Simulation of Matter under Extreme Conditions

By Shikang Ni

Contents

1 2018-19 (MOCK)

1.1 Q1

1. (Part I)
   (a) Mie-Grueisen EoS:

   $$p = \Gamma(\rho)\cdot\rho\cdot(\epsilon - \epsilon_{ref}(\rho)) + p_{ref}(\rho)$$

   where $p_{ref}(\rho)$ and $\epsilon_{ref}(\rho)$ is the reference pressure and reference energy, respectively. $\Gamma(\rho)$ is the Gruneisen parameter. ϵ is the specific internal energy. $e = \rho\epsilon \Rightarrow \epsilon = e\nu$

   (b)

   $$(\rho c)^2 = \rho^2\nu^2\left(-\frac{\partial p}{\partial v}\Big|_e + p\frac{\partial p}{\partial e}\Big|_v\right) \quad \text{and} \quad p = p_{ref}(\nu) + \frac{1}{\nu}\Gamma(\nu)(\epsilon - \epsilon_{ref}(\nu))$$

   $$\frac{\partial p}{\partial v}\Big|_e = \frac{\mathrm{d}p_{ref}}{\mathrm{d}\nu} - \frac{\Gamma(\nu)}{\nu}\frac{\mathrm{d}\epsilon_{ref}(\nu)}{\mathrm{d}\nu} + (\epsilon - \epsilon_{ref}(\nu))\frac{\mathrm{d}}{\mathrm{d}\nu}\left(\frac{\Gamma(\nu)}{\nu}\right)$$

   $$\boxed{\Gamma(\nu) = \nu\frac{\partial p}{\partial e}\Big|_\nu}$$

   So,

   $$\begin{aligned}(\rho c)^2 &= \overbrace{-\frac{\mathrm{d}p_{ref}(\rho)}{\mathrm{d}\nu} + \frac{\Gamma(\nu)}{\nu}\frac{\mathrm{d}\epsilon_{ref}(\nu)}{\mathrm{d}\nu} - (\epsilon - \epsilon_{ref}(\nu))\frac{\partial}{\partial\nu}\left(\frac{\Gamma(\nu)}{\nu}\right)} + \overbrace{p\frac{\Gamma(\nu)}{\nu}} \\ &= -\frac{\mathrm{d}p_{ref}(\rho)}{\mathrm{d}\nu} + \frac{\Gamma(\nu)}{\nu}\left[p_{ref}(\rho) + \frac{\mathrm{d}\epsilon_{ref}(\nu)}{\mathrm{d}\nu}\right] + \left[\frac{\Gamma(\nu)^2}{\nu^2} - \frac{\mathrm{d}}{\mathrm{d}\nu}\left(\frac{\Gamma(\nu)}{\nu}\right)\right](\epsilon - \epsilon_{ref}(\nu))\end{aligned}$$

   (c)
      i. Isentrope reference curve. Entropy is constant along the curve.
      ii.

      $$de = -pdv + Tds \Rightarrow ds = \frac{p}{T}dv + \frac{1}{T}de$$

      $$\frac{\partial s}{\partial v}\Big|_e = \frac{p}{T} \quad \text{and} \quad \frac{\partial s}{\partial e}\Big|_v = \frac{1}{T}$$

      $$\frac{\partial^2 s}{\partial e\,\partial v} = \frac{\partial}{\partial e}\left(\frac{p}{T}\right)\Big|_v \quad \text{and} \quad \frac{\partial^2 s}{\partial v\,\partial e} = \frac{\partial}{\partial v}\left(\frac{1}{T}\right)\Big|_e$$

      They are equal, hence proving the relationship.
      iii. Complete the EoS by providing a reference temperature.
      iv. Along isentrope, $ds = 0$,

      $$\boxed{\Gamma(\nu) = -\frac{\nu}{T}\frac{\partial T}{\partial\nu}\Big|_s = -\frac{\partial\ln T}{\partial\ln\nu}\Big|_s}$$

      $$\frac{1}{T}\frac{\partial T}{\partial\nu} = -\frac{\Gamma}{\nu} \quad \Rightarrow \quad \ln\left(\frac{T}{T_0}\right) = -\Gamma\ln\left(\frac{\nu}{\nu_0}\right)$$

      $$T_{\text{ref}}(\nu) = T_0\left(\frac{v}{v_0}\right)^{-\Gamma}$$

      Thus, $T(\nu) = \frac{e - e_{\text{ref}}(\nu)}{\Gamma c_v}\nu + T_{\text{ref}}(\nu)$.

(Part II)

(a)

$$F(v,T) = e - Ts$$
$$dF = Tds - pdv - Tds - sdT = -sdT - pdv$$
$$\frac{\partial F}{\partial T}\bigg|_v = -s \quad \text{and} \quad \frac{\partial F}{\partial v}\bigg|_T = -p$$
$$\frac{\partial^2 F}{\partial v\,\partial T} = -\frac{\partial s}{\partial v}\bigg|_T \quad \text{and} \quad \frac{\partial^2 F}{\partial T\,\partial v} = -\frac{\partial p}{\partial T}\bigg|_v$$

The two expressions are equal, proving the relationship.

(b)

$$\left(p + \frac{a}{v^2}\right)(v-b) = RT$$

Differentiate EoS w.r.t. T while keeping v constant:

$$(v-b)\frac{\partial p}{\partial T} = R$$

Consider **total derivative of s in terms of dT and dv**, motivated by part (a):

$$\begin{aligned} ds &= \frac{\partial s}{\partial T}dT + \frac{\partial s}{\partial v}dv \\ &= \frac{c_v}{T}dT + \frac{\partial p}{\partial T}dv \\ &= \frac{c_v}{T}dT + \frac{R}{v-b}dv \end{aligned}$$

We simply **integrate** to obtain an expression for s:

$$\int_{s_0}^{s} ds = c_v \int_{T_0}^{T} \frac{dT}{T} + R\int_{v_0}^{v} \frac{1}{v-b}dv$$

$$s - s_0 = c_v \ln\left(\frac{T}{T_0}\right) + R\ln\left(\frac{v-b}{v_0-b}\right)$$

Substituting Van der Waals's EoS and given $R = c_v(\gamma' - 1)$, we have:

$$s = s_0 + c_v \ln\left(\frac{(p+\frac{a}{v^2})(v-b)}{(p_0+\frac{a}{v_0^2})(v_0-b)}\right) + c_v(\gamma'-1)\ln\left(\frac{v-b}{v_0-b}\right)$$

$$s = s_0 + c_v \ln\left(\frac{(p+\frac{a}{v^2})(v-b)^{\gamma'}}{(p_0+\frac{a}{v_0^2})(v_0-b)^{\gamma'}}\right)$$

(c) Set a = b = 0.

1.2 Q2

2. (a) $\lambda \in [0,1]$. λ is the reaction progress variable, it tells us how much reactant has turned into products. At the beginning, we only have reactants, so $\lambda = 0$. At the end, assuming all reactants are converted to products, $\lambda = 1$.

   (b) Chemical energy can either appear as in source term or incorporated into EoS.

$$\frac{\partial}{\partial t}\left(\rho\left(\frac{1}{2}u^2 + \tilde{e} + \lambda Q\right)\right) + \frac{\partial}{\partial x}\left(\rho\left(\frac{1}{2}u^2 + \tilde{e} + \lambda Q\right)u + pu\right) = \rho R Q$$

$$\frac{\partial}{\partial t}\left(\rho\left(\frac{1}{2}u^2 + \tilde{e}\right)\right) + \frac{\partial}{\partial x}\left(\rho\left(\frac{1}{2}u^2 + \tilde{e}\right)u + pu\right) + \underbrace{\frac{\partial}{\partial t}(\rho\lambda Q) + \frac{\partial}{\partial x}(\rho\lambda Q u) = \rho R Q}_{\text{Evolution of } \lambda}$$

   So,

$$\frac{\partial}{\partial t}\left(\rho\left(\frac{1}{2}u^2 + \tilde{e}\right)\right) + \frac{\partial}{\partial x}\left(\rho\left(\frac{1}{2}u^2 + \tilde{e}\right)u + pu\right) = 0$$

   (c) i. The Rayleigh line is a straight line that connects the points corresponding to the initial and final states on a graph of **pressure versus specific volume** for a substance subjected to a shock wave.

      Side note: the RH condition is derived assuming $\boxed{\boldsymbol{w}_1 = (\rho_1, u_1 = 0, p_1 = 0)}$. Zero pressure (stress) make sense for solids, as under atmospheric conditions, a solid material is close to zero-stress condition.

      Essentially, we want to eliminate u_2 from momentum RH equation:

$$S - \frac{\rho_1 S}{\rho_2} = u_2 \quad \text{(mass equation)}$$

      Then,

$$\begin{aligned} p_2 - p_1 &= (\rho_2 S - \rho_1 S)\left(S - S + \frac{\rho_1 S}{\rho_2}\right) \\ &= S^2(\rho_2 - \rho_1)\frac{\rho_1}{\rho_2} \quad \text{(Rayleigh line)} \end{aligned}$$

      ii. No, it is not affected. The additional chemical energy source term only comes in through the energy equation.

iii. **Derivation of Hugoniot Equation/Curve** $[\varepsilon = \varepsilon(p, \nu)]$

From mass continuity RH equation:

$$S(\rho_2 - \rho_1) = \rho_2 u_2$$

$$S = \frac{\rho_2 u_2}{\rho_2 - \rho_1}$$

Substitute into momentum RH equation:

$$\frac{p_2 - p_1}{\rho_2 u_2} = \frac{\rho_2 u_2}{\rho_2 - \rho_1} - u_2$$

$$\frac{p_2 - p_2}{\rho_2 u_2} = \frac{\rho_1 u_2}{\rho_2 - \rho_1}$$

$$u_2^2 = \frac{(p_2 - p_1)(\rho_2 - \rho_1)}{\rho_1 \rho_2}$$

Then, we wish to eliminate u_2 and S from the energy RH condition:

$$p_2 u_2 = \rho_1 \frac{\rho_2 u_2}{\rho_2 - \rho_1} \left(\frac{(p_2 - p_1)(\rho_2 - \rho_1)}{2\rho_1 \rho_2} + e_2 - e_1 \right)$$

$$p_2 = \frac{\rho_1 \rho_2}{\rho_2 - \rho_1} \left(\frac{(p_2 - p_1)(\rho_2 - \rho_1)}{2\rho_1 \rho_2} + e_2 - e_1 \right)$$

$$p_2 = \frac{1}{2}(p_2 - p_1) + \frac{\rho_1 \rho_2}{\rho_2 - \rho_1}(e_2 - e_1)$$

$$\frac{1}{2}(p_2 + p_1) = \frac{\rho_1 \rho_2}{\rho_2 - \rho_1}(e_2 - e_1)$$

$$e_2 - e_1 = \frac{1}{2}(p_2 + p_1) \left(\frac{1}{\rho_1} - \frac{1}{\rho_2} \right)$$

$$e_2 - e_1 = \frac{1}{2}(p_2 + p_1)(\nu_1 - \nu_2)$$

iv. The Hugoniot equation gives all possible thermodynamic states behind the shock wave/discontinuity which satisfy the RH conditions.

v. The heat of detonation Q is involved in the reactive system. Take $e_2 = \tilde{e}_2 - \lambda Q$. The Hugoniot equation becomes:

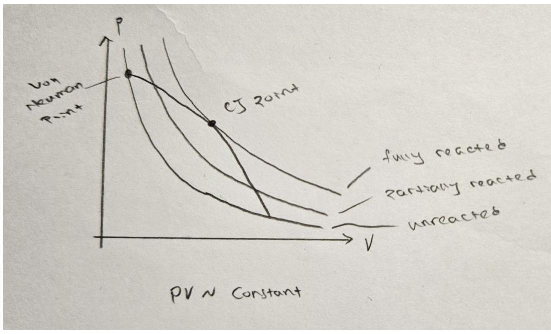
$$\tilde{e}_2 - e_1 = \frac{1}{2}(p_2 + p_1)(\nu_1 - \nu_2) + \lambda Q$$

ZND detonation model: a 1D model for the process of detonation of an explosive (proposed during WW1).

First, an infinitesimally thin shock wave compresses the explosive to a high pressure called the von Neumann spike, while remaining unreacted. It marks the onset of the zone of exothermic chemical reaction.

CJ point is a point at which the Rayleigh line is tangent to the Hugoniot curve.

vi.



vii. The CJ point is the end of the reaction zone (sonic locus, where $u = c$. The Von Neumann point is the highest attainable pressure and the beginning of the reaction zone in a ZND detonation.

1.3 Q3

3. (a) Take 1D flow to be along x-direction.

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

$$\frac{\partial \rho v_x}{\partial t} + \frac{\partial}{\partial x}\left(\rho v_x^2 + p + \frac{1}{2}(B_x^2 + B_y^2 + B_z^2) - B_x^2\right) = 0$$

$$\frac{\partial \rho v_y}{\partial t} + \frac{\partial}{\partial x}\left(\rho v_y v_x - B_y B_x\right) = 0$$

$$\frac{\partial \rho v_z}{\partial t} + \frac{\partial}{\partial x}\left(\rho v_z v_x - B_z B_x\right) = 0$$

$$\frac{\partial U}{\partial t} + \frac{\partial}{\partial x}\left((U + p + \frac{1}{2}(B_x^2 + B_y^2 + B_z^2))v_x - (v_x B_x + v_y B_y + v_z B_z)B_x\right) = 0$$

$$\frac{\partial B_x}{\partial t} = 0$$

$$\frac{\partial B_y}{\partial t} + \frac{\partial}{\partial x}(B_y v_x - v_y B_x)$$

$$\frac{\partial B_z}{\partial t} + \frac{\partial}{\partial x}(B_z v_x - v_z B_x)$$

(b) Doing it equation-by-equation:

- For ρ:

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

- For v_x:

$$\rho \frac{\partial v_x}{\partial t} + \underbrace{v_x \frac{\partial \rho}{\partial t} + 2\rho v_x \frac{\partial v_x}{\partial x} + v_x^2 \frac{\partial \rho}{\partial x}}_{\text{factor out } v_x} + \frac{\partial p}{\partial x} + \cancel{B_x \frac{\partial B_x}{\partial x}} + B_y \frac{\partial B_y}{\partial x} + B_z \frac{\partial B_z}{\partial x} - \cancel{2B_x \frac{\partial B_x}{\partial x}} = 0$$

since $\boldsymbol{\nabla} \cdot \boldsymbol{B} = \frac{\partial B}{\partial x} = 0$.

$$\frac{\partial v_x}{\partial t} + v_x \frac{\partial v_x}{\partial x} + \frac{1}{\rho} \frac{\partial p}{\partial x} + \frac{B_y}{\rho} \frac{\partial B_y}{\partial x} + \frac{B_z}{\rho} \frac{\partial B_z}{\partial x} = 0$$

- For v_y:

$$\rho \frac{\partial v_y}{\partial t} + \rho v_x \frac{\partial v_y}{\partial x} - \cancel{B_y \frac{\partial B_x}{\partial x}} - B_x \frac{\partial B_y}{\partial x} = 0$$

$$\frac{\partial v_y}{\partial t} + v_x \frac{\partial v_y}{\partial x} - \frac{B_x}{\rho} \frac{\partial B_y}{\partial x} = 0$$

- For v_z:

$$\frac{\partial v_z}{\partial t} + v_x \frac{\partial v_z}{\partial x} - \frac{B_x}{\rho} \frac{\partial B_z}{\partial x} = 0$$

- For p. Given:

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

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

$$\frac{1}{\gamma - 1} \frac{\partial p}{\partial t} + \frac{1}{\gamma - 1} \left(v_x \frac{\partial p}{\partial x} + p \frac{\partial v_x}{\partial x} \right) + p \frac{\partial v_x}{\partial x} = 0$$

$$\frac{\partial p}{\partial t} + v_x \frac{\partial p}{\partial x} + \cancel{p \frac{\partial v_x}{\partial x}} + \gamma p \frac{\partial v_x}{\partial x} - \cancel{p \frac{\partial v_x}{\partial x}} = 0$$

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

- For B_y:

$$\frac{\partial B_y}{\partial t} + B_y \frac{\partial v_x}{\partial x} + v_x \frac{\partial B_y}{\partial x} - \cancel{v_y \frac{\partial B_x}{\partial x}} - B_x \frac{\partial v_y}{\partial x} = 0$$

$$\frac{\partial B_y}{\partial t} + B_y \frac{\partial v_x}{\partial x} - B_x \frac{\partial v_y}{\partial x} + v_x \frac{\partial B_y}{\partial x} = 0$$

- For B_z:

$$\frac{\partial B_z}{\partial t} + B_z \frac{\partial v_x}{\partial x} - B_x \frac{\partial v_z}{\partial x} + v_x \frac{\partial B_z}{\partial x} = 0$$

Hence, in matrix form:

$$\frac{\partial}{\partial t}\begin{pmatrix}\rho\\ v_x\\ v_y\\ v_z\\ p\\ B_y\\ B_z\end{pmatrix}+\begin{pmatrix}v_x & \rho & 0 & 0 & 0 & 0 & 0\\ 0 & v_x & 0 & 0 & 1/\rho & B_y/\rho & B_z/\rho\\ 0 & 0 & v_x & 0 & 0 & -B_x/\rho & 0\\ 0 & 0 & 0 & v_x & 0 & 0 & -B_x/\rho\\ 0 & \rho c_s^2 & 0 & 0 & v_x & 0 & 0\\ 0 & B_y & -B_x & 0 & 0 & v_x & 0\\ 0 & B_z & 0 & -B_x & 0 & 0 & v_x\end{pmatrix}\frac{\partial}{\partial x}\begin{pmatrix}\rho\\ v_x\\ v_y\\ v_z\\ p\\ B_y\\ B_z\end{pmatrix}=0$$

(c) Ordered:

$$v_x - c_f \le v_x - c_a \le v_x - c_s \le v_x \le v_x + c_s \le v_x + c_a \le v_x + c_f$$

Need to prove $0 \le c_s \le c_a \le c_f$.

- For $0 \le c_s$. We observe that:

$$\sqrt{(a^2+c_a^2)^2 - 4\frac{a^2B_x^2}{\rho}} \le a^2 + c_a^2$$

  So, $0 \le c_s$.

- For $c_s \le c_a$. Consider:

$$a^2 + c_a^2 - \sqrt{(a^2+c_a^2)^2 - 4\frac{a^2B_x^2}{\rho}} \le 2c_a^2$$

$$a^2 - \sqrt{(a^2+c_a^2)^2 - 4\frac{a^2B_x^2}{\rho}} \le c_a^2$$

$$(a^2-c_a^2)^2 \le (a^2+c_a^2)^2 - 4\frac{a^2B_x^2}{\rho}$$

$$4\frac{a^2B_x^2}{\rho} \le 4a^2c_a^2$$

$$\frac{B_x^2}{\rho} \le c_a^2 = \frac{B_x^2+B_y^2+B_z^2}{\rho}$$

  The inequality holds.

- $c_a \le c_f$. Consider:

$$2c_a^2 \le a^2 + c_a^2 + \sqrt{(a^2+c_a^2)^2 - 4\frac{a^2B_x^2}{\rho}}$$

$$(c_a^2-a^2)^2 \le (a^2+c_a^2)^2 - 4\frac{a^2B_x^2}{\rho}$$

$$4\frac{a^2B_x^2}{\rho} \le 4a^2c_a^2$$

$$\frac{B_x^2}{\rho} \le c_a^2$$

  The inequality holds.

2 2019-20 (MOCK)

2.1 Q1

1. (Part I)

   (a)

$$\frac{\partial \rho}{\partial t} + \boldsymbol{\nabla}\cdot(\rho\boldsymbol{u}) = 0$$

$$\frac{\partial \rho\boldsymbol{u}}{\partial t} + \boldsymbol{\nabla}\cdot(\rho\boldsymbol{u}\otimes\boldsymbol{u} - \boldsymbol{\sigma}) = 0$$

$$\frac{\partial \rho(1/2u^2+e)}{\partial t} + \boldsymbol{\nabla}\cdot\left(\rho\left(\frac{1}{2}u^2+e\right)\boldsymbol{u} + p\boldsymbol{u}\right) = \boldsymbol{\nabla}\cdot(\boldsymbol{\sigma'}\cdot\boldsymbol{u} - \boldsymbol{q})$$

   (b) An incomplete EoS, $p = p(\rho, \varepsilon)$, provides closure between density, pressure and specific internal energy. However, heat flux is a function of temperature. An incomplete EoS cannot close the system, as T is not specified.

   (c) We recover the Euler equations, which is hyperbolic.

   (Part II)

   (a) $p_{\text{ref}}(\rho)$: reference pressure curve.
   $e_{\text{ref}}(\rho)$: reference energy curve.
   $\Gamma(\rho)$: Gruneisen coefficient/gamma.

   (b)
   - Isentrope, curve of constant entropy.
   - Hugoniot curve/shock locus, curve of thermodynamic states behind a shock wave which satisfy the Rankine-Hugoniot conditions.
   - No, it is missing a reference temperature, T_{ref}.

   (c) Stiffened gas:

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

   So, $\Gamma = \gamma - 1$, $p_{\text{ref}} = -\gamma p_\infty$ and $\varepsilon_{\text{ref}} = 0$.

   Ideal gas:

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

   So, $\Gamma = \gamma - 1$, $p_{\text{ref}} = 0$ and $\varepsilon_{\text{ref}} = 0$.

   (d) Isentrope: $ds = 0$. Ideal gas: $p = (\gamma-1)\rho\varepsilon$ and $pv = nRT$.

   i.

$$de = \cancel{Tds} - pdv = -pdv$$

$$de = -(\gamma-1)\rho e d\left(\frac{1}{\rho}\right)$$

$$\frac{1}{e}de = (\gamma-1)\frac{1}{\rho}d\rho$$

$$\ln\left(\frac{e}{e_0}\right) = (\gamma-1)\ln\left(\frac{\rho}{\rho_0}\right)$$

$$\Rightarrow e = e_0 \left(\frac{\rho}{\rho_0}\right)^{(\gamma-1)}$$

$$e = e_0 \left(\frac{\rho_0}{\rho}\right)^{-(\gamma-1)}$$

and, substituting $e = \frac{pv}{\gamma-1}$,

$$\frac{pv}{\gamma-1} = \frac{p_0 v_0}{\gamma-1}\left(\frac{\rho_0}{\rho}\right)^{-(\gamma-1)}$$

$$p = p_0 \frac{\rho}{\rho_0}\left(\frac{\rho}{\rho_0}\right)^{\gamma-1}$$

$$p = p_0 \left(\frac{\rho}{\rho_0}\right)^{\gamma}$$

ii.

$$c^2 = \frac{\partial p}{\partial \rho}\Big|_s$$

$$c^2 = \frac{\gamma p_0}{\rho_0}\left(\frac{\rho}{\rho_0}\right)^{(\gamma-1)} = \frac{\gamma p_0}{\rho}\left(\frac{\rho}{\rho_0}\right)^{\gamma} = \frac{\gamma p}{\rho}$$

$$\Rightarrow c^2 = c_0^2 \left(\frac{\rho}{\rho_0}\right)^{(\gamma-1)}$$

iii.

$$dp = c^2 d\rho$$

$$\begin{aligned}\int \frac{dp}{\rho c} &= \int \frac{c}{\rho} d\rho \\ &= \int c_0 \frac{\rho^{1/2(\gamma-3)}}{\rho_0^{1/2(\gamma-1)}} d\rho \\ &= \frac{c_0}{\rho_0^{1/2(\gamma-1)}} \frac{\rho^{1/2(\gamma-1)}}{1/2(\gamma-1)} \\ &= \frac{2c}{\gamma-1}\end{aligned}$$

2.2 Q2

2\. (a) CJ theory: consider detonation as a shock wave and assume chemical reaction to be completed instantaneously.

ZNH theory: considers the structure of the detonation wave and assume reaction is not instantaneous.

(b)

$$p_2u_2 = \rho_1 S\left(\frac{1}{2}u_2^2 + e_2 - \lambda Q - e_1\right)$$

(c)

$$\frac{p_2v_2}{\gamma-1} - \lambda Q - \frac{p_1v_1}{\gamma-1} = \frac{1}{2}(p_2+p_1)(v_1-v_2)$$

(d) For reactive, we have the augmented Euler equation.

$$\frac{\partial}{\partial t}\begin{pmatrix}\rho\\ \rho u\\ \rho\left(\frac{1}{2}u^2+e\right)\\ \rho\lambda\end{pmatrix} + \frac{\partial}{\partial x}\begin{pmatrix}\rho u\\ \rho u^2+p\\ \rho\left(\frac{1}{2}u^2+e\right)u+pu\\ \rho\lambda u\end{pmatrix} = \begin{pmatrix}0\\0\\0\\ \rho K\end{pmatrix} \quad \text{or} \quad \begin{pmatrix}0\\0\\ \rho KQ\\ \rho K\end{pmatrix}$$

with,

$$\rho e = \frac{p}{\gamma-1} - \rho\lambda Q \quad \text{or} \quad \rho e = \frac{p}{\gamma-1}$$

where K is the reactive rate law and Q is the heat of detonation. The chemical energy can either be incorporated into the total energy or appear as a source term.

(e) Add a fourth row.

$$\boldsymbol{U}_K^* = \rho_K\left(\frac{S_K-u_K}{S_K-S^*}\right)\begin{pmatrix}1\\ S^*\\ \frac{e_K}{\rho_K} + (S^*-u_K)\left[S^* + \frac{p_K}{\rho_K(S_K-u_K)}\right]\\ \frac{1}{\rho_K}\left(\frac{S_K-S^*}{S_K-u_K}\right)\lambda_K\end{pmatrix}$$

Proof: Jump conditions: $f^* - f_K = S(U^* - U_K)$.

$$\begin{gathered}\rho_L^*\lambda_L^*S^* - \rho_L\lambda_Lu_L = S_L(\rho_L^*\lambda_L^* - \rho_L\lambda_L)\\ \rho_L^*\lambda_L^*(S^*-S_L) = \rho_L\lambda_L(u_L-S_L)\\ \lambda_L^* = \frac{S_L-u_L}{S_L-S^*}\frac{\rho_L}{\rho_L^*}\lambda_L\\ \lambda_L^* = \lambda_L\end{gathered}$$

Physical reasoning: λ can only jump across contact discontinuity where the material change.

(f) 4 waves. Eigenvalues:

$$\lambda_{1,2} = u,\ \lambda_{3,4} = u \pm c_s$$

where c_s is the sound speed. u is a repeated eigenvalue.

(g) To solve hyperbolic PDE with source terms, we use **operator splitting**, where we separate the conservation law update and the source term update. Consider two operations to give a first-order update:

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

where Δt is the stable time step.

- $\mathcal{C}^{(\Delta t)}$: ignore the source term and solve the conservation law PDE over time Δt, to get an intermediate state $\bar{\boldsymbol{u}}^{n+1}$. We could use HLLC solver here.

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

- $\mathcal{S}^{(\Delta t)}$: ignore the divergence operator and solve the balance law ODE over Δt, to get final state $\boldsymbol{u}^{n+1}$. We could use RK4 or Heun method here.

$$\left.\begin{array}{ll}\text{ODE:} & \frac{\mathrm{d}\boldsymbol{u}}{\mathrm{d}t} = \boldsymbol{s}(\boldsymbol{u}) \\ \text{IC:} & \bar{\boldsymbol{u}}^{n+1}\end{array}\right\} = \boldsymbol{u}^{n+1}$$

Side note: for second order,

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

Source terms are modelling physical behaviour not included in the conservation law, so they will have their own timescale. E.g. diffusion timescale is $\Delta t_s = \frac{(\Delta x)^2}{2D}$. If the source term is stiff ($\Delta t_s < \Delta t_{CFL}$). E.g. chemical reactions. In general, the stable time step is $\Delta t = \min(\Delta t_{CFL}, \Delta t_s)$. We do not want to integrate both equations with the smaller source term time step, as it leads to greater computational cost and unnecessary accumulation or error. we could use:

- **Subcycling**: If source term involve solving a rapid physical process, ODE solver need to be operated at a smaller optimal time step (Δt_s) than the hyperbolic solver. Hence, we run the ODE solver several times for each single time step (Δt_{CFL}) in the hyperbolic solver.
- **Stable implicit scheme**: although implicit schemes are more computationally expensive than explicit schemes, if $\Delta t_s \ll \Delta t_{CFL}$, solving the source term implicitly and evolving the hyperbolic system with Δt_{CFL} may be more efficient. It is useful for parabolic source terms which have infinite propagation speed and lack of discontinuities.

See 2021-22 (Exam) Q2. Link

(h) We would use the same augmented euler equations as in (d) but now ρ would describe the density of the mixture. λ would be the mass fraction of the reactants and the mixture rules we would need are: $e = \lambda e_1 + (1-\lambda)e_2$ and $v = \lambda v_1 + (1-\lambda)v_2$. We need pressure and temperature equilibrium to close the system.

2.3 Q3

3. (a) We compute electric field using equation (5), then we can use equation (7) to compute the charge density directly.

   (b)

$$\frac{\partial}{\partial t} \sim \frac{v}{a}$$

   (c) From equation (4),

$$\frac{v|B|}{a} \sim -\frac{|E|}{a} \Rightarrow |E| \sim v|B|$$

   Consider equation (5), time derivative has dimensions:

$$\frac{1}{c^2}\frac{\partial E}{\partial t} \sim \frac{v^2|B|}{c^2 a} \ll 1$$

   We can neglect time derivative in equation (5) and it reduces to:

$$\boldsymbol{J} = \mu_0^{-1} \boldsymbol{\nabla} \times \boldsymbol{B}$$

   From equation (7), $\tau \sim \frac{\epsilon_0|E|}{a}$, Consider equation (2),

$$\tau E \sim \frac{\epsilon_0 v^2|B|^2}{a} = \frac{v^2|B|^2}{c^2\mu_0} \ll 1$$

   We can neglect the $\tau\boldsymbol{E}$ component in equation (2).

   Since charge density no longer appears in any of the evolution equation, we no longer need equation (7). OR We can use $\eta\boldsymbol{J} = \boldsymbol{E} + \boldsymbol{v} \times \boldsymbol{B}$ to remove $\boldsymbol{E}$ from all evolution equations, and we do not need any τ in any equation. So, we no longer need equation (7).

   (d) Zero resistivity / perfect conductivity ($\eta = 0$).

(e) **Astrophysical plasma v.s. lightning**

System of Equations

- Astrophysical application uses the non-relativistic ideal MHD. The ideal approximation is valid as the length scales are large, and the material is fully ionised. We have 4 evolution equation for density, momentum, energy and magnetic field.
- Lightning produces current-induced plasma, which act on timescales comparable to the speed of light ($\sim 0.3c$). This means the magnetic field is evolving much faster than the hydrodynamics of the system. From the fluid variable perspective, as they evolve, it appears the magnetic field nearly instantaneously "relax" to match their evolution. We adopt an electrostatic approach and ignore the magnetic field evolution equation. We have 3 evolution equation, and additional equations to compute magnetic field from current distribution. ($\boldsymbol{\nabla} \cdot \boldsymbol{J} = 0$ and $\mu_0 \boldsymbol{J} = -\nabla^2 \boldsymbol{A}$)

What can be considered negligible or non-negligible

- For astrophysical, ideal MHD
- For lightning, resistivity is non-negligible. Air might be partially-ionised.

Equation of State

- Astrophysical plasma is fully ionised, can consider ideal gas EoS $p = (\gamma - 1)\rho\varepsilon$ with $\gamma = 5/3$.
- Lightning is partially ionised, and the level of ionisation substantially changes the physical properties of the plasma. Air contains different components which needs to be captured by the EoS, or we could use a tabulated EoS.

Additional Source Terms

- Astrophysical plasma may require gravitational terms.
- Lightning reaches high enough temperatures that energy loss due to radiative emission cannot be neglected.

3 2019-20 (EXAM)

3.1 Q1

1. (Part I)

(a)

$$\text{Aim: } ds = C_v d\ln(pv^\gamma)$$

$$\text{Ideal gas: } de = Tds - pdv \quad , \quad e = C_vT = \frac{pv}{\gamma-1} \quad , \quad pv = RT$$

I want to get rid of de.

$$de = \frac{pdv}{\gamma-1} + \frac{vdp}{\gamma-1}$$

So,

$$\begin{aligned} ds &= \frac{1}{T}de + \frac{p}{T}dv \\ &= \frac{1}{T(\gamma-1)}(pdv + vdp) + \frac{p}{T}dv \\ &= \left(\frac{p}{T(\gamma-1)} + \frac{p}{T}\right)dv + \frac{v}{T(\gamma-1)}dp \\ &= \frac{\gamma p}{T(\gamma-1)}dv + \frac{v}{T(\gamma-1)}dp \end{aligned}$$

With,

$$T(\gamma-1) = \frac{pv}{C_v}$$

$$\begin{aligned} ds &= \frac{C_v\gamma p}{pv}dv + \frac{C_v v}{pv}dp \\ &= \frac{C_v\gamma}{v}dv + \frac{C_v}{p}dp \\ &= C_v\left(\gamma\frac{dv}{v} + \frac{dp}{p}\right) \\ &= C_v\left(\gamma d(\ln v) + d\ln(p)\right) \\ &= C_v d\ln(pv^\gamma) \end{aligned}$$

Integrating to get expression for s,

$$\int ds = \int C_v d\ln(pv^\gamma)$$

$$s = s_0 + C_v\frac{pv^\gamma}{p_0v_0^\gamma}$$

(b)

$$\text{Sound speed: } c^2 = \frac{\partial p}{\partial \rho}\bigg|_s$$

$$0 = \frac{\gamma dv}{v} + \frac{dp}{p}$$

$$\frac{dp}{p} = -\gamma\frac{dv}{v} = -\gamma\frac{d(1/\rho)}{v} = \frac{\gamma\rho d\rho}{\rho^2}$$

$$c^2 = \frac{\partial p}{\partial \rho}\bigg|_s = \frac{\gamma p}{\rho} \quad \Rightarrow \quad \frac{p}{\rho} = \frac{c^2}{\gamma}$$

$$\begin{aligned} h &= \frac{c^2}{\gamma} + e \\ &= \frac{c^2}{\gamma} + \frac{p}{\rho(\gamma-1)} \\ &= c^2\left(\frac{1}{\gamma} + \frac{1}{\gamma(\gamma-1)}\right) \\ &= \frac{c^2}{\gamma-1} \end{aligned}$$

(c) A reference temperature curve, T_{ref} have to be provided. For example,

$$T = \frac{e}{C_v} \quad \rightarrow \quad T = \frac{e}{C_v} + T_{\text{ref}}$$

(d) At low temperatures, intermolecular forces becomes significant and kinetic energy of the particles decreases. As a result, potential energy is not much lower than kinetic energy and the ideal gas approximation no longer holds.

Assumptions of ideal gas EoS:

i. Gas is made up of non-interacting point particles.
ii. Intermolecular forces result in a potential energy that is much lower than the kinetic energy of the particles.
iii. Constant specific heats.

Advantages:

- Derived from laws of thermodynamics.
- Applies to a wide range of gases and plasmas, over a wide range of conditions. E.g. air and noble gases at atm, plasma for astrophysical or fusion models and interior of neutron stars.

(e) For steady flows, time derivative vanishes,

$$\begin{pmatrix} \rho u \\ \rho u^2 + p \\ (\rho E + p)u \end{pmatrix}_x = \mathbf{0}$$

(f)

$$\text{Note: } E = e + \frac{1}{2}u^2$$

$$\frac{\partial}{\partial x}(\rho u) = 0 \quad , \quad \frac{\partial}{\partial x}(\rho u^2 + p) = 0 \quad , \quad \frac{\partial}{\partial x}\left(\left(\rho e + \frac{1}{2}\rho u^2 + p\right)u\right) = 0$$

From equation (3),

$$\rho u \frac{\partial}{\partial x}\left(e + \frac{1}{2}u^2 + p\nu\right) + \cancel{\left(e + \frac{1}{2}u^2 + p\nu\right)\frac{\partial}{\partial x}(\rho u)} = 0$$

$$\frac{\partial}{\partial x}\left(e + \frac{1}{2}u^2 + p\nu\right) = 0$$

So,

$$e + \frac{1}{2}u^2 + p\nu = \text{constant}$$

(g) For isentropic flow, $ds = 0$,

$$de = -pd\nu$$

$$\begin{aligned} d(e + p\nu) &= de + pd\nu + \nu dp \\ &= \nu dp \\ &= \frac{dp}{\rho} \end{aligned}$$

So,

$$e + p\nu = \int \frac{dp}{\rho}$$

$$e + p\nu + \frac{1}{2}u^2 = \frac{1}{2}u^2 + \int \frac{dp}{\rho}$$

(Part II)

(a) A material undergoes deformation when subjected to stress. Strain provides a measure of the deformation. Deformation is the transformation of a body from a reference configuration to the current configuration. This transformation can be described using the deformation gradient:

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

where F_{ij} transforms an infinitesimal particle from its reference configuration $d\boldsymbol{X}$ to its current Eulerian position $d\boldsymbol{x}$.

Why deformation gradient?

- Not affected by translation or rotation.
- Length scales are accounted for.

Closure

- Stress is related to strain, strain to deformation gradient, deformation gradient to density. A relationship between strain and conserved variables is essential for closing the solid system of equations.

(b) Longitudinal deformation of a rod is:

$$e = \frac{\delta l}{l_0}$$

where e is the strain and δl is the absolute elongation, $\delta l = l - l_0$. The absolute elongation cannot be used by itself, as length scales need to be accounted for. For example, for the same absolute elongation of 1cm, rods of length 10cm and 5cm should be in different states.

(c)

$$F_{ij} = \frac{\partial x_i}{\partial \xi_j} \quad , \quad u_i = \frac{\mathrm{d}x_i}{\mathrm{d}t}$$

$$\begin{aligned}
\frac{\mathrm{d}F_{ij}}{\mathrm{d}t} = \frac{\mathrm{d}}{\mathrm{d}t}\left(\frac{\partial x_i}{\partial \xi_j}\right) &= \frac{\partial u_i}{\partial \xi_j} \\
&= \frac{\partial u_i}{\partial x_k}\frac{\partial x_k}{\partial \xi_j} \\
&= \frac{\partial u_i}{\partial x_k} F_{kj} \\
&= (\nabla_k u_i) F_{kj}
\end{aligned}$$

where,

$$L_{ik} = \nabla_k u_i$$

(d) In addition:

$$\frac{\partial \rho}{\partial t} + \nabla_k(\rho u_k) = 0 \quad , \quad \frac{\mathrm{d}}{\mathrm{d}t} = \frac{\partial}{\partial t} + u_k \nabla_k$$

We also have,

$$\begin{aligned}
\frac{\mathrm{d}F_{ij}}{\mathrm{d}t} - \nabla_k u_i F_{kj} &= 0 \\
\frac{\partial F_{ij}}{\partial t} + u_k \nabla_k F_{ij} - \nabla_k u_i F_{kj} &= 0
\end{aligned}$$

Consider,

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

$$\frac{\partial \rho F_{ij}}{\partial t} + \nabla_k(\rho u_k F_{ij}) - \cancel{F_{ij}\nabla_k(\rho u_k)} - \nabla_k(u_i \rho F_{kj}) + u_i \nabla_k(\rho F_{kj}) + \cancel{F_{ij}\nabla_k(\rho u_k)} = 0$$

$$\frac{\partial \rho F_{ij}}{\partial t} + \nabla_k(\rho u_k F_{ij}) - \nabla_k(u_i \rho F_{kj}) = -u_i \nabla_k(\rho F_{kj})$$

$$\frac{\partial \rho F_{ij}}{\partial t} + \nabla_k(u_k \rho F_{ij} - u_i \rho F_{kj}) = -u_i \nabla_k(\rho F_{kj})$$

We can impose an additional constraint, if

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

for the initial data, then this relationship holds true all the time. This means that for appropriately chosen initial data, we have a conservation law for $\boldsymbol{F}$.

3.2 Q2

2. (a)

$$\boldsymbol{B} \to \frac{\boldsymbol{B}}{\sqrt{\mu_0}} \quad , \quad \boldsymbol{E} \to \frac{\boldsymbol{E}}{\sqrt{\mu_0}} \quad , \quad \boldsymbol{J} \to \sqrt{\mu_0}\boldsymbol{J}$$

(b) For non-relativistic, $v \ll c$. Assume non-negligible B and v.

Equation (7) gives $|E| \sim v|B|$. We also have, $\nabla \sim \frac{1}{a}$ and $\frac{\partial}{\partial t} \sim \frac{v}{a}$ where a and t are the characteristic length and timescale.

The Poisson's equation for $\boldsymbol{E}$ is $\boldsymbol{\nabla} \cdot \boldsymbol{E} = \frac{\tau}{\epsilon_0}$. We have $\frac{|E|}{a} = \tau \mu_0 c^2$, $\tau = \frac{v|B|}{a\mu_0 c^2}$. Then, the term $\tau \boldsymbol{E} \sim \frac{v^2|B|^2}{c^2 a \mu_0} \ll 1$. We can discard the $\tau \boldsymbol{E}$ term in the momentum equation under non-relativistic assumption.

After scaling:

$$\boldsymbol{J} \times \boldsymbol{B} \to \sqrt{\mu_0}\boldsymbol{J} \times \boldsymbol{B}/\sqrt{\mu_0} \to \boldsymbol{J} \times \boldsymbol{B}$$

$$\frac{\partial \boldsymbol{B}}{\partial t} + \boldsymbol{\nabla} \times \boldsymbol{E} = 0 \to \frac{1}{\sqrt{\mu_0}} \frac{\partial \boldsymbol{B}}{\partial t} + \frac{1}{\mu_0} \boldsymbol{\nabla} \times \boldsymbol{E} = 0 \to \frac{\partial \boldsymbol{B}}{\partial t} + \boldsymbol{\nabla} \times \boldsymbol{E} = 0$$

$$\boldsymbol{J} = \mu_0^{-1} \boldsymbol{\nabla} \times \boldsymbol{B} \to \sqrt{\mu_0}\boldsymbol{J} = \frac{1}{\sqrt{\mu_0}} \boldsymbol{\nabla} \times \boldsymbol{B} \to \boldsymbol{J} = \boldsymbol{\nabla} \times \boldsymbol{B}$$

(c)

$$U = \rho e + \frac{1}{2}\rho u^2 + \frac{1}{2}B^2$$

$$\begin{aligned}
\frac{\partial U}{\partial t} &= \frac{\partial (\rho e)}{\partial t} + \frac{\partial}{\partial t}\left(\frac{1}{2}\rho u_i u_i\right) + \frac{\partial}{\partial t}\left(\frac{1}{2}B_i B_i\right) \\
&= \frac{\partial (\rho e)}{\partial t} + \frac{1}{2}u_i u_i \frac{\partial \rho}{\partial t} + \frac{1}{2}\rho u_i \frac{\partial u_i}{\partial t} + \frac{1}{2}\rho u_i \frac{\partial u_i}{\partial t} + \frac{1}{2}B_i \frac{\partial B_i}{\partial t} + \frac{1}{2}B_i \frac{\partial B_i}{\partial t} \\
&= \frac{\partial (\rho e)}{\partial t} + \frac{1}{2}u_i u_i \frac{\partial \rho}{\partial t} + \rho u_i \frac{\partial u_i}{\partial t} + B_i \frac{\partial B_i}{\partial t} \\
&= \frac{\partial (\rho e)}{\partial t} + \frac{1}{2}u_i u_i \frac{\partial \rho}{\partial t} + u_i \frac{\partial \rho u_i}{\partial t} - u_i u_i \frac{\partial \rho}{\partial t} + B_i \frac{\partial B_i}{\partial t} \\
&= \frac{\partial (\rho e)}{\partial t} - \frac{1}{2}u_i u_i \frac{\partial \rho}{\partial t} + u_i \frac{\partial \rho u_i}{\partial t} + B_i \frac{\partial B_i}{\partial t} \\
&= \frac{\partial (\rho e)}{\partial t} - \frac{1}{2}u^2 \frac{\partial \rho}{\partial t} + \boldsymbol{u} \cdot \frac{\partial \rho \boldsymbol{u}}{\partial t} + \boldsymbol{B} \cdot \frac{\partial \boldsymbol{B}}{\partial t}
\end{aligned}$$

We have the evolution equation for momentum and magnetic field. This allows us to obtain the evolution equation for energy by performing the dot product of velocity with the momentum evolution equation and dot product of magnetic field with the magnetic field evolution equation.

It identifies how to bring the non-conservative equations into conservative form for the energy equation.

(d) Consider,

$$\begin{aligned}\boldsymbol{\nabla}\times\boldsymbol{E} &= -\boldsymbol{\nabla}\times(\boldsymbol{v}\times\boldsymbol{B})\\ &= -\epsilon_{ijk}\nabla_j\epsilon_{klm}v_lB_m\\ &= -\epsilon_{kij}\epsilon_{klm}\nabla_j(v_lB_m)\\ &= -(\delta_{il}\delta_{jm}-\delta_{im}\delta_{jl})\nabla_j(v_lB_m)\\ &= -\nabla_j(v_iB_j)+\nabla_j(v_jB_i)\\ &= \nabla_j(B_iv_j-v_iB_j)\\ &= \boldsymbol{\nabla}\cdot(\boldsymbol{B}\otimes\boldsymbol{v}-\boldsymbol{v}\otimes\boldsymbol{B})\end{aligned}$$

So,

$$\frac{\partial\boldsymbol{B}}{\partial t}+\boldsymbol{\nabla}\cdot(\boldsymbol{B}\otimes\boldsymbol{v}-\boldsymbol{v}\otimes\boldsymbol{B})=0$$

(e) HLL approximate Riemann solver - ideal MHD v.s. compressible Euler,

Similarities:

- We assume the Rankine-Hugoniot conditions govern the intermediate state for both MHD and Euler.
$$\boldsymbol{f}^{HLL}-\boldsymbol{f}_{L/R}=S_{S/L}(\boldsymbol{u}^{HLL}-\boldsymbol{u}_{L/R})$$
- Intermediate flux still is:
$$\boldsymbol{f}^{HLL}=\frac{S_R\boldsymbol{f}_L-S_L\boldsymbol{f}_R+S_LS_R(\boldsymbol{u}_R-\boldsymbol{u}_L)}{S_R-S_L}$$

Differences:

- Wave speed estimate for S_L and S_R, instead of sound speed, we use the fast wave speed:
$$S_L=\min(v_L,v_R)-\max(c_{f,L},c_{f,R})\quad,\quad S_R=\min(v_L,v_R)+\max(c_{f,L},c_{f,R})$$

(f) HLLC v.s. HLL approximate Riemann solver,

If the normal component of the magnetic field is non-zero, a contact discontinuity in MHD has only a density discontinuity, thereby requiring continuous tangential fluid velocities and magnetic field components.

No change:

- Wave speed estimates do not change, nor do the estimates for the intermediate states of the fluid variables (ρ, v, U, p).

Changes:

- The standard HLLC states cannot be used for the magnetic field variables [$B_{y,z}$ and $B_xB_{y,z}$ and $\boldsymbol{B}\cdot\boldsymbol{v}$], because the resultant scheme is not consistent with integral form of the conservation law.
- For these variables, the HLL value is used. $B^*_{y,z}=B^{HLL}_{y,z}$ and $(\boldsymbol{B}\cdot\boldsymbol{u})^*=\boldsymbol{B}^{HLL}\cdot\boldsymbol{u}^{HLL}$.

Extra note:

- $$S^* = \frac{\rho_R v_{x,R}(S_R - v_{x,R}) - \rho_L v_{x,L}(S_L - v_{x,L}) + (p_L - B_{x,L}^2) - (p_R - B_{x,R}^2)}{\rho_R(S_R - v_{x,R}) - \rho_L(S_L - v_{x,L})}$$

  also,

  $$p^* = \rho(S_K - v_{x,K})(S^* - v_{x,K}) + p - B_{x,K}^2 + (B_{x,K}^{HLLC})^2$$

  To satisfy the assumption $p_L^* = p_R^*$ with the definition of S^*, we need $B_{x,L}^* = B_{x,R}^*$.
- In order to satisfy the consistency condition as follows:

  $$\frac{S^* - S_L}{S_R - S_L}\boldsymbol{u}_L^{HLLC} + \frac{S_R - S^*}{S_R - S_L}\boldsymbol{u}_R^{HLLC} = \frac{S_R\boldsymbol{u}_R - S_L\boldsymbol{u}_L - (\boldsymbol{f}_R - \boldsymbol{f}_L)}{S_R - S_L} = \boldsymbol{u}^{HLL}$$

  We need $B_{x,L}^* B_{y,L}^* = B_{x,R}^* B_{y,R}^*$ and $B_{x,L}^* B_{z,L}^* = B_{x,R}^* B_{z,R}^*$.

  Hence, $B_{y,L}^* = B_{y,R}^*$ and $B_{z,L}^* = B_{z,R}^*$.

- Finally, we just assign HLL states to them: $B_x^* = B_x^{HLL}$, $B_y^* = B_y^{HLL}$ and $B_z^* = B_z^{HLL}$.
- Consider the consistency condition for energy equation, we get: $(\boldsymbol{B}\cdot\boldsymbol{v})_L^* = (\boldsymbol{B}\cdot\boldsymbol{v})_R^*$. Assigning HLL values to them, $(\boldsymbol{B}\cdot\boldsymbol{v})^* = \boldsymbol{B}^{HLL}\cdot\boldsymbol{v}^{HLL}$.

  $\therefore$ Magnetic field components and $\boldsymbol{B}\cdot\boldsymbol{v}$ is continuous across the contact discontinuity.

(g) Mathematically, provided the initial data obeys the divergence constraint $\boldsymbol{\nabla}\cdot\boldsymbol{B} = 0$, then all the solutions will continue to obey the constraint.

(h) Numerically, numerical errors can cause violation of $\boldsymbol{\nabla}\cdot\boldsymbol{B} = 0$ (the divergence does not completely vanish), and these errors grow. Lead to instability and conservation errors.

(i) **Divergence cleaning**: the idea is to evolve away any errors that appear in the divergence constraint. We do this by introducing a new variable ψ in the evolution equation of $\boldsymbol{B}$, and also it evolved itself:

$$\begin{cases} \frac{\partial\boldsymbol{B}}{\partial t} + \boldsymbol{\nabla}\cdot(\boldsymbol{B}\otimes\boldsymbol{v} - \boldsymbol{v}\otimes\boldsymbol{B}) + \boldsymbol{\nabla}\psi = 0 \\ \mathcal{D}(\psi) + \boldsymbol{\nabla}\cdot\boldsymbol{B} = 0 \end{cases}$$

where $\mathcal{D}$ is chosen such that the divergence errors are transported to the domain boundaries with the maximal admissible speed (advection term) and are damped (diffusion term) at the same time.

$$\Rightarrow \quad \mathcal{D}(\psi) = \frac{1}{c_h^2}\frac{\partial\psi}{\partial t} + \frac{1}{c_p^2}\psi$$

where c_h is the hyperbolic wave speed and is the speed of propagation of the divergence errors. We choose c_h to be the maximum possible wave speed:

$$c_h = \max(|v_x| + c_{f,x}, |v_y| + c_{f,y}, |v_z| + c_{f,z})$$

c_p is the parabolic damping term for ψ. They have the relationship:

$$c_p^2 = 0.18 \times c_h$$

3.3 Q3

3. (a)

$$\alpha = \frac{x_B - x_{i-1/2}}{\Delta x}$$

(b)

$$\Delta t = C\frac{\alpha x}{a_{\max}}$$

(c) The stabilised flux is defined such that the timestep of the overall simulation is not reduced by a factor of $\frac{1}{\alpha}$. It tackles the small cell problem, where existence of small cells constrain the explicit stable Δt.

(d) We extend the influence of the cut cell to the regular cell size Δx, we have a stable but not conservative update formula:

$$\bar{u}_i^{n+1} = u_i^n + \frac{\Delta t}{\Delta x}(f_{i-1/2}^n - f_B^n)$$

The conservative update accounts for the size of cut cell, but we now have an unknown flux:

$$\hat{u}_i^{n+1} = u_i^n + \frac{\Delta t}{\alpha\Delta x}(f_{i-1/2}^{*,n} - f_B^n)$$

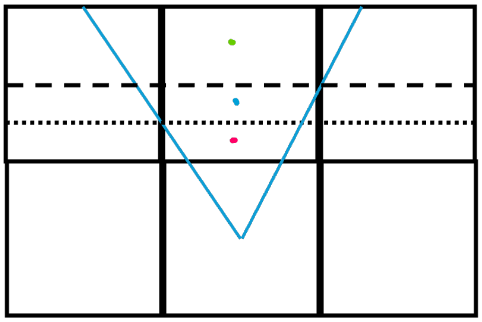
We solve for the unknown stabilised flux,

$$f_{i-1/2}^n - f_B^n = \frac{1}{\alpha}(f_{i-1/2}^{*,n} - f_B^n)$$

$$f_{i-1/2}^{*,n} = f_B^n + \alpha(f_{i-1/2}^n - f_B^n)$$

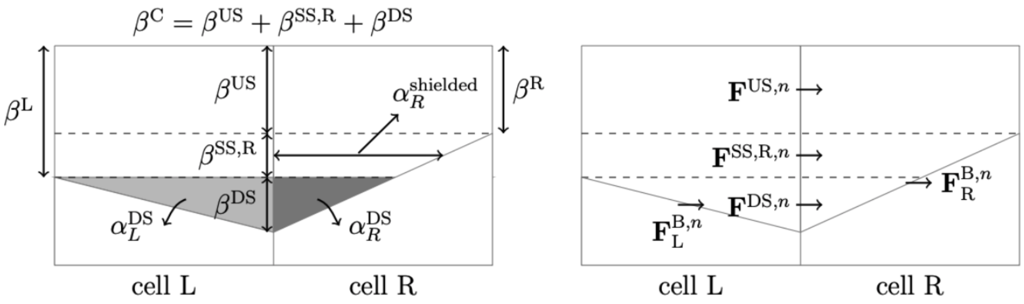
As $\alpha \to 1$, $f_{i-1/2}^{*,n} \to f_{i-1/2}^n$.
As $\alpha \to 0$, $f_{i-1/2}^{*,n} \to f_B^n$.

(e)



- Shielded flux: red and blue dot.
- Unshielded flux: green dot.

(f)



[1]

- 4 possible values for α: two for a cell cut along at least one x-edge, two for a cell cut along at least one y-edge. In each case, there is a volume fraction corresponding to the region between the shielded flux (singly or doubly) and the cut, and between two unshielded edges.
- 4 possible values of β: two for the regions along the x-axis not occupied by the rigid object, and two along the y-axis. Unshielded and shielded.
- 2 possible values for the average distance to the interface:

Total flux is the area weighted average:

$$F_C = \frac{1}{\beta_C}\left(\beta_{US}F^{US,n} + \beta_{SS,L}F^{SS,L,n} + \beta_{SS,R}F^{SS,R,n} + \beta_{DD}F^{DS,n}\right)$$

where $\beta_C = \beta_{US} + \beta_{SS} + \beta_{DS}$.

(g)

$$f_{i-1/2,j} = \beta_{i+1/2,j} f^{US}_{i-1/2,j} + (\beta_{i-1/2,j} - \beta_{i+1/2,j}) f^{SS}_{i-1/2,j}$$

(h) A doubly shielded cell is where a concave feature exists in the cut cell geometry. It is a region that face the boundary from the left and right sides.

4 2020-21 (EXAM)

4.1 Q1

1. (a) Hyperbolic conservation laws are solved using explicit update and hence will be limited by the CFL condition. This means the maximum stable time step is proportional to the size of the smallest cell. The "small cell problem" happens when the existence of a small cell cause the maximum stable time step to become too small. As a result, the numerical solution becomes too computationally expensive and inefficient.

   (b) **Cell merging**: combining cut cells with their neighbours to produce a larger cell with α at least 0.5, to bypass the CFL stability restriction.

   Advantage: Conceptually simple solution.
   Disadvantage: Difficult to program, as cell merging modifies the Cartesian state and flux data structure, and we have to keep track of merged cells. Reduces the accuracy of the solution at the boundary.

   Alternatives to avoid the problem of tracking merged cells:

   Cell merging variants

   - **Cell linking**: keep cut cells distinct in the data structure, but algorithmically treat them as merged during time integration.
   - **State mixing**: keep cut cells distinct in the data structures, and cell merged states are attained using mixing terms.
   - **State redistribution**: similar to state mixing but allow overlapping merging neighbourhoods.

   Others

   - **Flux redistribution**: apply only α times the explicit flux update to the cut cell, while redistributing the remaining flux to the neighbours. (first order at boundary)
   - **Flux stabilisation**: modifies the flux at the cut cell to produce a stable update for the cut cell using KBN or LPFS procedure. Dimensionally split, simple to implement and can be extended to 3D problems. (first order at boundary)

   (c) Conservative update (may not be stable):

$$U_{-1}^{n+1} = U_{-1}^{n} + \frac{a\Delta t}{\alpha\Delta x}(U_{-2}^{n} - U_{-1}^{n})$$

$$U_{0}^{n+1} = U_{0}^{n} + \frac{a\Delta t}{\Delta x}(U_{-1}^{n} - U_{0}^{n})$$

$$U_{1}^{n+1} = U_{1}^{n} + \frac{a\Delta t}{\alpha\Delta x}(U_{0}^{n} - U_{1}^{n})$$

$$U_{2}^{n+1} = U_{2}^{n} + \frac{a\Delta t}{\Delta x}(U_{1}^{n} - U_{2}^{n})$$

(d) After merging procedure:

$$
\begin{aligned}
&\Delta x \left(M_{-1} + \alpha M_{-1} + \frac{1}{2}(M_{-1} + M_1) + \alpha M_1 + M_1 \right) \\
&= \Delta x \left(\frac{3}{2} + \alpha \right) (M_{-1} + M_1) \\
&= \Delta x \left(\frac{3/2 + \alpha}{2 + \alpha} \right) (U_{-2}^{n+1} + \alpha U_{-1}^{n+1} + 2U_0^{n+1} + \alpha U_1^{n+1} + U_2^{n+1}) \\
&= \Delta x \left(\frac{3 + 2\alpha}{2(2 + \alpha)} \right) (U_{-2}^{n+1} + \alpha U_{-1}^{n+1} + 2U_0^{n+1} + \alpha U_1^{n+1} + U_2^{n+1}) \\
&\neq \text{pre-merged mass}
\end{aligned}
$$

The naive cell merging procedure is not conservative.

(e)

$$
\begin{aligned}
&\hat{U}_1^{n+1} = M_1^* \\
&= \frac{1}{\Delta x/2 + \alpha \Delta x + \Delta x/3} \left(\frac{\Delta x}{2}(U_2^n + c(U_1^n - U_2^n)) + \alpha \Delta x \left(U_1^n + \frac{c}{\alpha}(U_0^n - U_1^n) \right) + \frac{\Delta x}{3} U_0^{n+1} \right) \\
&= \frac{1}{5/6 + \alpha} \left(\frac{1}{2}(1 - c)U_2^n + \left(\frac{1}{2}c + \alpha - c \right) U_1^n + cU_0^n + \frac{1}{3}(U_0^n + c(U_{-1}^n) - U_0^n) \right) \\
&= \frac{6}{5 + 6\alpha} \left(\frac{1}{2}(1 - c)U_2^n + \left(\alpha - \frac{1}{2}c \right) U_1^n + \left(\frac{1}{3} + \frac{2}{3}c \right) U_0^n + \frac{1}{3}cU_{-1}^n \right) \\
&= \frac{6}{5 + 6\alpha} \left(\frac{2 + 4c}{6} U_0^n + \frac{6\alpha - 3c}{6} U_1^n + \frac{3 - 3c}{6} U_2^n + \frac{2c}{6} U_{-1}^n \right) \\
&= \frac{2 + 4c}{5 + 6\alpha} U_0^n + \frac{6\alpha - 3c}{5 + 6\alpha} U_1^n + \frac{3 - 3c}{5 + 6\alpha} U_2^n + \frac{2c}{5 + 6\alpha} U_{-1}^n
\end{aligned}
$$

where $c = \frac{a\Delta t}{\Delta x}$ is the Courant number.

4.2 Q2

2. ADER Procedure:

   (a) First-order reconstruction polynomial:

   $$p_i(x) = u_i^n + (x - x_i)\Delta_i \quad \text{and} \quad p_{i+1}(x) = u_{i+1}^n + (x - x_{i+1})\Delta_{i+1}$$

   where $\Delta_i =$

   (b) GRP: PDE + IV

   $$\text{PDE: } \partial_t u + \lambda \partial_x u = \beta u$$

   $$IV : u(x,0) = \begin{cases} p_i(x) & \text{if} \quad x < 0 \\ p_{i+1}(x) & \text{if} \quad x > 0 \end{cases}$$

   (c) Approximate solution at the cell interface to find Godunov state, using Taylor expansion in time:

   $$u_{i+1/2}(\tau) = \underbrace{u(0,0_+)}_{\substack{\text{leading-order} \\ \text{term}}} + \underbrace{\sum_{k=1}^{m} \left[\partial_t^{(k)} u(0,0_+) \frac{\tau^k}{k!} \right]}_{\text{higher-order term}}$$

   where

   $$u(0,0_+) = \lim_{t \to 0_+} u(0,t)$$

   The location of the interface is at $x = 0$. 0_+ is the time slightly above $t = 0$.

   Keeping only terms to first-order derivative in t:

   $$u_{i+1/2}(\tau) = u(0,0_+) + \tau \frac{\partial u(0,0_+)}{\partial t}$$

   (d) For the leading-order term, we get it by solving the classical piece-wise constant RP:

   $$\text{PDE: } \partial_t u + \lambda \partial_x u = 0$$

   $$\text{IC: } u(x,0) = \begin{cases} p_i(0) = u_i^n + \frac{1}{2}\Delta_i \Delta x & \text{if} \quad x < 0 \\ p_{i+1}(0) = u_{i+1/2}^n - \frac{1}{2}\Delta_{i+1}\Delta x & \text{if} \quad x > 0 \end{cases}$$

   One-wave solution for linear-advection equation (eigenvalue = λ):

   $$d_{i+1/2}(x/t) = \begin{cases} u_i^n + \frac{1}{2}\Delta_i \Delta x & \text{if} \quad x/t < \lambda \\ u_{i+1/2}^n - \frac{1}{2}\Delta_{i+1}\Delta x & \text{if} \quad x/t > \lambda \end{cases}$$

   Hence, along the interface where $x/t = 0$:

   $$u(0,0_+) = \begin{cases} u_i^n + \frac{1}{2}\Delta_i \Delta x & \text{if} \quad \lambda > 0 \\ u_{i+1}^n - \frac{1}{2}\Delta_{i+1}\Delta x & \text{if} \quad \lambda < 0 \end{cases}$$

   Since $\lambda > 0$, $u(0,0_+) = u_i^n + \frac{1}{2}\Delta_i \Delta x$

(e) For the higher-order terms, we first use the Cauchy-Kovalevskaya procedure to relate temporal to spatial derivative:

$$\partial_t u = -\lambda \partial_x u$$

So,

$$u_{i+1/2}(\tau) = u(0,0_+) + \tau(-\lambda\partial_x u)$$

$$\frac{u_{i+1/2}(\tau) - u(0,0_+)}{\tau} + \lambda\partial_x u = 0$$

$$\partial_t u + \lambda\partial_x u = 0$$

$$\partial_t(\partial_x u) + \lambda\partial_x(\partial_x u) = 0$$

We then need to solve the classical RP for spatial derivatives:

$$\text{PDE: } \partial_t(\partial_x u) + \lambda\partial_x(\partial_x u) = 0$$

$$\text{IC: } \partial_x u = \begin{cases} \Delta_i & \text{if} \quad x < 0 \\ \Delta_{i+1} & \text{if} \quad x > 0 \end{cases}$$

(f) Solution to the classical RP for spatial derivative:

$$\partial_x d_{i+1/2}(x/t) = \begin{cases} \Delta_i & \text{if} \quad x/t < \lambda \\ \Delta_{i+1} & \text{if} \quad x/t > \lambda \end{cases}$$

Hence, the Godunov state at the interface is:

$$\partial_x u(0,0_+) = \begin{cases} \Delta_i & \text{if} \quad \lambda > 0 \\ \Delta_{i+1} & \text{if} \quad \lambda < 0 \end{cases}$$

Since $\lambda > 0$, $\partial_x u(0,0_+) = \Delta_i$.

$$u_{i+1/2}(\tau) = u_i^n + \frac{1}{2}\Delta_i\Delta x + \tau\left(-\lambda\Delta_i + \beta\left(u_i^n + \frac{1}{2}\Delta_i\Delta x\right)\right)$$

So, with $\tau = \frac{1}{2}\Delta t$

$$f_{i+1/2} = \lambda\left(u_i^n + \frac{1}{2}\Delta_i\Delta x - \frac{1}{2}c\Delta_i\Delta x + \frac{1}{2}c\Delta_i\Delta x - \tau\lambda\Delta_i + \frac{1}{2}r\left(u_i^n + \frac{1}{2}\Delta_i\Delta x\right)\right)$$

$$f_{i+1/2} = \lambda\left(u_i^n + \frac{1}{2}(1-c)\Delta_i\Delta x + \cancel{\frac{1}{2}c\Delta_i\Delta x - \frac{1}{2}c\Delta x\Delta_i} + \frac{1}{2}r\left(u_i^n + \frac{1}{2}\Delta_i\Delta x\right)\right)$$

$$f_{i+1/2} = \lambda\left(u_i^n + \frac{1}{2}(1-c)\Delta_i\Delta x + \frac{1}{2}r\left(u_i^n + \frac{1}{2}\Delta_i\Delta x\right)\right)$$

(g) Consider first-order temporal Taylor expansion and Cauchy-Kovalevskaya procedure,

$$u_i(x_i,\tau) = u_i(x_i,0_+) + \tau\partial_t(x_i,0_+)$$

$$u_i(x_i,\tau) = u_i(x_i,0_+) + \tau(-\lambda\partial_x u_i(x_i,0_+) + \beta u_i(x_i,0_+))$$

We know $u_i(x_i,0_+) = u_i^n$ (not at interface) and $\partial_x(x_i,0_+) = \Delta_i$.

$$s_i = \beta u_i(x_i,\tau)$$

$$= \beta\left(u_i^n + \frac{1}{2}\Delta t(-\lambda\Delta_i + \beta u_i^n)\right)$$

(h)

$$\begin{aligned}
u_i^{n+1} &= u_i^n - \frac{\Delta t}{\Delta x}(f_{i+1/2} - f_{i-1/2}) + \Delta t s_i \\
f_{i+1/2} &= \lambda \left(u_i^n + \frac{1}{2}(1-c)\Delta_i \Delta x + \frac{1}{2} r \left(u_i^n + \frac{1}{2}\Delta_i \Delta x \right) \right) \\
f_{i-1/2} &= \lambda \left(u_{i-1}^n + \frac{1}{2}(1-c)\Delta_{i-1} \Delta x + \frac{1}{2} r \left(u_{i-1}^n + \frac{1}{2}\Delta_{i-1} \Delta x \right) \right) \\
s_i &= \beta \left(u_i^n + \frac{1}{2}\Delta t(-\lambda \Delta_i + \beta u_i^n) \right)
\end{aligned}$$

Hence,

$$\begin{aligned}
u_i^{n+1} = u_i^n - c\Big[(u_i^n - u_{i-1}^n) + \frac{1}{2}(1-c)\Delta x(\Delta_i - \Delta_{i-1}) + \frac{1}{2} r (u_i^n - u_{i-1}^n) \\
+ \frac{1}{4} r \Delta x (\Delta_i - \Delta_{i-1}))\Big] \\
+ \Delta t \beta \left(u_i^n + \frac{1}{2}\Delta t(-\lambda \Delta_i + \beta u_i^n) \right)
\end{aligned}$$

$$\begin{aligned}
u_i^{n+1} = u_i^n &- c\Big[(u_i^n - u_{i-1}^n) + \frac{1}{2}(1-c)\Delta x(\Delta_i - \Delta_{i-1})\Big] \\
&- cr\Big[\frac{1}{2}(u_i^n - u_{i-1}^n) + \frac{1}{4}\Delta x(\Delta_i - \Delta_{i-1}))\Big] \\
&+ r \left(u_i^n - \frac{1}{2} c \Delta x \Delta_i + \frac{1}{2} r u_i^n \right)
\end{aligned}$$

$$\begin{aligned}
u_i^{n+1} = u_i^n &- c \left[(u_i^n - u_{i-1}^n) + \frac{1}{2}(1-c)\Delta x(\Delta_i - \Delta_{i-1}) \right] \\
&- cr \left[\frac{1}{2}(u_i^n - u_{i-1}^n) + \frac{1}{4}\Delta x(\Delta_i - \Delta_{i-1})) \right] \\
&+ r \left[\left(1 + \frac{1}{2} r \right) u_i^n - \frac{1}{2} c \Delta x \Delta_i \right]
\end{aligned}$$

4.3 Q3

3. (a) Reference state: the shape of the solid when not subjected to any stress.

(b)
- **Elastic deformation**: When the applied stress is removed, the solid will relax back to its reference state. Can be linear elastic (stress $\propto$ strain), hyperelastic (non-linear stress-strain) or Cauchy-elastic (path-dependent deformation).
- **Plastic deformation**: When the applied stress is removed, the solid will not fully recover to its reference state but remain deformed to some extent permanently. Flow plasticity theory.
- **Fracture**: Due to the applied stress, the solid cracks and undergoes damage. New interfaces are formed. With sufficient damage, the solid fails and some part of this material disconnects with some other parts.

(c)

$$\rho = \frac{m}{V} = \frac{m}{\det\left(\frac{\partial x_i}{\partial X_j}\right) V_0(X_j)} = \frac{\rho_0}{\det(F_{ij})}$$

where the deformation gradient is defined as:

$$F_{ij} = \frac{\partial x_i}{\partial X_j}$$

$V(x_i) = \det\left(\frac{\partial x_i}{\partial X_j}\right) V_0(X_j) = \det(F_{ij}) V_0(X_j)$, essentially the deformation gradient acts as the Jacobian for converting between these two frames of reference.

(d) 2 reasons:

- EoS: stress is generally a function of deformation gradient and specific internal energy.

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

[No longer $p = (\gamma - 1)\rho\varepsilon$. Pressure is a function of density and specific internal energy]

- We can express density in terms of the deformation gradient trivially, but we cannot obtain the deformation gradient (matrix) from density (scalar).

Specifically,

$$\sigma_{ij} = \rho F_{ik} \frac{\partial \varepsilon}{\partial F_{kj}} \quad \text{and} \quad \varepsilon = \varepsilon(\boldsymbol{F}, s)$$

(e) Flow plasticity theory: total deformation (gradient) can be decomposed into elastic deformation (gradient) and plastic deformation (gradient):

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

(f)

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

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

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

$$F^e_{ik}\frac{\mathrm{d}F^p_{kl}}{\mathrm{d}t}(F^p_{lj})^{-1} + \frac{\mathrm{d}F^e_{ik}}{\mathrm{d}t}F^p_{kl}(F^p_{lj})^{-1} - (\nabla_k v_i)F^e_{kl}F^p_{lj}(F^p_{lj})^{-1} = 0$$

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

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

$$\frac{\mathrm{d}F^e_{ij}}{\mathrm{d}t} - (\nabla_k v_i)F^e_{kj} = -F^e_{ik}\frac{\mathrm{d}F^p_{kl}}{\mathrm{d}t}(F^p_{lj})^{-1}$$

(g) **Yield strength**: In a simple stress-strain curve, the yield strength is the point at which the material stops behaving elastically.

Yield surface: a 6D surface in stress-strain space which define the region inside which the material behaves elastically. Stressed states outside this surface are not physically permitted.

(h) If the evolution equation results in stresses outside the yield surface,

- these can be remapped back to the yield surface
- Effectively, we relax the stress, and increase plastic deformation.
- Assuming the deviations beyond the yield surface are small, they can be recovered by taking the steepest path (in 6D) back to the surface (Miller and Colella).
- Ideal plasticity assumes plastic behaviour can only happen beyond the yield surface.

(i) Small plastic deformation can occur within the yield surface. One example is work hardening, which introduces an additional advected quantity.

5 2021-22 (EXAM)

5.1 Q1

1. (a) ρ is density. $\boldsymbol{v}$ is the velocity. $\boldsymbol{B}$ is the magnetic field. p is the pressure. $U = \rho\varepsilon + \frac{1}{2}\rho v^2 + \frac{1}{2}B^2$ is the total energy. $\rho\boldsymbol{v}$ is momentum. $B^2 = \boldsymbol{B}\cdot\boldsymbol{B}$ is the magnitude square of magnetic field.

   (b) Mass equation:

$$\frac{\partial \rho}{\partial t} + \nabla_i(\rho v_i) = 0$$
$$\frac{\partial \rho}{\partial t} + \frac{\partial \rho v_x}{\partial x} + \frac{\partial \rho v_y}{\partial y} + \frac{\partial \rho v_z}{\partial z} = 0$$

Momentum equation:

$$\frac{\partial \rho v_j}{\partial t} + \nabla_i\left[\rho v_j v_i + \left(p + \frac{1}{2}B^2\right)\delta_{ij} - B_j B_i\right] = 0$$
$$\frac{\partial \rho v_j}{\partial t} + \frac{\partial}{\partial x}\left[\rho v_j v_x + \left(p + \frac{1}{2}B^2\right)\delta_{jx} - B_j B_x\right] + \frac{\partial}{\partial y}\left[\rho v_j v_y + \left(p + \frac{1}{2}B^2\right)\delta_{jy} - B_j B_y\right] + \frac{\partial}{\partial z}\,[\text{z-term}]$$

Energy equation:

$$\frac{\partial U}{\partial t} + \nabla_i\left[\left(U + p + \frac{1}{2}B^2\right)v_i - v_j B_j B_i\right] = 0$$
$$\frac{\partial U}{\partial t} + \frac{\partial}{\partial x}\left[\left(U + p + \frac{1}{2}B^2\right)v_x - (\boldsymbol{v}\cdot\boldsymbol{B})B_x\right] + \frac{\partial}{\partial y}\left[\left(U + p + \frac{1}{2}B^2\right)v_y - (\boldsymbol{v}\cdot\boldsymbol{B})B_y\right] + \frac{\partial}{\partial x}\,[\text{z-term}] = 0$$

Magnetic field equation:

$$\frac{\partial B_j}{\partial t} + \nabla_i(B_j v_i - v_j B_i) = 0$$
$$\frac{\partial B_j}{\partial t} + \frac{\partial}{\partial x}(B_j v_x - v_j B_x) + \frac{\partial}{\partial y}(B_j v_y - v_j B_y) + \frac{\partial}{\partial z}(B_j v_z - v_j B_z) = 0$$

Hence, collecting everything:

$$\boldsymbol{f}(\boldsymbol{u}) = \begin{pmatrix} \rho v_x \\ \rho v_x^2 + \left(p + \frac{1}{2}B^2\right) - B_x^2 \\ \rho v_y v_x - B_y B_x \\ \rho v_z v_x - B_z B_x \\ \left(U + p + \frac{1}{2}B^2\right)v_x - (\boldsymbol{v}\cdot\boldsymbol{B})B_x \\ 0 \\ B_y v_x - v_y B_x \\ B_z v_x - v_z B_x \end{pmatrix}, \quad \boldsymbol{g}(\boldsymbol{u}) = \begin{pmatrix} \rho v_y \\ \rho v_x v_y - B_x B_y \\ \rho v_y^2 + \left(p + \frac{1}{2}B^2\right) - B_y^2 \\ \rho v_z v_y - B_z B_y \\ \left(U + p + \frac{1}{2}B^2\right)v_y - (\boldsymbol{v}\cdot\boldsymbol{B})B_y \\ B_x v_y - v_y B_x \\ 0 \\ B_z v_y - v_z B_y \end{pmatrix}$$

$$\boldsymbol{h}(\boldsymbol{u}) = \begin{pmatrix} \rho v_z \\ \rho v_x v_z - B_x B_z \\ \rho v_y v_z - B_y B_z \\ \rho v_z^2 + \left(p + \frac{1}{2}B^2\right) - B_z^2 \\ \left(U + p + \frac{1}{2}B^2\right)v_z - (\boldsymbol{v}\cdot\boldsymbol{B})B_z \\ B_x v_z - v_z B_x \\ B_y v_z - v_y B_z \\ 0 \end{pmatrix}$$

(c) In 1D, we have 7 evolution equations.

$$\frac{\partial \boldsymbol{g}}{\partial y} = \frac{\partial \boldsymbol{h}}{\partial z} = 0$$

The evolution equation for B_x becomes:

$$\frac{\partial B_x}{\partial t} = 0$$

Hence, B_x is always constant in time and its evolution equation disappears.

(d) Maximum number of waves is 7. None of these waves are degenerate as we would find 7 distinct, real eigenvalues of the system.

(e) We have one contact discontinuity, two fast waves, two Alfvén waves and two slow waves.

$$\lambda = v_x \, , \; v_x \pm c_{sl} \, , \; v_x \pm c_a \, , \; v_x \pm c_f$$

Properties of MHD waves:

- Across contact discontinuity, only density jumps. Magnetic field, pressure and velocity is continuous.

$$\{\enclose{circle}{\rho} \, , \, v_\perp \, , \, v_\parallel \, , \, p \, , \, B_\perp \, , \, B_\parallel\}$$

- Slow waves can be a shock, rarefaction or tangential discontinuity.

  In the limiting case, it is a tangential discontinuity when velocity and magnetic field are parallel to the wave. All variables jump except pressure and normal velocity.

$$\{\enclose{circle}{\rho} \, , \, v_\perp \, , \, \enclose{circle}{v_\parallel} \, , \, p \, , \, \enclose{circle}{B_\perp} \, , \, \enclose{circle}{B_\parallel}\}$$

- Alfvén waves are rotational discontinuities. Across a rotational discontinuity, only magnetic field components jump, while the rest are continuous including magnitude of magnetic field.

$$\{\rho \, , \, v_\perp \, , \, v_\parallel \, , \, p \, , \, |B| \, , \, \enclose{circle}{B_x} , \, , \, \enclose{circle}{B_y} , \, , \, \enclose{circle}{B_z}\}$$

- Fast waves can be a shock or rarefaction.

  Across a shock wave, all variables jump.
  Across a rarefaction, no variables jump, all are continuous.

Note: possible variables: $\{\rho \, , \, v_\perp \, , \, v_\parallel \, , \, p \, , \, B_\perp \, , \, B_\parallel\}$.

(f) Divergence Constraint

The **divergence constraint** is:

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

- It is a constraint on the solution to avoid magnetic monopoles.
- Numerical errors building up can cause violation of the divergence constraint.
- Solutions which violate the divergence constraint may not be stable.
- Over time, errors build up and may lead to oscillations.

(g) c_h is the **hyperbolic wave speed**, which is the speed of propagation of divergence error, chosen to be the maximum wave speed over the entire domain:

$$c_h=\max(|v_x|+c_{f,x},|v_y|+c_{f,y},|v_z|+c_{f,z})$$

c_p is the **parabolic damping term**, found through numerical experiment to be:

$$c_p^2=0.18c_h$$

The effect of the divergence cleaning treatment is that the divergence errors are transported to the domain boundaries with the maximal admissible speed and are damped at the same time.

(h) A hyperbolic system has real and distinct eigenvalues.

The divergence cleaning treatment introduces a new unknown ψ which couples the divergence constraint to the hyperbolic system. This introduces an additional evolution equation into the MHD equations and modifies the evolution equation for B_x:

$$\frac{\partial\psi}{\partial t}+c_h^2\frac{\partial B_x}{\partial x}=-\frac{c_h^2}{c_p^2}\psi \quad\text{and}\quad \frac{\partial B_x}{\partial t}+\frac{\partial\psi}{\partial x}=0$$

We can express the new MHD system of equations as:

$$\partial_t\boldsymbol{W}+A(\boldsymbol{W})\partial_x\boldsymbol{W}=0$$

where $\boldsymbol{W}=(\rho,u_x,u_y,u_z,U,B_x,B_y,B_z,\psi)^T$. Looking at the eigenstructure of A, we see that these two equations has no dependence on u_x, this means that the equations of B_x and ψ can be decoupled from the remaining system.

We now have:

$$\frac{\partial}{\partial t}\begin{pmatrix}B_x\\ \psi\end{pmatrix}+\begin{pmatrix}0&1\\ c_h^2&0\end{pmatrix}\frac{\partial}{\partial x}\begin{pmatrix}B_x\\ \psi\end{pmatrix}=-\frac{c_h^2}{c_p^2}\begin{pmatrix}0\\ \psi\end{pmatrix}\quad\text{and}\quad\underbrace{\partial_t\boldsymbol{W'}+A'(\boldsymbol{W'})\partial_x\boldsymbol{W'}=0}_{\text{original 1D MHD}}$$

The eigenvalues of the subsystem are trivially obtained , $\lambda=c_h,-c_h$. The eigenvalues of the subsystem are distinct from the eigenvalues of the original 1D MHD if c_h is sufficiently large. We have 9 real and distinct eigenvalues. Hence, the system is hyperbolic.

(i) Alternative approach: **constrained transport**.

- *Description*: it uses a staggered grid to store magnetic fields
- *Advantage*: we can show this is divergence free by construction. (imitates the analytical fact that the divergence of a curl equals zero)
- *Disadvantage*: more difficult to implement as it requires code structure to be written to follow this staggered grid approach - may need to start from scratch.

(j) In 1D, all y- and z- derivatives vanish. So the divergence constraint is:

$$\boldsymbol{\nabla} \cdot \boldsymbol{B} = \frac{\partial B_x}{\partial x} = 0$$

Also in 1D, $B_x =$ constant in time. Hence, the divergence constraint will never be violated.

5.2 Q2

2. (a) **Advected tracer**

$$\boldsymbol{s}(\boldsymbol{u}) = \begin{pmatrix} 0 & 0 & 0 & 0 \end{pmatrix}^T$$

Augmented Euler Equations

- The system describes a variable which simply moves with the material velocity.
- An advected tracer quantity has similar properties as the underlying material i.e. it has same equation of state as the underlying material.
- This equation will then model the concentration of this quantity as it moves with the flow.
- E.g. the spreading of food colouring in water.

Reactions: to achieve a model for reactions (e.g. detonation/reactive material), we simply have:

$$\boldsymbol{s}(\boldsymbol{u}) = \begin{pmatrix} 0 & 0 & \text{rate of energy change} & \text{rate of reaction} \end{pmatrix}^T$$

The reaction rate is commonly modelled by an Arrhenius law or a pressure-based law.

(b) λ is the reaction progress variable which tells us how much of the reactants has turned into products.

(c)
- The augmented Euler equations can model either the reactant or the product.
- As a result, energy may be added or removed from the material depending on whether it is being created or not.
- Energy can either be released (exothermic) or absorbed (endothermic) during the reaction.

(d) **Source term and stable time step**

How source term adversely affect stable time step:

- Source term model a physical process which is not included in the conservation law i.e. described through the gradient of material quantities.
- It will have its own timescale, which may be different from the acoustic time scales of the simulation.
- If the source term timescale is much smaller than one obtained from the CFL condition, the choice of a minimum stable time step $\Delta t = \min(\Delta t_{CFL}, \Delta t_s)$ gives a lower time step than necessary.
- This leads to many iterations of the conservation law part of the system, resulting in unnecessary accumulation of error and greater computational expense.

Two techniques to avoid this error:

i. **Implicit scheme**:

- A timestep independent scheme can be used to update the source term.
- Most applicable for diffusive (parabolic) sources.
- These can have contribution across the entire numerical domain due to infinite propagation speed.
- Requires a computationally expensive matrix inversion procedure.

- If $\Delta t_s \ll \Delta t_{CFL}$, it may be more efficient to solve the source term implicitly.
- If error accumulation for explicit update is large, then for the same accuracy, implicit schemes might be more efficient.

ii. **Subcycling (explicit scheme)**:

- Update the source term at its own stable time step Δt_s multiple times for each acoustic timestep (Δt_{CFL}) of the system.
- The evolution must be stopped once the Δt_{CFL} is reached, and the states now exists at the same time.
- Most appropriate when there is local behaviour based on the properties of a single cell e.g. chemical reaction (where the speed of conversion of reactants into products is much faster than the speed with which the material moves).

Decision: which scheme can achieve a given accuracy fastest?

(e) Use subcycling, due to the fact that the reaction occurs through a chemical, cell-based process.

(f) For cylindrically symmetric, ignore θ terms, we only have dependence on r and z.

$$\boldsymbol{\nabla} \cdot \boldsymbol{f} = \frac{\partial f_r}{\partial r} + \frac{\partial f_z}{\partial z} + \frac{f_r}{r}$$

For mass equation:

$$\frac{\partial \rho}{\partial t} + \nabla_i(\rho v_i) = 0$$

$$\frac{\partial \rho}{\partial t} + \frac{\partial}{\partial r}(\rho v_r) + \frac{\partial}{\partial z}(\rho v_z) + \frac{\rho v_r}{r} = 0$$

For momentum equation:

$$\frac{\partial \rho v_i}{\partial t} + \nabla_j(\rho v_i v_j) + \nabla_i(p) = 0$$

$$\frac{\partial \rho v_i}{\partial t} + \frac{\partial}{\partial r}(\rho v_i v_r + p\delta_{ir}) + \frac{\partial}{\partial z}(\rho v_i v_z + p\delta_{iz}) + \frac{\rho v_i v_r}{r} = 0$$

The pressure term is a gradient, not a divergence, so it does not appear in the source term.

For energy equation:

$$\frac{\partial E}{\partial t} + \nabla_i((E+p)v_i) = \pm \rho K Q$$

$$\frac{\partial E}{\partial t} + \frac{\partial (E+p)v_r}{\partial r} + \frac{\partial (E+p)v_z}{\partial z} + \frac{(E+p)v_r}{r} = \pm\rho K Q$$

For tracer/reaction rate equation:

$$\frac{\partial \rho\lambda}{\partial t} + \nabla_i(\rho\lambda v_i) = \rho K$$

$$\frac{\partial \rho\lambda}{\partial t} + \frac{\partial}{\partial r}(\rho\lambda v_r) + \frac{\partial}{\partial z}(\rho\lambda v_z) + \frac{\rho\lambda v_r}{r} = \rho K$$

Combining everything:

$$\frac{\partial}{\partial t}\begin{pmatrix}\rho\\ \rho v_r\\ \rho v_z\\ E\\ \rho\lambda\end{pmatrix} + \frac{\partial}{\partial r}\begin{pmatrix}\rho v_r\\ \rho v_r^2+p\\ \rho v_z v_r\\ (E+p)v_r\\ \rho\lambda v_r\end{pmatrix} + \frac{\partial}{\partial z}\begin{pmatrix}\rho v_z\\ \rho v_r v_z\\ \rho v_z^2+p\\ (E+p)v_z\\ \rho\lambda v_z\end{pmatrix} = -\frac{1}{r}\begin{pmatrix}\rho v_r\\ \rho v_r^2\\ \rho v_z v_r\\ (E+p)v_r\\ \rho\lambda v_r\end{pmatrix} + \begin{pmatrix}0\\ 0\\ 0\\ \pm\rho K Q\\ \rho K\end{pmatrix}$$

The source terms are made up of a physical source term and geometric source term.

(g) **Operator splitting** separates the conservation law update and the source term update. Consider two operations to give a first-order update:

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

- First, $\mathcal{C}^{(\Delta t)}$: ignore the source term and solve the PDE as a conservation law over time Δt to get an intermediate state $\bar{\boldsymbol{u}}^{n+1}$.

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

- Then, $\mathcal{S}^{(\Delta t)}$: ignore the divergence operator and solve the balance law ODE over Δt using the intermediate state to get final state $\boldsymbol{u}^{n+1}$.

$$\left.\begin{array}{ll}\text{ODE:} & \frac{\mathrm{d}\boldsymbol{u}}{\mathrm{d}t} = \boldsymbol{s}(\boldsymbol{u})\\ \text{IC:} & \bar{\boldsymbol{u}}^{n+1}\end{array}\right\} = \boldsymbol{u}^{n+1}$$

First order is:

$$\boldsymbol{u}^{n+1} = \bar{\boldsymbol{u}}^{n+1} + \Delta t\boldsymbol{s}$$

(h) Solve the ODE using a Runge-Kutta scheme (slope approximation).

- **Fourth-order explicit RK4** (original RK method):
  - Start with a first-order step.
  - Perform subsequent evolutions with this.
  - Eventual update is a weighted average of these four evolution steps.

$$\boldsymbol{K}_1 = \Delta t\cdot\boldsymbol{s}(\bar{\boldsymbol{u}}^{n+1})$$

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

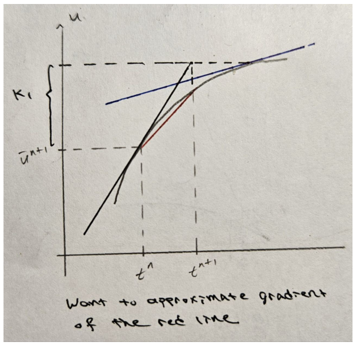
$$\boldsymbol{K}_4 = \Delta t\cdot\boldsymbol{s}(\bar{\boldsymbol{u}}^{n+1} + \boldsymbol{K}_3)$$

Then,

$$\boldsymbol{u}^{n+1} = \bar{\boldsymbol{u}}^{n+1} + \frac{1}{6}(\boldsymbol{K}_1 + 2\boldsymbol{K}_2 + 2\boldsymbol{K}_3 + \boldsymbol{K}_4)$$

- Second-order accuracy (Heun's method):

$$\boldsymbol{K}_1 = \Delta t \cdot \boldsymbol{s}(\bar{\boldsymbol{u}}^{n+1}) \quad \text{and} \quad \boldsymbol{K}_2 = \Delta t \cdot \boldsymbol{s}(\bar{\boldsymbol{u}}^{n+1} + \boldsymbol{K}_1)$$



Want to approximate gradient of the red line

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

5.3 Q3

3. Same question as 2024-25 (Mock) Q3. Link

6 2023-24 (EXAM)

6.1 Q1

1. Same question 2024-25 (Mock) Q1. Link

6.2 Q2

2. (a) First, extend influence of cut cell to full cell length using stable time-step Δt and the update is (stable, not conservative):

$$\boldsymbol{U}_i^{n+1} = \boldsymbol{U}_i^n - \frac{\Delta t}{\Delta x}(\boldsymbol{F}^{b,n} - \boldsymbol{F}_{i-1/2}^n)$$

Then, realise that the desired conservative update is obtained using the stabilised flux (conservative, not stable):

$$\boldsymbol{U}_i^{n+1} = \boldsymbol{U}_i^n - \frac{\Delta t}{\alpha \Delta x}(\boldsymbol{F}^{b,n} - \boldsymbol{F}_{i-1/2}^{KBN,n})$$

Equating:

$$\boldsymbol{F}^{b,n} - \boldsymbol{F}_{i-1/2}^n = \frac{1}{\alpha}(\boldsymbol{F}^{b,n} - \boldsymbol{F}_{i-1/2}^{KBN,n})$$
$$\boldsymbol{F}_{i-1/2}^{KBN,n} = \boldsymbol{F}^{b,n} + \alpha(\boldsymbol{F}_{i-1/2}^n - \boldsymbol{F}^{b,n})$$

(b) It represents the propagation of information from cell x_i where the slope of the line is the maximum wave speed.

(c) To ensure stability, we increase the influence of the cut cell by just enough to $\alpha_2 \Delta x$ (rather than to the full cell length in a typical KBN flux), such that waves in the cell x_i do not overlap with waves in the cell x_{i-1} in a single time-step. Repeating the same procedure as for KBN flux:

$$\boldsymbol{U}_i^{n+1} = \boldsymbol{U}_i^n - \frac{\Delta t}{\alpha_2 \Delta x}(\boldsymbol{F}^{b,n} - \boldsymbol{F}_{i-1/2}^n) \quad \text{and} \quad \boldsymbol{U}_i^{n+1} = \boldsymbol{U}_i^n - \frac{\Delta t}{\alpha \Delta x}(\boldsymbol{F}^{b,n} - \boldsymbol{F}_{i-1/2}^{KBN,mod,n})$$

We get:

$$\boldsymbol{F}_{i-1/2}^{KBN,mod,n} = \boldsymbol{F}^{b,n} + \frac{\alpha}{\alpha_2}(\boldsymbol{F}_{i-1/2}^n - \boldsymbol{F}^{b,n})$$

(d) $\alpha \in [0, 1]$. $\alpha_2 \in [\alpha, 1]$

(e) It means we get:

$$\boldsymbol{F}_{i-1/2}^{KBN,mod,n} = \boldsymbol{F}_{i-1/2}^n$$

there is no need for flux stabilisation of the cut cell. This happens when the maximum wave speed in the cut cell is

$$a_{max,i} = \alpha \frac{\Delta x}{\Delta t}$$

where α is coincidentally the Courant number.

(f) LPFS flux goes further to propose that no flux stabilisation is required for the fraction of time $\frac{\Delta t_{cc}}{\Delta t}$, in which the wave from cell i has yet to reach the neighbouring cell. For the remaining fraction of time $1 - \frac{\Delta t_{cc}}{\Delta t}$, the flux is stabilised using the modified KBN method. Hence,

$$\boldsymbol{F}_{i-1/2}^{LPFS,n} = \frac{\Delta t_{cc}}{\Delta t}\boldsymbol{F}_{i-1/2}^{n} + \left(1 - \frac{\Delta t_{cc}}{\Delta t}\right)\boldsymbol{F}_{i-1/2}^{KBN,mod,n}$$

(g) Characteristic speed for linear advection is a. We consider the stable time-step for a regular cell and the cut cell:

$$\Delta t_{cc} = C\frac{\alpha \Delta x}{a_{max,i}} \quad \text{and} \quad \Delta t = C\frac{\Delta x}{a_{max}}$$

Dividing,

$$\frac{\Delta t_{cc}}{\Delta t} = \alpha \frac{a_{max}}{a_{max,i}}$$

For linear advection, the characteristic speed is the same everywhere ($a_{max} = a_{max,i}$). Hence,

$$\frac{\Delta t_{cc}}{\Delta t} = \alpha$$

Also, by geometry we get

$$\frac{\Delta t_{cc}}{\Delta t} = \frac{\alpha}{\alpha_2}$$

Hence, $\alpha_2 = 1$.

(h)

$$\begin{aligned}
\boldsymbol{F}_{i-1/2}^{LPFS,n} &= \alpha\boldsymbol{F}_{i-1/2}^{n} + (1-\alpha)\boldsymbol{F}_{i-1/2}^{KBN,mod,n} \\
&= \alpha\boldsymbol{F}_{i-1/2}^{n} + (1-\alpha)\left[\boldsymbol{F}^{b,n} + \alpha(\boldsymbol{F}_{i-1/2}^{n} - \boldsymbol{F}^{b,n})\right] \\
&= \alpha\boldsymbol{F}_{i-1/2}^{n}(1 + 1 - \alpha) + (1-\alpha)[\boldsymbol{F}^{b,n}(1-\alpha)] \\
&= \alpha(2-\alpha)\boldsymbol{F}_{i-1/2}^{n} + (\alpha - 1)^2\boldsymbol{F}^{b,n}
\end{aligned}$$

From $\boldsymbol{U}_i^{n+1} = \boldsymbol{U}_i^n - \frac{\Delta t}{\alpha_2 \Delta x}(\boldsymbol{F}^{b,n} - \boldsymbol{F}_{i-1/2}^{n})$, if $\alpha_2 = 1$, it becomes the familiar cell update with $\boldsymbol{F}^{b,n} = \boldsymbol{F}_{i+1/2}^{n}$,

$$\boldsymbol{F}_{i-1/2}^{LPFS,n} = \alpha(2-\alpha)\boldsymbol{F}_{i-1/2}^{n} + (\alpha-1)^2\boldsymbol{F}_{i+1/2}^{n}$$

(i) For $\boldsymbol{F}_{i+1/2}^{n} = 0$,

$$\boldsymbol{F}_{i-1/2}^{LPFS,n} = \alpha(2-\alpha)(\boldsymbol{F}_{i-1/2}^{n})$$

What is consistency? Local truncation error of method vanish as $\Delta t, \Delta x \to 0$.

$$\begin{aligned}
U_i^{n+1} &= U_i^n - \frac{\Delta t}{\alpha \Delta x}(\cancel{F^{b,n}} - F_{i-1/2}^{LPFS,n}) \\
&= U_i^n + \frac{\Delta t}{\alpha \Delta x}\left[\alpha(2-\alpha)F_{i-1/2}^{n}\right] \\
&= U_i^n + (2-\alpha)\frac{\Delta t}{\Delta x}F_{i-1/2}^{n} \\
&= U_i^n + (2-\alpha)\frac{a\Delta t}{\Delta x}U_{i-1}^{n}
\end{aligned}$$

Consider truncation error analysis:

$$
\begin{aligned}
Lu_i &= \frac{u_i^{n+1} - u_i^n}{\Delta t} - a(2-\alpha)\frac{u_{i-1}^n}{\Delta x} \\
&= u_t(x_i, t^n) - a(2-\alpha)\frac{u_i^n - \frac{1+\alpha}{2}\Delta x u_x(x_i, t^n)}{\Delta x} + \mathcal{O}(\Delta x, \Delta t) \\
&= -au_x(x_i, t^n) - a(2-\alpha)\frac{u_i^n}{\Delta x} + a(2-\alpha)\frac{1+\alpha}{2}u_x(x_i, t^n) + \mathcal{O}(\Delta x, \Delta t) \\
&= au_x(x_i, t^n)\left(-1 + 1 - \frac{1}{2}\alpha + \alpha - \frac{1}{2}\alpha^2\right) - \frac{a(2-\alpha)}{\Delta x}u_i^n + \mathcal{O}(\Delta x, \Delta t) \\
&= \frac{1}{2}\alpha(1-\alpha)au_x(x_i, t^n) - \frac{a(2-\alpha)}{\Delta x}u_i^n + \mathcal{O}(\Delta x, \Delta t)
\end{aligned}
$$

The truncation error does not vanish as $\Delta x, \Delta t \to 0$, the method is not consistent.

(j) **Supraconvergence**

- Although truncation error analysis fails to prove the consistency of the numerical method, numerical tests show that LPFS does converge with first order accuracy.
- The aim is to find another grid function w which differs from the grid function of u (real solution) by an $\mathcal{O}(\Delta x)$ amount, and for which the truncation error in all cells is $\mathcal{O}(\Delta t, \Delta x)$.

  $$w = u + \mathcal{O}(\Delta x)$$

  Our consistency analysis is now:

  $$|w_i - U_i| = \mathcal{O}(\Delta x, \Delta t)\ \forall i$$

- Although our numerical scheme is not consistent with our exact solution u_i, we can show that it does consistently solve for another grid function w_i.
- Ultimately, we are concerned with the behaviour of the method as $\Delta x \to 0$. By showing consistency with w_i, our method is effectively consistent in the desired limit $\Delta x \to 0$.

It shows that LPFS is consistent.

6.3 Q3

3. (a) Deformation gradient:

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

(b)

$$I_1 = \mathrm{Tr}(\boldsymbol{A})$$

$$I_2 = \frac{1}{2}(\mathrm{Tr}(\boldsymbol{A})\,\mathrm{Tr}(\boldsymbol{A}) - \mathrm{Tr}(\boldsymbol{A}\boldsymbol{A}))$$

(c) Symmetric means $\boldsymbol{A}^T = \boldsymbol{A}$. Consider

$$\boldsymbol{C}^T = (\boldsymbol{F}^{-T}\boldsymbol{F}^{-1})^T = (\boldsymbol{F}^{-1})^T(\boldsymbol{F}^{-T})^T = \boldsymbol{F}^{-T}\boldsymbol{F}^{-1} = \boldsymbol{C}$$

The finger tensor is symmetric.

(d) For Finger tensor,

$$\begin{aligned} I_3 &= \det(\boldsymbol{C}) \\ &= \det\left(\boldsymbol{F}^{-T}\boldsymbol{F}^{-1}\right) \\ &= \det\left(\boldsymbol{F}^{T}\right)^{-1}\det(\boldsymbol{F})^{-1} \\ &= \det(\boldsymbol{F})^{-1}\det(\boldsymbol{F})^{-1} \\ &= \det(\boldsymbol{F})^{-2} \\ &= \frac{\rho^2}{\rho_0^2} \end{aligned}$$

(e)

$$\frac{\partial I_{C,1}}{\partial C_{ij}} = \frac{\partial C_{kk}}{\partial C_{ij}} = \delta_{ij}$$

Only differentiates to 1 iff $i = j$.

(f) Consider,

$$\begin{aligned} \frac{\partial I_{C,2}}{\partial C_{ij}} &= \frac{1}{2}\left[\frac{\partial(C_{kk}C_{mm} - C_{km}C_{mk})}{\partial C_{ij}}\right] \\ &= C_{kk}\frac{\partial C_{kk}}{\partial C_{ij}} - \underbrace{\frac{1}{2}C_{km}\frac{\partial C_{mk}}{\partial C_{ij}} - \frac{1}{2}C_{mk}\frac{\partial C_{km}}{\partial C_{ij}}}_{\boldsymbol{C}\text{ is symmetric}} \\ &= I_{C,1}\delta_{ij} - C_{km}\frac{\partial C_{km}}{\partial C_{ij}} \end{aligned}$$

and

$$\begin{aligned} \frac{\partial I_{C,3}}{\partial C_{ij}} &= \frac{\partial \det(C_{ij})}{\partial C_{ij}} \\ &= \det(C_{ij})(C^{-1})_{ji} \\ &= I_{C,3}(C^{-1})_{ji} \end{aligned}$$

$$\begin{aligned}
\sigma_{ij} &= -2\rho C_{ik}\frac{\partial I_{C,l}}{\partial C_{kj}}\frac{\partial \varepsilon}{\partial I_{C,l}} \\
&= -2\rho C_{ik}\left[\frac{\partial I_{C,1}}{\partial C_{kj}}\frac{\partial \varepsilon}{\partial I_{C,1}} + \frac{\partial I_{C,2}}{\partial C_{kj}}\frac{\partial \varepsilon}{\partial I_{C,2}} + \frac{\partial I_{C,3}}{\partial C_{kj}}\frac{\partial \varepsilon}{\partial I_{C,3}}\right] \\
&= -2\rho C_{ik}\left[\delta_{kj}\frac{\partial \varepsilon}{\partial I_{C,1}} + \left(I_{C,1}\delta_{kj} - C_{lm}\frac{\partial C_{lm}}{\partial C_{kj}}\right)\frac{\partial \varepsilon}{\partial I_{C,2}} + I_{C,3}(C^{-1})_{jk}\frac{\partial \varepsilon}{\partial I_{C,3}}\right] \\
&= -2\rho\left[C_{ij}\frac{\partial \varepsilon}{\partial I_{C,1}} + I_{C,1}C_{ij}\frac{\partial \varepsilon}{\partial I_{C,2}} - C_{ik}C_{lm}\frac{\partial C_{lm}}{\partial C_{kj}}\frac{\partial \varepsilon}{\partial I_{C,2}} + I_{C,3}C_{ik}C_{jk}^{-1}\frac{\partial \varepsilon}{\partial I_{C,3}}\right] \\
&= -2\rho\left[\left(\frac{\partial \varepsilon}{\partial I_{C,1}} + I_{C,1}\frac{\partial \varepsilon}{\partial I_{C,2}}\right)C_{ij} - C_{ij}C_{lm}\delta_{lk}\delta_{mj}\frac{\partial \varepsilon}{\partial I_{C,2}} + I_{C,3}\delta_{ij}\frac{\partial \varepsilon}{\partial I_{C,3}}\right] \\
&= -2\rho\left[\left(\frac{\partial \varepsilon}{\partial I_{C,1}} + I_{C,1}\frac{\partial \varepsilon}{\partial I_{C,2}}\right)C_{ij} - C_{ij}C_{kj}\frac{\partial \varepsilon}{\partial I_{C,2}} + I_{C,3}\frac{\partial \varepsilon}{\partial I_{C,3}}\delta_{ij}\right]
\end{aligned}$$

(g)

$$\frac{\partial \varepsilon}{\partial I_{C,1}} = \frac{b_0^2 I_{C,3}^{\beta_R/2}}{3} I_{C,1}$$

$$\frac{\partial \varepsilon}{\partial I_{C,2}} = -\frac{b_0^2 I_{C,3}^{\beta_R/2}}{2}$$

$$\begin{aligned}
\frac{\partial \varepsilon}{\partial I_{C,3}} &= \frac{K_0}{\alpha_R^2}(I_{C,3}^{\alpha_R/2} - 1)\frac{\alpha_R}{2}I_{C,3}^{\alpha_R/2-1} + c_V T_0\frac{\gamma_R}{2}I_{C,3}^{\gamma_R/2-1}(e^{s/C_V} - 1) + \frac{b_0^2}{2}\frac{\beta_R}{2}I_{C,3}^{\beta_R/2-1}\left(\frac{I_{C,1}^2}{3} - I_{C,2}\right) \\
&= \frac{K_0}{2\alpha_R}(I_{C,3}^{\alpha_R/2} - 1)I_{C,3}^{\alpha_R/2-1} + \frac{c_V T_0 \gamma_R}{2}(e^{s/C_V} - 1)I_{C,3}^{\gamma_R/2-1} + \frac{b_0^2\beta_R}{4}\left(\frac{I_{C,1}^2}{3} - I_{C,2}\right)I_{C,3}^{\beta_R/2-1}
\end{aligned}$$

$$\sigma_{ij} = -2\rho\left[\left(\frac{b_0^2 I_{C,3}^{\beta_R/2}}{3} - \frac{b_0^2 I_{C,3}^{\beta_R/2}}{2}I_{C,1}\right)C_{ij} + \left(\frac{b_0^2 I_{C,3}^{\beta_R/2}}{2}\right)C_{ij}C_{kj} + I_{C,3}\frac{\partial \varepsilon}{\partial I_{C,3}}\delta_{ij}\right]$$

(h)
- Linear elastic: stress $\propto$ strain.
- Hyperelastic: non-linear stress-strain e.g. high strain rate simulation of solid materials.
- Cauchy-elastic: path-dependent work done by stress.

7 2024-25 (Mock)

7.1 Q1

1. Solve on paper during Mock exam.

7.2 Q2

2. Same question as 2021-22 (Exam) Q1. Link

7.3 Q3

3. (a)

$$\gamma_{adia} = -\frac{\nu}{p}\frac{\partial p}{\partial \nu}\bigg|_s = \frac{\rho}{p}\frac{\partial p}{\partial \rho}\bigg|_s \quad \text{and} \quad \frac{\partial p}{\partial \rho}\bigg|_s = \frac{p}{\rho^2 \frac{\partial \varepsilon}{\partial p}} - \frac{\frac{\partial \varepsilon}{\partial \rho}}{\frac{\partial \varepsilon}{\partial p}}$$

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

$$\frac{\partial \varepsilon}{\partial p} = \frac{1}{\rho(\gamma-1)} \quad \text{and} \quad \frac{\partial \varepsilon}{\partial \rho} = -\frac{p}{\rho^2(\gamma-1)}$$

$$\begin{aligned}\frac{\partial p}{\partial \rho}\bigg|_s &= \frac{p}{\rho^2 \frac{\partial \varepsilon}{\partial p}} - \frac{\frac{\partial \varepsilon}{\partial \rho}}{\frac{\partial \varepsilon}{\partial p}} \\ &= \frac{p\rho(\gamma-1)}{\rho^2} + \frac{\rho(\gamma-1)p}{\rho^2(\gamma-1)} \\ &= \frac{p(\gamma-1)}{\rho} + \frac{p}{\rho} \\ &= \frac{\gamma p}{\rho}\end{aligned}$$

$$\Rightarrow \gamma_{adia} = \frac{\rho}{p} \times \frac{\gamma p}{\rho} = \gamma$$

Hence, the γ in the equation of state is the same as the adiabatic index.

(b) If $\Gamma > 0$:

- Temperature varies monotonically along an isentrope
- EoS provides a unique parametrisation of thermodynamic space,
- meaning specific volume, specific internal energy and pressure $p(\nu, \varepsilon)$, $\varepsilon(\nu, p)$ and $\nu(\varepsilon, p)$ are all single-valued functions of the other two variables.

(c)

$$\Gamma = -\frac{\nu}{T}\frac{\partial T}{\partial \nu}\Big|_s = -\frac{\nu}{T}\left[\frac{\partial T}{\partial \rho}\Big|_\varepsilon \frac{\partial \rho}{\partial \nu}\Big|_s + \frac{\partial T}{\partial \varepsilon}\Big|_\rho \frac{\partial \varepsilon}{\partial \nu}\Big|_s\right]$$

$$\Gamma = -\frac{1}{T\rho}\left[\frac{\partial T}{\partial \rho}\Big|_\varepsilon \left(-\frac{1}{\nu^2}\right) + \frac{\partial T}{\partial \varepsilon}\Big|_\rho (-p)\right]$$

$$\Gamma = \frac{\rho}{T}\left[\frac{\partial T}{\partial \rho}\Big|_\varepsilon + \frac{p}{\rho^2}\frac{\partial T}{\partial \varepsilon}\Big|_\rho\right]$$

where for $ds = 0$,

$$T ds = d\varepsilon + p d\nu \Rightarrow d\varepsilon = -p d\nu$$

(d) Ideal gas:

$$p\nu = nRT \quad , \quad p = (\gamma - 1)\rho\varepsilon$$

$$\frac{\partial s}{\partial \varepsilon}\Big|_\nu = \frac{1}{T} \quad \text{and} \quad \frac{\partial s}{\partial \nu}\Big|_\varepsilon = \frac{p}{T}$$

$$\frac{\partial^2 s}{\partial \nu\,\partial \varepsilon} = \frac{\partial}{\partial \nu}\left(\frac{1}{T}\right)\Big|_\varepsilon \quad \text{and} \quad \frac{\partial^2 s}{\partial \varepsilon\,\partial \nu} = \frac{\partial}{\partial \varepsilon}\left(\frac{p}{T}\right)\Big|_\nu$$

$$-\frac{1}{T^2}\frac{\partial T}{\partial \nu}\Big|_\varepsilon = -\frac{p}{T^2}\frac{\partial T}{\partial \varepsilon}\Big|_\nu + \frac{1}{T}\frac{\partial p}{\partial \varepsilon}\Big|_\rho$$

$$\frac{\rho^2}{T^2}\frac{\partial T}{\partial \rho}\Big|_\varepsilon = -\frac{p}{T^2}\frac{\partial T}{\partial \varepsilon}\Big|_\rho + \frac{1}{T}(\gamma - 1)\rho$$

$$\frac{\partial T}{\partial \rho}\Big|_\varepsilon = -\frac{p}{\rho^2}\frac{\partial T}{\partial \varepsilon}\Big|_\rho + \frac{T(\gamma - 1)}{\rho}$$

Hence, for ideal gas:

$$\Gamma = \frac{\rho}{T}\left(\cancel{\frac{p}{\rho^2}\frac{\partial T}{\partial \varepsilon}\Big|_\rho - \frac{p}{\rho^2}\frac{\partial T}{\partial \varepsilon}\Big|_\rho} + \frac{T(\gamma - 1)}{\rho}\right)$$

$$\Gamma = \gamma - 1 > 0$$

OR

Ideal gas:

$$\varepsilon = c_V T \quad \Rightarrow \quad T = \frac{\varepsilon}{c_V}$$

Using expression from previous question,

$$\Gamma = \frac{\rho}{T}\left[\frac{p}{\rho^2}\frac{1}{c_V}\right] = \frac{p}{T\rho c_V}$$

All quantities are non-negative.

(e) Stiffened gas EoS:

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

where ρ is density, p is pressure, ε is specific internal energy. p_∞ is a reference pressure, a stiffening parameter to model resistance to compression. ε_∞ is the reference energy from heat of formation. γ is constant.

(f)

$$\gamma_{adia} = \frac{\rho}{p} c_s^2 \quad \text{and} \quad c_s^2 = \frac{p}{\rho^2 \frac{\partial \varepsilon}{\partial p}} - \frac{\frac{\partial \varepsilon}{\partial \rho}}{\frac{\partial \varepsilon}{\partial p}}$$

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

$$\frac{\partial \varepsilon}{\partial p} = \frac{1}{(\gamma - 1)\rho} \quad \text{and} \quad \frac{\partial \varepsilon}{\partial \rho} = -\frac{p + \gamma p_\infty}{\rho^2 (\gamma - 1)}$$

$$\begin{aligned} c_s^2 &= \frac{p(\gamma - 1)}{\rho} + \frac{(\gamma - 1)\rho(p + \gamma p_\infty)}{\rho^2(\gamma - 1)} \\ &= \frac{p(\gamma - 1)}{\rho} + \frac{p + \gamma p_\infty}{\rho} \\ &= \frac{\gamma(p + p_\infty)}{\rho} \end{aligned}$$

Hence,

$$\gamma_{adia} = \frac{\rho}{p} \frac{\gamma(p + p_\infty)}{\rho} = \gamma_{SG} \left(1 + \frac{p_\infty}{p} \right)$$

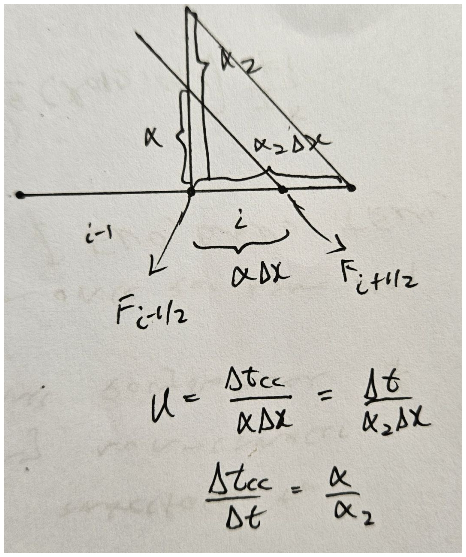
(g)

$$\begin{aligned} \Gamma &= -\frac{\nu}{T} \frac{\partial T}{\partial \nu} \Big|_s \\ &= -\frac{\nu}{T} \frac{\partial}{\partial \nu} \left(\frac{\varepsilon + \varepsilon_\infty - \nu p_\infty}{c_v} \right) \Big|_s \\ &= -\frac{\nu}{c_v T} \left(\frac{\partial \varepsilon}{\partial \nu} \Big|_s - p_\infty \right) \\ &= -\frac{\nu}{c_v T} (-p - p_\infty) \\ &= \frac{p + p_\infty}{c_v T \rho} \end{aligned}$$

(h) In order to have a real sound speed, p is bounded by $-p_\infty$ i.e. $p + p_\infty > 0$. Also, density, temperature and c_V are always non-negative. Hence, the minimum value of Γ is 0.

8 Appendix

8.1 Ideas of KBN and LPFS method



1. Spatial stabilisation by considering extending influence to $\alpha_2 \Delta x$ instead of Δx (chosen to give stable Δt):

$$F'_{i-1/2} - F_b = \frac{\alpha}{\alpha_2}(F_{i-1/2} - F_b)$$

   KBN method.

2. Temporal stabilisation (LPFS)?:

$$F''_{i-1/2} = \left(1 - \frac{\alpha}{\alpha_2}\right) F'_{i-1/2} + \frac{\alpha}{\alpha_2} F_{i-1/2}$$

$$F''_{i-1/2} - F'_{i-1/2} = \frac{\alpha}{\alpha_2}(F_{i-1/2} - F'_{i-1/2})$$

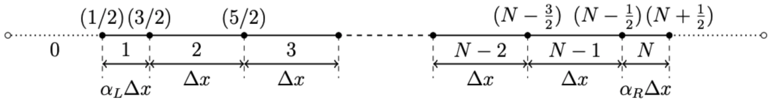
   For the fraction $\frac{\alpha}{\alpha_2}$ of the time step, no flux stabilisation is necessary. So we can do a linear combination of stabilised and unstabilised flux. The ultimate aim is to reduce diffusion of numerical solution.

3. Overall:

$$F^{LPFS}_{i-1/2} = f_b + \frac{\alpha}{\alpha_2}\left(2 - \frac{\alpha}{\alpha_2}\right)(f_{i-1/2} - f_b)$$

   where $\alpha_2 = \frac{a\Delta x}{\Delta t}$.

8.2 Derivation of Update Formulas under LPFS



General Flux update: $U_i^{n+1} = U_i^n - \frac{\Delta t}{\Delta x}\left(f_{i+1/2}^n - f_{i-1/2}^n\right)$

General LPFS Flux: $F_{i-1/2}^{LPFS} = f_b + \frac{\alpha}{\alpha_2}\left(2 - \frac{\alpha}{\alpha_2}\right)(f_{i-1/2} - f_b)$

Note: for linear advection: $\alpha_2 = 1$ and $f_{i+1/2}^n = f(U_i^n) = aU_i^n$ for backward difference. The stabilised flux are $f_{3/2}^{LPFS}$ and $f_{N-1/2}^{LPFS}$, which affects cells 1, 2, N-1 and N.

$$F_{N-1/2}^{LPFS} = f_{N+1/2} + \alpha_R(2-\alpha_R)(f_{N-1/2} - f_{N+1/2})$$

$$F_{3/2}^{LPFS} = f_{1/2} + \alpha_L(2-\alpha_L)(f_{3/2} - f_{1/2})$$

Cell N:

$$\begin{aligned}
U_N^{n+1} &= U_N^n - \frac{\Delta t}{\alpha_R\Delta x}\left(f_{N+1/2} - F_{N-1/2}^{LPFS}\right)\\
&= U_N^n - \frac{\Delta t}{\cancel{\alpha_R}\Delta x}\left(-\cancel{\alpha_R}(2-\alpha_R)\left(f_{N-1/2} - f_{N+1/2}\right)\right)\\
&= U_N^n + c(2-\alpha_R)(U_{N-1}^n - U_N^n)
\end{aligned}$$

Cell N-1:

$$\begin{aligned}
U_{N-1}^{n+1} &= U_{N-1}^n - \frac{\Delta t}{\Delta x}\left(F_{N-1/2}^{LPFS} - f_{N-3/2}\right)\\
&= U_{N-1}^n - \frac{\Delta t}{\Delta x}\left(f_{N+1/2} + \alpha_R(2-\alpha_R)(f_{N-1/2} - f_{N+1/2}) - f_{N-3/2}\right)\\
&= U_{N-1}^n - c[U_N^n + \alpha_R(2-\alpha_R)(U_{N-1} - U_N^n) - U_{N-2}^n]\\
&= U_{N-1}^n + c[U_{N-2}^n - \alpha_R(2-\alpha_R)(U_{N-1}^n - U_N^n) - U_N^n]\\
&= U_{N-1}^n + c[U_{N-2}^n - \alpha_R(2-\alpha_R)U_{N-1}^n - (\alpha_R^2 - 2\alpha_R + 1)U_N^n]\\
&= U_{N-1}^n + c[U_{N-2}^n - \alpha_R(2-\alpha_R)U_{N-1}^n - (\alpha_R^2 - 1)^2U_N^n]
\end{aligned}$$

Cell 1:

$$\begin{aligned}
U_1^{n+1} &= U_1^n - \frac{\Delta t}{\alpha_L\Delta x}\left(F_{3/2}^{LPFS} - f_{1/2}\right)\\
&= U_i^n - \frac{\Delta t}{\cancel{\alpha_L}\Delta x}(\cancel{\alpha_L}(2-\alpha_L)(f_{3/2} - f_{1/2}))\\
&= U_i^n + c(2-\alpha_L)(U_0^n - U_1^n)
\end{aligned}$$

Likewise for Cell 2 by substitution.

8.3 Derivation Relating to Gruneisen coefficient

Derivation:

$$\Gamma = -\frac{\nu}{T}\frac{\partial T}{\partial \nu}\Big|_s = \nu \frac{\partial p}{\partial \varepsilon}\Big|_\nu$$

How do we link them? They have different independent variables, (s, ν) and (ε, ν).

$$\frac{\partial T}{\partial \nu}\Big|_s \quad \leftrightarrow \quad \frac{\partial p}{\partial \varepsilon}\Big|_\nu$$

Consider,

$$d\varepsilon(s,\nu) = Tds - pd\nu \quad , \quad Tds(\varepsilon,\nu) = pd\nu + d\varepsilon$$

We see that the LHS can be extracted using Maxwell's relations,

$$\frac{\partial T}{\partial \nu}\Big|_s = \frac{\partial^2 \varepsilon}{\partial s\, \partial \nu}$$

We attempt to extract the RHS by holding ε constant, we obtain:

$$p = T\frac{\partial s}{\partial \nu}\Big|_\varepsilon$$

Then, differentiate w.r.t. ε while **holding $\boldsymbol{\nu}$ constant**,

$$\frac{\partial p}{\partial \varepsilon}\Big|_\nu = T\frac{\partial^2 s}{\partial \varepsilon\, \partial \nu} + \frac{\partial T}{\partial \varepsilon}\Big|_\nu \frac{\partial s}{\partial \nu}\Big|_\varepsilon = T\frac{\partial^2 s}{\partial \varepsilon\, \partial \nu} + \cancel{\frac{\partial}{\partial \varepsilon}\left(\frac{\partial \varepsilon}{\partial s}\right)\Big|_\nu \frac{\partial s}{\partial \nu}\Big|_\varepsilon} = T\frac{\partial^2 s}{\partial \varepsilon\, \partial \nu}$$

where $T = \frac{\partial \varepsilon}{\partial s}\big|_\nu$ from $d\varepsilon = Tds$ at constant volume.

$$\begin{aligned}
\frac{\partial p}{\partial \varepsilon}\Big|_\nu &= T\frac{\partial}{\partial \nu}\left(\frac{\partial s}{\partial \varepsilon}\right) \\
&= T\frac{\partial}{\partial \nu}\left(\frac{\partial \varepsilon}{\partial s}\right)^{-1} \\
&= -T\left(\frac{\partial \varepsilon}{\partial s}\right)^{-2}\Big|_\nu \frac{\partial^2 \varepsilon}{\partial \nu\, \partial s} \\
&= -T\frac{1}{T^2} \times \frac{\partial T}{\partial \nu}\Big|_s \\
&= -\frac{1}{T}\frac{\partial T}{\partial \nu}\Big|_s
\end{aligned}$$

Note: make use of the symmetric property of mixed second-order partial derivatives.

$$\Gamma = -\frac{\nu}{T}\left(-T\frac{\partial p}{\partial \varepsilon}\Big|_\nu\right) = \nu\frac{\partial p}{\partial \varepsilon}\Big|_\nu$$

8.4 Derivation of Entropy of Ideal Gas

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

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

Find $s = s(p, \nu)$,

$$\begin{aligned} Tds &= d\varepsilon + pd\nu \\ &= \frac{pd\nu + \nu dp}{\gamma - 1} + pd\nu \\ \frac{p\nu}{c_V(\gamma - 1)} ds &= \left(\frac{p}{\gamma - 1} + p \right) d\nu + \frac{\nu}{\gamma - 1} dp \\ \frac{1}{c_V} ds &= \frac{\gamma}{\nu} d\nu + \frac{1}{p} dp \\ ds &= \frac{c_p}{\nu} d\nu + \frac{c_V}{p} dp \end{aligned}$$

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

Find $s = s(\varepsilon, \nu)$,

$$\begin{aligned} Tds &= d\varepsilon + pd\nu \\ \frac{\varepsilon}{c_V} ds &= d\varepsilon + (\gamma - 1)\rho\varepsilon d\nu \\ ds &= \frac{c_V}{\varepsilon} d\varepsilon + \frac{(\gamma - 1)c_V}{\nu} d\nu \\ ds &= \frac{c_V}{\varepsilon} d\varepsilon + \frac{R}{\nu} d\nu \end{aligned}$$

$$\Rightarrow s = c_V \ln \varepsilon + R \ln \nu + \text{const.}$$

8.5 Equation of States

Isentropes: lines of constant entropy.

$$d\varepsilon = -p d\nu \quad \text{and} \quad c_s = \sqrt{\left.\frac{\partial p}{\partial \rho}\right|_s}$$

- **Adiabatic index**: $p\nu^\gamma = \text{const.}$

$$\gamma_{adia} = -\frac{\nu}{p}\left.\frac{\partial p}{\partial \nu}\right|_s = -\left.\frac{\partial \ln p}{\partial \ln \nu}\right|_s$$

- **Gruneisen coefficient**:

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

- **Fundamental derivative**: curvature of isentrope $\sim \frac{\partial^2 \nu}{\partial p^2}$ in $p - \nu$ plane written in non-dimensional form.

$$\mathcal{G} = \frac{c^4}{2\nu^3}\left.\frac{\partial^2 \nu}{\partial p^2}\right|_s \quad \text{and} \quad c^2 = \left.\frac{\partial p}{\partial \rho}\right|_s = -\nu^2\left.\frac{\partial p}{\partial \nu}\right|_s$$

$$\begin{aligned}
\mathcal{G} &= \frac{c^4}{2\nu^3}\frac{\partial}{\partial p}\left(\frac{\partial \nu}{\partial p}\right)\Big|_s \\
&= \frac{c^4}{2\nu^3}\frac{\partial \nu}{\partial p}\frac{\partial}{\partial \nu}\left(\frac{\partial p}{\partial \nu}\right)^{-1}\Big|_s \\
&= \frac{c^4}{2\nu^3}\frac{\partial \nu}{\partial p}(-1)\left(\frac{\partial p}{\partial \nu}\right)^{-2}\left.\frac{\partial^2 p}{\partial \nu^2}\right|_s \\
&= \frac{c^4}{2\nu^3}\frac{\nu^2}{c^2}\frac{\nu^4}{c^4}\left.\frac{\partial^2 p}{\partial \nu^2}\right|_s \\
&= \frac{\nu^3}{2c^2}\left.\frac{\partial^2 p}{\partial \nu^2}\right|_s \\
&= \frac{\nu^2}{2\gamma p}\left.\frac{\partial^2 p}{\partial \nu^2}\right|_s = \frac{1}{2}\frac{\rho^2}{\gamma p}\frac{\partial c_s^2}{\partial \rho} = \frac{1}{2}\frac{\rho}{c_s}2c_s\frac{\partial c_s}{\partial \rho} = \rho\left.\frac{\partial c_s}{\partial \rho}\right|_s
\end{aligned}$$

If $\mathcal{G} > 0$, isentropes are convex, and we get:

1. Compressive, entropy-increasing shock waves.
2. Expansive rarefactions.

This means sound speed increases across shock waves and decreases across rarefactions.

1. **Ideal gas EoS**:
$$p = (\gamma - 1)\rho\varepsilon$$

2. **Stiffened gas EoS**: model high-pressure liquids (useful to deal with shock waves)
$$p = (\gamma - 1)\rho\varepsilon - \gamma p_\infty$$
If you have a reactive liquid *e.g. explosive liquids*, you include a reference energy to account for the heat of formation.
$$p = (\gamma - 1)\rho(\varepsilon - \varepsilon_\infty) - \gamma p_\infty$$

3. **Mie-Grüneisen EoS**: model high-pressure solids. Obtain EoS by integrating Gruineisen parameter, $\Gamma = \nu\frac{\partial p}{\partial \varepsilon}\big|_\nu$. It represents a family of models from which many EoS are derived.
$$p(\rho, \varepsilon) = \Gamma(\rho)\rho(\varepsilon - \varepsilon_{\text{ref}}(\rho)) + p_{\text{ref}}(\rho)$$
Usually we are given p_{ref} and we have to compute ε_{ref} by assuming a **reference curve**.
   (a) Along isentrope: integrate $d\varepsilon = -pd\nu$
   (b) Along isotherm:
   (c) Along shock locus: use the Hugoniot equation obtained after eliminating shock speed and velocity. It gives all the possible thermodynamic states behind the shock wave/discontinuity which satisfy the RH conditions.
   $$\varepsilon_2 - \varepsilon_1 = \frac{1}{2}(p_1 + p_2)(\nu_1 - \nu_2)$$
   For derivation, see 2018-19M Q2(c)(iii) Link

4. **JWL EoS**: model explosives, usually for the products of a detonation. It is a Mie-Grüneisen type EoS with constant Γ, and uses an **isentrope reference**. It has a region of validity.

5. **Hugoniot EoS**: model solids under shock. Any EoS that uses the **shock locus** as the reference curve for pressure. It represents the locus of all states which can be reached by shocking a material from a given initial state. It is popular because of linear relationship between shock velocity and particle velocity in many solids, $S \propto v_2 \Rightarrow S = c_0 + sv_2$, where c_0 is the bulk sound speed. ε_{ref} is obtained from Hugoniot equation, and derive p_{ref} from RH conditions using reference state $(\rho_0, 0, 0)^T$:

   For compression: i.e. $\rho \geq \rho_0$ so $\eta > 0$, we define:
   $$p = K_0\eta(1 + K_1\eta + K_2\eta^2 + K_3\eta^3 + ... + K_M\eta^M)$$
   From RH condition for mass:
   $$\rho v = S(\rho - \rho_0) \quad \Rightarrow \quad v = (c_0 + sv)\eta \quad \Rightarrow \quad v = \frac{c_0\eta}{1 - s\eta}$$

From RH condition for momentum:

$$\rho v^2 + p = S\rho v \quad \Rightarrow \quad p = (c_0 + sv)\rho v - \rho v^2 = \frac{\rho c_0 \eta}{1 - s\eta}\left(c_0 + \frac{s c_0 \eta}{1 - s\eta} - \frac{c_0 \eta}{1 - s\eta}\right)$$

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

Taylor expanding the denominator:

$$p_{\text{ref}} = \rho_0 c_0^2 \eta\left[1 + 2(s\eta) + 3(s\eta)^2 + 4(s\eta)^3 + ...\right]$$

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

So, $K_n = (n+1)s^n$ for $n \geq 1$.

For expansion i.e. $\rho < \rho_0$ so $\eta < 0$:

$$p_{\text{ref}} = K_0 \eta$$

$$\varepsilon_{\text{ref}} = \frac{K_0 \eta^2}{2\rho_0} + \varepsilon_0$$

6. **Tabulated EoS**:

8.6 Derivation of Thermodynamic Var. for Complete Stiffened Gas EoS

$$\begin{aligned} F(\nu, T) &= \underbrace{\varepsilon - Ts}_{F_{\text{ideal}}} + p_\infty \nu + \epsilon_\infty \\ &= \underbrace{(\varepsilon + \varepsilon_\infty + \nu p_\infty)}_{\substack{\text{identify as} \\ \text{modified U}}} - Ts \end{aligned}$$

From reference and proof, $(p + p_\infty)\nu = (\gamma - 1)c_v T$ and we know: $p = (\gamma - 1)\rho(\varepsilon - \varepsilon_\infty) - \gamma p_\infty$.

$$\begin{aligned} \cancel{(\gamma - 1)} c_V T &= \nu[(\gamma - 1)\rho(\varepsilon - \varepsilon_\infty) - \gamma p_\infty + p_\infty] \\ &= \nu \cancel{(\gamma - 1)}(\rho(\varepsilon - \varepsilon_\infty) - p_\infty) \\ c_V T &= \varepsilon - \varepsilon_\infty - \nu p_\infty \end{aligned}$$

Hence,

$$T = \frac{\varepsilon - \varepsilon_\infty - \nu p_\infty}{c_v}$$

Consider,

$$ds = \frac{\partial s}{\partial \nu} d\nu + \frac{\partial s}{\partial T} dT \quad \text{and} \quad p = (\gamma - 1)\rho(\varepsilon - \varepsilon_\infty) - \gamma p_\infty$$

Also from Maxwell's relations:

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

Differentiate EoS w.r.t. T while keeping ν constant,

$$\left.\frac{\partial p}{\partial T}\right|_\nu = (\gamma - 1)\rho \frac{\partial \varepsilon}{\partial T} = (\gamma - 1)\rho c_v$$

Then,

$$\begin{aligned} ds &= \left.\frac{\partial p}{\partial T}\right|_\nu d\nu + \frac{c_v}{T} dT \\ &= (\gamma - 1)\rho c_v d\nu + \frac{c_v}{T} dT \\ \int_{s_0}^{s} ds &= (\gamma - 1)c_v \int_{\nu_0}^{\nu} \frac{1}{\nu} d\nu + c_v \int_{T_0}^{T} \frac{1}{T} dT \\ s - s_0 &= (\gamma - 1)c_v \ln\left(\frac{\nu}{\nu_0}\right) + c_v \ln\left(\frac{T}{T_0}\right) \\ s &= s_0 + c_v \left((\gamma - 1)\ln\left(\frac{\nu}{\nu_0}\right) + \ln\left(\frac{T}{T_0}\right)\right) \end{aligned}$$

$$s = s_0 + c_v \ln\left(\frac{\frac{T}{\nu}\nu^\gamma}{\frac{T_0}{\nu_0}\nu_0^\gamma}\right)$$

$$s = s_0 + c_v \ln\left(\frac{(p + p_\infty)\nu^\gamma}{(p_0 + p_\infty)\nu_0^\gamma}\right)$$

8.7 Derivations of Sound Speeds

1. Stiffened Gas:

$$p = (\gamma - 1)\rho\varepsilon - \gamma p_\infty \quad \Rightarrow \quad \varepsilon = \frac{p + \gamma p_\infty}{(\gamma - 1)\rho}$$

$$c_s^2 = \frac{p}{\rho^2 \frac{\partial \varepsilon}{\partial p}} - \frac{\frac{\partial \varepsilon}{\partial \rho}}{\frac{\partial \varepsilon}{\partial p}}$$

$$\frac{\partial \varepsilon}{\partial p} = \frac{1}{(\gamma - 1)\rho} \quad \text{and} \quad \frac{\partial \varepsilon}{\partial \rho} = -\frac{p + \gamma p_\infty}{(\gamma - 1)\rho^2}$$

$$\begin{aligned}[c_s^2 &= \rho(\gamma - 1)\left[\frac{p}{\rho^2} + \frac{p + \gamma p_\infty}{(\gamma - 1)\rho^2}\right] \\ &= \rho(\gamma - 1)\frac{\gamma(p + p_\infty)}{\rho^2(\gamma - 1)} \\ &= \frac{\gamma(p + p_\infty)}{\rho}\end{aligned}$$

8.8 Recommended Papers to Read

1. **Divergence cleaning**: Dedner, A. et al. Hyperbolic Divergence Cleaning for the MHD Equations. Journal of Computational Physics 175, 645–673 (2002). Link
2. **LPFS Flux**: Gokhale, N., Nikiforakis, N. & Klein, R. A dimensionally split Cartesian cut cell method for hyperbolic conservation laws. Journal of Computational Physics 364, 186–208 (2018). Link
3. **Fundamental Derivative**: Thompson, P. A. A Fundamental Derivative in Gasdynamics. The Physics of Fluids 14, 1843–1849 (1971). Link
4. **Hugoniot Equation of State**: 1. Robinson, A. C. The Mie-Gruneisen Power Equation of State. https://www.osti.gov/biblio/1762624 (2019) doi:10.2172/1762624. Link
5. **HLLC Solver for Magnetohydrodynamics**: Li, S. An HLLC Riemann solver for magneto-hydrodynamics. Journal of Computational Physics 203, 344–357 (2005). Link