seen, the heat, Q , is 'hidden' in the specific heat quantities
- The specific heats, at constant volume and pressure respectively, are

$$c_v = \frac{1}{M} \left. \frac{dQ}{dT} \right|_V, \quad c_p = \frac{1}{M} \left. \frac{dQ}{dT} \right|_p$$

- Here, M is the total mass within a given control volume
- One of the key additional assumptions of the ideal gas model is that the specific heats **are constant**

Derivation of the ideal gas EoS

- At constant volume, the first law becomes $dQ = dU$, hence we have

$$dU = Mc_V dT \quad \Rightarrow \quad U = Mc_V T$$

- At constant pressure, the ideal gas law, when considering **changes** in material quantities, becomes

$$pdV = nRdT \quad \Rightarrow \quad dQ = Mc_V dT + nRdT$$

- Therefore we can write

$$c_p = \frac{(Mc_V + nR) dT}{M dT} = c_V + \frac{nR}{M}$$

- At this point, it is worth noting that the quantity n/M is the **molar mass**, and that $R_{\text{specific}} = nR/M$ is the **specific gas constant** of the gas in question

Derivation of the ideal gas EoS

$$c_p = \frac{(Mc_V + nR) dT}{M dT} = c_V + \frac{nR}{M}$$

- Using the relationships defined so far, we can remove temperature dependence from the ideal gas law

$$pV = \frac{nRU}{Mc_V} = \frac{(c_p - c_V)U}{c_V} = (\gamma - 1)U$$

- Here, we have defined the adiabatic constant $\gamma = c_p/c_V$
- The final step is to divide through by volume, giving internal energy per unit volume, $e = \rho\varepsilon = U/V$

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

- This is the form of the ideal gas law we quoted previously

- With the ideal gas law, and the laws of thermodynamics, it is worth revisiting the mysterious quantity, entropy, and investigating where some previous definitions come from
- Entropy is an important quantity in various aspects of CFD, but is somewhat abstract, and not a natural quantity to work with
- Despite this, understanding entropy is essential for understanding the thermodynamic behaviour resulting from our choice of equation of state
- Additionally, it can be essential in ensuring that we have unique solutions around discontinuities, by providing additional constraints on permissible behaviour
- Definitions of entropy are numerous, including it being a **measure of disorder** of a system

- For continuum systems, entropy is governed by the second law of thermodynamics

$$dU = -pdV + TdS$$

- It is common to work with **specific entropy**, s (entropy per unit mass)

$$d\varepsilon = -pd\nu + Tds$$

- Though in much literature, s and S are used interchangeably
- Here, we also have **specific volume**, $\nu = V/(\rho V) = 1/\rho$ (volume per unit mass)
- From this, we can derive the expression we gave previously for entropy,

$$s = c_V \ln p - c_p \ln \rho + \text{const.}$$

Entropy of an ideal gas

$$s = c_V \ln p - c_p \ln \rho + \text{const.}$$

- We start with the second law of thermodynamics and the ideal gas EoS

$$d\varepsilon = -pd\nu + Tds, \quad p = (\gamma - 1) \rho \varepsilon = (\gamma - 1) \frac{\varepsilon}{\nu}$$

- Using the equation of state, note that

$$\varepsilon = c_V T \quad d\varepsilon = \frac{pd\nu + \nu dp}{\gamma - 1}$$

- This enables us to rewrite the second law of thermodynamics as

$$\frac{pd\nu + \nu dp}{\gamma - 1} = -pd\nu + \frac{1}{c_V} \frac{p\nu}{\gamma - 1} ds$$

Entropy of an ideal gas

- Simplifying the expression for the second law on the previous slide gives

$$\frac{1}{p}dp + \gamma \frac{1}{\nu}d\nu = \frac{1}{c_V}ds \quad \Rightarrow \quad c_V d(\ln p) + c_p d(\ln \nu) = ds$$

- Integrating through this statement then gives the expected result

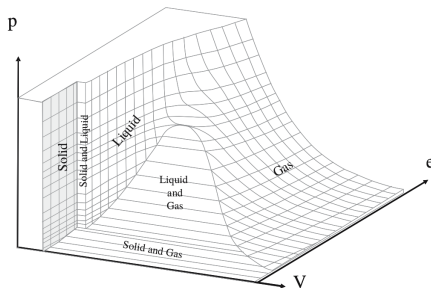
$$c_V \ln p + c_p \ln \nu = s + \text{const.}$$

or

$$c_V \ln p - c_p \ln \rho = s + \text{const.}$$

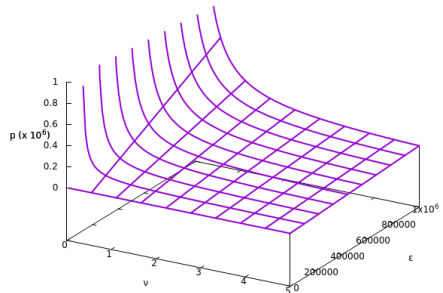
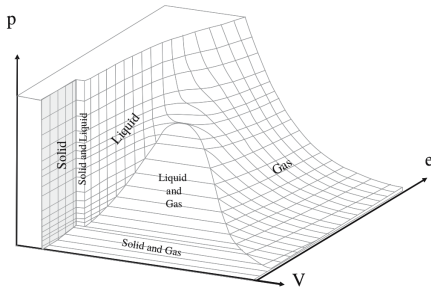
- We do not know the value of this constant, but we are generally concerned with the **change in entropy** of a system, so it is enough to know that it is constant

Phase diagram for an ideal gas



- We can now consider how the ideal gas EoS fits into this phase diagram schematic
- Obviously it can't cover everything - none of the assumptions about intermolecular forces hold for solids or liquids
- But since we have $p = (\gamma - 1)\epsilon/\nu$, this is just a function we can plot

Phase diagram for an ideal gas



- The similarities between the 'gas' region and the phase diagram for the ideal gas EoS are clear
- Here we have plotted here with $\gamma = 1.4$

Why do we need this equation of state?

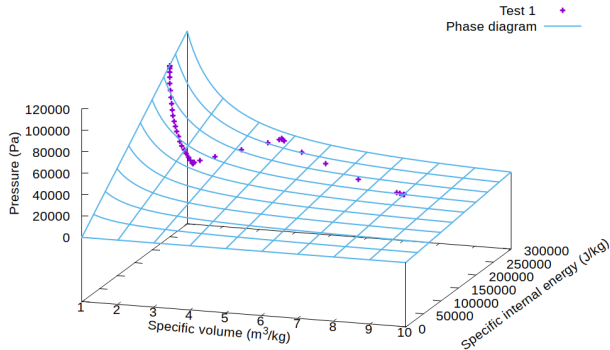
- Quite a lot of the phase diagram looks quite flat, do we really need such a 'complex' model
- Back at the start of Numerical Methods for Compressible Fluid Dynamics, we considered various simplifications of the full Navier Stokes equations
- These often simplified to a single, complete equation with no need for an EoS
- But this required assumptions such as constant density or constant pressure
- However, in a flat region of an EoS, we **may** be able to use $p = p(\rho)$ or $p = p(\rho, \varepsilon)$ rather than $p = p(\rho, \varepsilon)$
- We investigate whether this is possible with Toro's tests

Why do we need this equation of state?

- We use slight modifications to the standard tests
- In Toro's book, they are 'non-dimensionalised' ($p \propto 1$), to get true equation of state we revert to atmospheric-like conditions
- For the full unit conversion, pressure is multiplied by 10^5 , and velocity by $\sqrt{10^5}$ (since the units of pressure are $\text{kg}/(\text{m s}^2)$)
- Final time can then be divided by the same $\sqrt{10^5}$ conversion factor
- We can then make a ν - ε - p plot to see where variables lie on the phase diagram

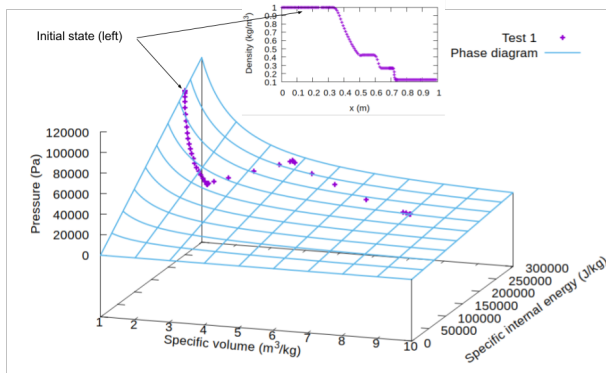
Plotting on the phase diagram

- We start with the dimensionalised Toro test 1



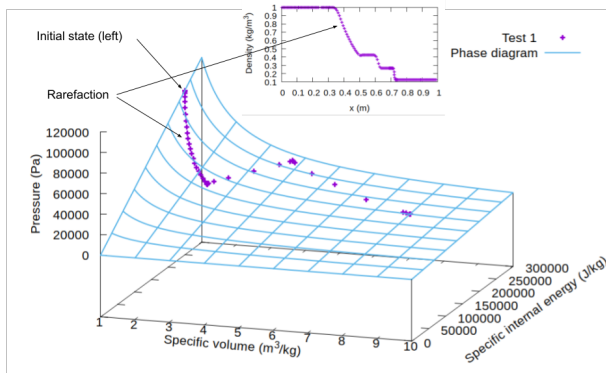
Plotting on the phase diagram

- We start with the dimensionalised Toro test 1



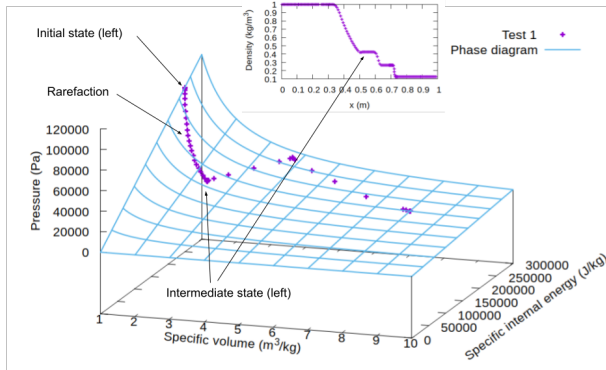
Plotting on the phase diagram

- We start with the dimensionalised Toro test 1



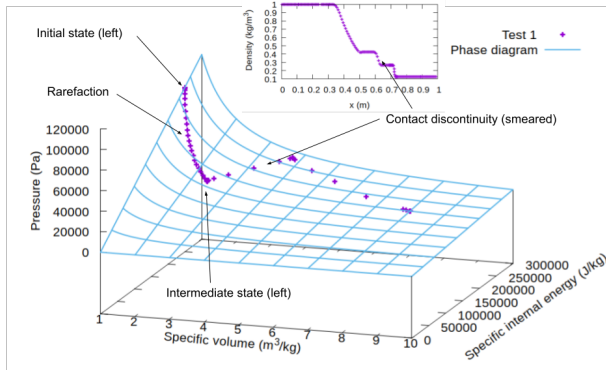
Plotting on the phase diagram

- We start with the dimensionalised Toro test 1



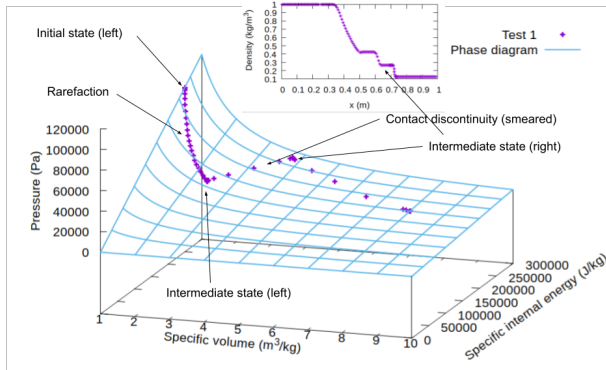
Plotting on the phase diagram

- We start with the dimensionalised Toro test 1



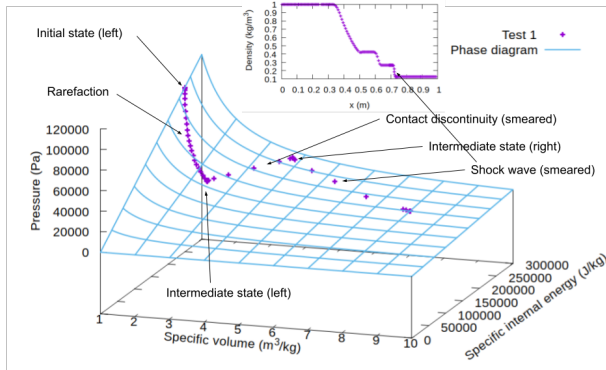
Plotting on the phase diagram

- We start with the dimensionalised Toro test 1



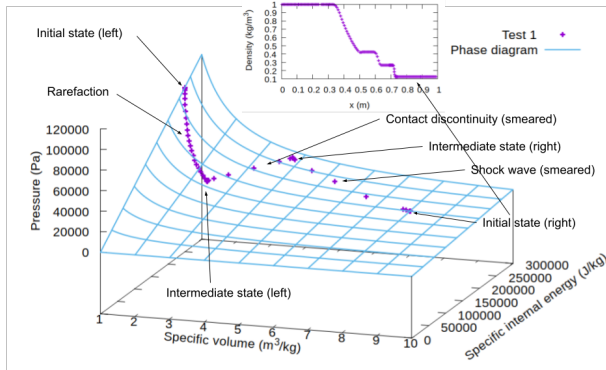
Plotting on the phase diagram

- We start with the dimensionalised Toro test 1



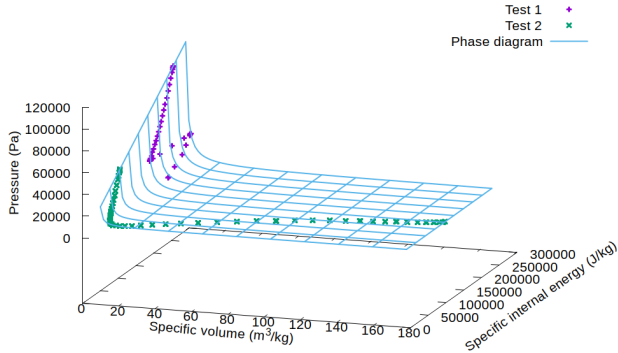
Plotting on the phase diagram

- We start with the dimensionalised Toro test 1



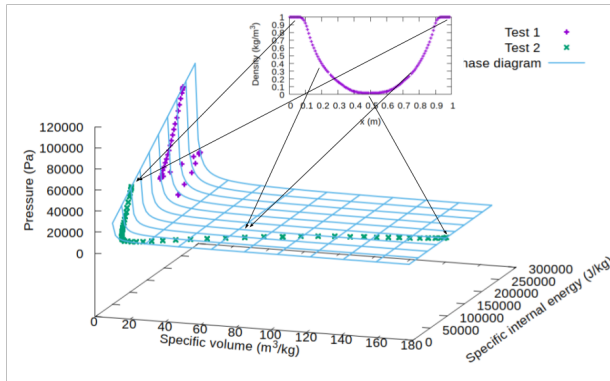
Plotting on the phase diagram

- We can now include the dimensionalised Toro test 2



Plotting on the phase diagram

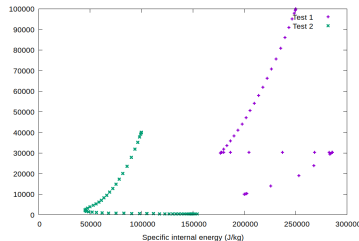
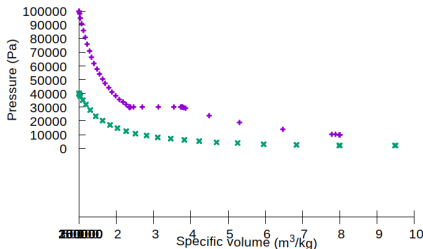
- We can now include the dimensionalised Toro test 2



Plotting on the phase diagram

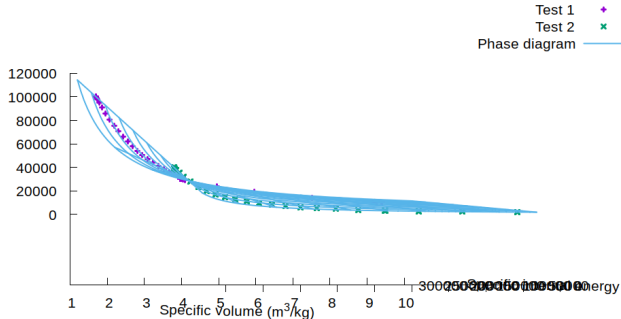
- We would like to find $p = p(w)$ for any single variable w
- It is clear that we cannot get $p = p(\rho)$ or $p = p(\varepsilon)$

Test 1 \times
Test 2 \times



Plotting on the phase diagram

- Even trying to be clever with how we define the variable w , we cannot get $p = p(w)$
- And this is just for two relatively mild cases - full compressible material modelling always requires an equation of state



Outline

- 1 Source terms
- 2 Equation of state
- 3 Ideal gas equation of state
- 4 Beyond ideal gases

General equations of state

- Unsurprisingly, a wide range of materials cannot be modelled with an ideal gas equation of state
- Is it possible to do a calculation taking a molecular description of molecules in a volume, and use this to obtain an EoS, like we did of ideal gas?
- Unfortunately, the complex molecular interactions, largely absent from an ideal gas, get in the way here
- Equations of state do exist for other materials, but they are largely empirical
- This means that sometimes they are valid only for a much smaller regime, and more than one EoS may exist for a material
- The choice depends on the behaviour in the problem you are modelling
- We first define a few important quantities

The isentrope

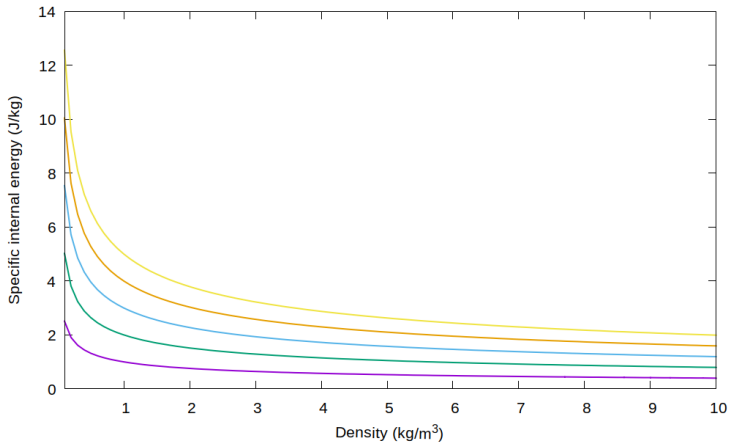
- Isentropes are simply lines of constant entropy, but they come up a lot when describing equations of state
- For example, in a Riemann problem, entropy is constant through a rarefaction (and in constant regions) - isentropes can be used to identify fluid variables here
- Speed of sound is also defined as a derivative assuming constant entropy

$$c_s = \sqrt{\left. \frac{\partial p}{\partial \rho} \right|_s}$$

- The second law of thermodynamics allows us to define the isentrope:

$$d\varepsilon = -pd\nu + Tds \quad \Rightarrow \quad d\varepsilon = -pd\nu$$

Isentrope for an ideal gas



Why do we care about the isentrope?

- We have said that going beyond ideal gases requires experimental measurements to derive an EoS
- It is rare that one (or two) measurements are enough to parameterise these more complex materials
- Instead a series of controlled measurements are required
- It is relatively easy to conduct isentropic experiments on a wide variety of materials
- One example is the Rüchardt experiment which can be used to determine some isentropic properties of gases



Source: Stephan Riediker,

<https://commons.wikimedia.org/w/index.php?curid=10382752>

The adiabatic index

- We introduced the **adiabatic index** $\gamma = c_p/c_V$ for the ideal gas
- A general form for the adiabatic index of an equation of state is

$$\gamma = -\frac{\nu}{p} \frac{\partial p}{\partial \nu} \bigg|_s = -\frac{\partial \ln p}{\partial \ln \nu} \bigg|_s$$

- In general, γ does not have to be constant
- However, when it is, along an isentrope, we have $p \propto v^{-\gamma}$ - hence this is sometimes called the **adiabatic exponent**
- This is also the slope of $\ln p$ - $\ln \nu$ space, even for non-constant γ , if you are close enough to a given reference state the above result holds - you can predict some behaviour based on your knowledge of an isentrope

The Grüneisen coefficient

- Another dimensionless coefficient for an equation of state, and one that also arises in isentropic situations is the **Grüneisen coefficient** Γ (sometimes called the Grüneisen Gamma)

$$\Gamma = - \left. \frac{\nu}{T} \frac{\partial T}{\partial \nu} \right|_s = - \left. \frac{\partial \ln T}{\partial \ln \nu} \right|_s$$

- As with the adiabatic index, we have a relationship $T \propto \nu^{-\Gamma}$
- Provided we know the temperature and density of a reference state close to a given state, we can use this to compute temperature within our system
- When $\Gamma > 0$, temperature varies monotonically along an isentrope and the EoS provides a unique parameterisation of the thermodynamic space, i.e. $p(\nu, e)$, $e(p, \nu)$ and $\nu(e, p)$ are all single valued

A brief note on convexity of isentropes

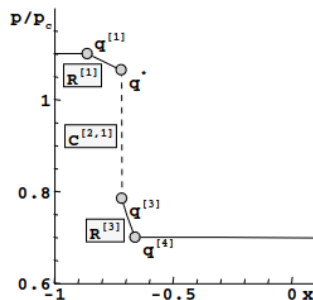
- Yet another dimensionless coefficient is the **fundamental derivative**

$$\mathcal{G} = \frac{1}{2} \frac{\nu^2}{\gamma p} \frac{\partial^2 p}{\partial \nu^2} \bigg|_s$$

- If $\mathcal{G} > 0$ then isentropes are **convex**
- Mathematically, a convex EoS is required for the wave structure we have seen in the Riemann problem:
 - Compressive, entropy-increasing shock waves
 - Expansive rarefactions
- Normally, this means sound speed increases across shock waves, and decreases across rarefactions - a non-convex EoS has a regime where this is reversed

Non-convex equations of state

- We shall not go into any detail about non-convex equations of state in this course, but we shall motivate why they may be of interest
- One common class of material described by a non-convex EoS are Bethe, Zel'dovich and Thompson (BZT) fluids
- These include heavy hydrocarbons such as decane, and some refrigerant liquids
- Such materials are widely studied, and Riemann problem solutions do exist
- Things get much more complicated though - we can now have **composite waves**



Source: Müller and Voß(2006)

Complete and incomplete equations of state

- When we were deriving the ideal gas EoS, we ended up with various expressions, e.g.

$$p = p(\rho, \varepsilon), \quad T = T(\rho, p), \quad s = s(\rho, p)$$

- We are able to freely change independent variables in these equations
- This description is a **complete equation of state** - all thermodynamic quantities are specified
- However, to close the system of equations, all we needed was

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

- For some equations of state, this is all that is provided - an **incomplete equation of state**
- This is a minimum requirement to solve the system of equations, but you will not have e.g. **temperature information**

When do you need a complete EoS?

- The basic answer is when you need to know something about temperature, this could include:
 - Temperature diffusion or convection is non-negligible in your system
 - You are dealing with freezing, melting, evaporation or condensation
 - You have temperature-dependent chemistry (e.g. detonations)
- There are also cases in which you may need to know about entropy (or, at least, changes in entropy):
 - Investigating stability of a numerical method
 - Investigation of shock wave properties

Completing an equation of state

- In the absence of a description of material properties from statistical mechanics, thermodynamic potentials can be used
- For example, the **Helmholtz free energy**, $F(\nu, T)$ or the **Gibbs free energy**, $G(p, T)$
- If **one of these** is known for a material in question, then we have either

$$dF(\nu, T) = -sdT - p d\nu$$

$$dG(p, T) = -sdT + \nu dp$$

- Coupled with the second law of thermodynamics, this gives us enough information to complete the equation of state, e.g. for the Helmholtz free energy, we have

$$p(\nu, T) = -\frac{\partial F}{\partial \nu}, \quad s(\nu, T) = -\frac{\partial F}{\partial T}$$