A KINETIC REINTERPRETATION OF THERMODYNAMIC RESTRICTIONS OF CONTINUA

We aim to give a kinematic interpretation of the theory of thermodynamic continua developed by PROF. RAJAGOPAL and collaborators. Our starting point will be the BOLTZMAN EQUATION, i.e.

$$\underbrace{\partial_t f + \underline{v}\cdot\nabla_x f}_{\text{ADVECTION}} = \underbrace{Q[f,f]}_{\text{COLLISION}}$$

where $f(\underline{x},\underline{v},t)$ is the one-particle distribution function i.e. the probability density of finding one particle of an ensamble at the position $(\underline{x},\underline{v})$ of the phase space at instant t. Furthermore the collision operator $Q[f,f]$ is defined as

$$Q[f,f] := \int_{\mathbb{R}^3} dv_* \int_{\mathbb{S}^2} d\theta\, d\varphi\, \overbrace{B(\theta,\varphi,|\underline{v}-v_*|)}^{\text{COLLISIONAL KERNEL}} \left[f(\underline{x},\underline{v}',t)\, f(\underline{x},v'_*,t) - f(x,v,t)\, f(x,v_*,t) \right]$$

where v' and v'_* are the post collisional velocities, which we assume can be computed from v and v_* by means of a binary low, i.e. $\underline{v}' = \underline{v}'(v,v_*)$ $\quad \underline{v}'_* = \underline{v}'_*(v,v_*)$.

For the moment being we will consider the BGK approximation of $Q[f,f]$, i.e. $Q[f,f] \simeq -\frac{1}{\tau}(f - f^{(0)})$

COLLISIONAL FREQUENCY $\longrightarrow$

where $f^{(0)}$ is the MAXWELLIAN DISTRIBUTION defined as,

$$f^{(0)}(\underline{x},\underline{v},t) = \frac{\rho(\underline{x},t)}{(2\pi R\theta)^{3/2}} \exp\left(-|\underline{v}-\underline{u}(\underline{x},t)|^2 / 2R\theta\right)$$

$$= \frac{\rho(\underline{x},t)}{\left(\frac{4}{3}\pi e(\underline{x},t)\right)^{3/2}} \exp\left(-\frac{|\underline{v}-u(\underline{x},t)|^2}{\frac{4}{3}e}\right)$$

EQUIPARTITION OF ENERGY THEOREM $e = \frac{3}{2}R\theta$ $\longrightarrow$ $=$

$\frac{2}{3}e = R\theta$

where $\rho(\underline{x},t)$, $\underline{u}(\underline{x},t)$ and $e(\underline{x},t)$ are respectively the density, the macroscopic velocity and internal energy defined as,

$$\rho(\underline{x},t) = m\, n(\underline{x},t) := m \int_{\mathbb{R}^d} f(\underline{x},\underline{v},t)\, d\underline{v}$$

$$u(\underline{x},t) = \frac{1}{n(\underline{x},t)} \int_{\mathbb{R}^d} \underline{v}\, f(\underline{x},\underline{v},t)\, d\underline{v}$$

$$e(\underline{x},t) = \frac{1}{n(\underline{x},t)}\, \frac{1}{2} \int_{\mathbb{R}^d} \underline{w}\cdot\underline{w}\, f(\underline{x},\underline{v},t)\, d\underline{v}\,, \text{ with } \underline{w} := \underline{v} - \underline{u}\,.$$

An other macroscopic quantity that will be of primal importance even if not involved in the definition of $f^{(0)}$ is the ENTROPY, i.e.

$$\eta(\underline{x},t) = \frac{1}{n(\underline{x},t)} \int_{\mathbb{R}^d} f(\underline{x},\underline{v},t) \log[f(\underline{x},\underline{v},t)]\, d\underline{v}$$

Thus the BGK operator is constructed in such a way to conserve the density, linear momentum and energy of f. Furthermore as we will see later it is constructed to mimic another property of $Q[f,f]$, i.e. the relaxation to the Maxwellian $f^{(0)}$.

BALANCE LAWS Testing the Boltzmann equation with the 3 (5 scalars) collision invariants, at the level of the binary interactions, we thus obtain:

$$\int_{\mathbb{R}^3} \psi(\underline{v})\, Q[f,f] = \int_{\mathbb{R}} \psi(\underline{v})\, Q_{BGK}[f,f] = 0 \quad \forall \psi \in \{m, vm, \tfrac{1}{2}m|v|^2\}.$$

This gives us 3 different balance laws, i.e.

$\psi = m)$ $\quad \partial_t \rho + \nabla_x \cdot (\rho \underline{u}) = 0$ CONTINUITY EQUATION / BALANCE LAW OF MASS

$\psi = m\underline{v})$ $\quad \rho[\partial_t \underline{u} + (\nabla u)\underline{u}] + \nabla_x \cdot \mathbb{T} = 0$ BALANCE LAW OF LINEAR MOMENTUM where $\Pi(\underline{x},t) = \int_{\mathbb{R}^3} m\, \underline{w} \otimes \underline{w}\, f(\underline{x},\underline{v},t)$ is the Cauchy stress tensor.

$\psi = \frac{1}{2} m |\underline{v}|^2$) $\partial_t \left(\frac{1}{2}\rho|\underline{u}|^2 + \rho e\right) + \nabla_x \cdot \left(\frac{1}{2}\rho |u|^2 \underline{u} + \rho e \underline{u} + \Pi u + Q\right) = 0$

This is the BALANCE LAW OF TOTAL ENERGY, where we have defined the HEAT FLUX VECTOR as,

$$Q(\underline{x},t) := \int_{\mathbb{R}^3} \frac{1}{2} m\, |\underline{w}|^2\, \underline{w}\, f(\underline{x},\underline{v},t)\, d\underline{v}.$$

This also implies the BALANCE LAW OF INTERNAL ENERGY, i.e.

$$\rho(\partial_t e + \nabla_x e \cdot \underline{u}) + \Pi : \nabla_x u + \nabla_x \cdot Q = 0.$$

Similarly testing by $\varphi(\underline{x},\underline{v},t) = \log(f(\underline{x},\underline{v},t))$ we can obtain an evolution equation for the ENTROPY, i.e.

$$\rho(\partial_t \eta + \nabla_x \eta \cdot \underline{u}) + \nabla_x \cdot \Phi = \zeta \quad (*)$$ where

$\Phi(\underline{x},t) = \int_{\mathbb{R}^3} w \log(f) f \, d\underline{v}$ ENTROPY FLUX

$\zeta(\underline{x},t) = \int_{\mathbb{R}^3} \frac{1}{2}(f^{(0)} - f) \log(f)\, d\underline{v}$ ENTROPY PRODUCTION

THERMODYNAMICS A key aspect of the Boltzmann equation is the so called Boltzmann inequality. Let us consider

$$\int d\underline{v}\, \frac{1}{2}(f^{(0)} - f)\log(f)\, d\underline{v} = \int dv\, \frac{1}{2}(f^{(0)} - f)\log(f) - \int dv\, \frac{1}{2}(f^{(0)} - f)\log(f^{(0)}) + \underbrace{\int dv\, \frac{1}{2}(f^{(0)} - f)\log(f^{(0)})}_{\text{VANISH}}$$

$$= \int dv\, \frac{1}{2}(f^{(0)} - f)\left(\log(f) - \log(f^{(0)})\right) \leq 0$$

This implies that the ENTROPY PRODUCTION is always NEGATIVE, which is a form of the second law of thermodynamics. We can also obtain an other form of the II law of thermodynamics, introducing

$H(t) := \int_{\Omega} \eta(x,t)\, dx$ where Ω is the volume occupied by the system of particles under consideration.

Integrating $(*)$ we thus get

$$\frac{dH}{dt} \le \underbrace{\int_{\partial\Omega} \underline{n} \cdot \underline{\Phi}}$$

This term vanish when the system is termodynamically isolated and thus we are left with the constant decrease of entropy $\frac{dH}{dt} \le 0$.

In particular we observe that $\frac{dH}{dt} = 0 \iff f = f^{(0)}$ since obviously when $f = f^{(0)}$, $\mathfrak{z} \equiv 0$. Suggesting that a system at thermodynamic isolation reaches equilibrium after enough time thus thermalising to a Maxwellian $f^{(0)}$.

Since we know that at thermodynamic equilibrium $f \searrow f^{(0)}$ we might think that near thermodynamic equilibrium f must be a perturbation around $f^{(0)}$.

This idea is formolised by the CHAPMAN-ENSKOG EXPANSION where we assume that $f = \sum_{k=0}^{\infty} (K_n)^k f^{(k)}$ with

$$K_n := \frac{\overset{\text{MEAN FREE PATH}}{\lambda}}{\underset{\text{CHARACHTERISTIC MACROSCOPIC LENGTH.}}{L}}$$

being the KNUDSEN NUMBER.

Using the relation between the thermal speed $v_T := \sqrt{2R\Theta}$, the mean free path λ and the collision frequency one has

$$\boxed{\lambda = v_\Theta z} \Rightarrow \boxed{K_n = \frac{v_\Theta z}{L}} \Rightarrow \boxed{z = \frac{K_n L}{v_T}} \Rightarrow \mathfrak{z} \sim \Theta\left(\frac{1}{K_n}\right).$$

ZEROTH - ORDER CHAPMAN - ENSKOG

We begin assuming that we are sufficently close to the equilibrium that $f \simeq f^{(0)}$. Thus we proceed deriving an equation of state, i.e.

$$\rho\eta^{(0)} = \int dv \log(f^{(0)})\, f^{(0)} = \frac{3}{2}\log\left(\frac{2}{3}e(\underset{\sim}{x},t)\rho(\underset{\sim}{x},t)^{-2/3}\right)\rho$$

thus implying that, $\eta^{(0)}(\underset{\sim}{x},t) = \frac{3}{2}\log\left(\frac{2}{3}e(\underset{\sim}{x},t)\rho(\underset{\sim}{x},t)^{-2/3}\right)$ and also by inverting this relation that,

$$e^{(0)}(\underset{\sim}{x},t) = \frac{3}{2}\exp\left(\frac{2}{3}\eta^{(0)}(\underset{\sim}{x},t)\right)\rho(\underset{\sim}{x},t)^{2/3} = e^{(0)}(\eta,\rho).$$

We now use the BALANCE LAW OF INTERNAL ENERGY, and the one for the ENTROPY to obtain the following:

$$\frac{d}{dt}e = \underbrace{\frac{\partial e}{\partial\rho}}\frac{d\rho}{dt} + \overbrace{\frac{\partial e}{\partial\eta}}\frac{d\eta}{dt}$$

By the thermodynamic definition of temperature $\frac{\partial e}{\partial\eta} = \Theta$

By the thermodynamic definition of pressure, $\hat{p} = \rho^2\frac{\partial e}{\partial\eta}$

thus we have that, $\frac{d\eta}{dt} = \frac{1}{\Theta}\left[\frac{de}{dt} - \hat{p}/\rho^2\,\overset{-\rho\nabla\cdot u}{\overbrace{\frac{d\rho}{dt}}}\right].$

Hence we have, $\frac{d\eta}{dt} = \frac{1}{\theta}\left[-\frac{1}{\rho}(\Pi:\nabla_x u + \nabla_x\cdot Q) + \hat{p}/\rho\,\nabla\cdot u\right]$

$$\begin{array}{l}\rho\dfrac{d\eta^{(0)}}{dt} = \dfrac{1}{\theta}\left[\hat{p}(\nabla\cdot u) - \Pi:\nabla_x u - \nabla_x\cdot Q\right]\\ \quad\| \\ \nabla_x\cdot\Phi^{(0)} - \zeta^{(0)} \quad\Rightarrow\quad \Theta(\nabla_x\cdot\Phi - \zeta) = \left[\hat{p}(\nabla\cdot u) - \Pi:\nabla_x u - \nabla_x\cdot Q\right]\end{array}$$

We now compute $\zeta^{(0)}$ and $\Phi^{(0)}$, notice that $\zeta^{(0)}$ is trivially zero and that we can compute

$$\underline{\Phi}^{(0)}(\underline{x},t) = +\int w \underbrace{\log(f^{(0)})} f^{(0)}\, d\underline{w}$$

$$\hookrightarrow \log(n(x,t)) + \log(C(x,t)) - \frac{|\underline{w}|^2}{\cancel{\text{[illegible]}}}\frac{3}{4}e^{-1}$$

$$\underline{\Phi}^{(0)}(\underline{x},t) = \underbrace{\int \underline{w} \log(n(x,t)) f^{(0)} dw}_{\overset{\shortparallel}{0}} + \underbrace{\int \underline{w} \log(c(x,t)) f^{(0)}}_{\overset{\shortparallel}{0}}$$

$$+ \int \underline{w}\, |\underline{w}|^2 \frac{3}{4} e^{-1} f^{(0)}\, d\underline{w} = Q/_{4/3}\, e$$

Notice now that $Q^{(0)} = \int w\,|w|^2\, dw = 0$ because the skewness of a Gaussian is zero. Thus we are left with the constraint,

$$\hat{p}\,(\nabla \cdot u) - \Pi : \nabla_x u = 0$$

$$\underline{\underline{I}}\,\hat{p} = \underline{\underline{\Pi}},$$ since this must be valid $\forall\, u$.

REMARK

FIRST ORDER CHAPMAN-ENSKOG

We will now assume that the Kn is sufficently small that we can write the truncated CHAPMAN-ENSKOG EXPANSION $f = f^{(0)} + (K_n) f^{(1)}$.

We thus introduce multiple time variables, i.e. $t_0 = t$ $t_1 = K_n t$ and treat f as a function of each time time scale, i.e. $f = f(\underline{x}, \underline{v}, t_0, t_1)$ and thus expanding the BOLTZMANN EQUATION we obtain,

$$(\partial_{t_0} + K_n \partial_{t_1})(f^{(0)} + K_n f^{(1)}) + \underline{v} \cdot \nabla_x (f^{(0)} + K_n f^{(1)}) = \frac{1}{\hat{\tau}} f^{(1)} \qquad (*)$$

where we have rescaled the collisional frequency by Kn. For this expansion to be unique we need to ask that the following solvability condition are satisfied,

$$\int d\underline{v}\, f^{(1)} = 0, \quad \int dv\, \underline{w} f^{(1)} = 0, \quad \int dv \tfrac{1}{2} |\underline{w}|^2 f^{(1)} = 0.$$

Collecting the zero-th order term in Kn in (*) we obtain,

$$f^{(1)} = (\partial_{t_0} f^{(0)} + \underline{v} \cdot \nabla_x f^{(0)}).$$

Which we can compute explicetly to be,

$$f^{(1)}_{BGK} = -\hat{\tau} f^{(0)} \left[\frac{m}{\frac{2}{3} e} (\underline{w} \otimes \underline{w}) : \mathbb{S} + \left(\frac{m\, \underline{w} \cdot \underline{w}}{2/3\, e} - \frac{5}{2} \right)^2 \underline{w} \cdot \frac{\nabla e}{e} \right]$$

where $\mathbb{S} = \frac{1}{2}(\nabla u + \nabla u^T) - \frac{1}{3}(\nabla \cdot u) \underline{\underline{\mathbb{I}}}$.

Notice that we now want to compute an equation of state similarly to before and we do so as follows,

We notice that $\log(1+x) = x + \mathcal{O}(x^2)$ thus if $x = K_n \frac{f^{(1)}}{f^{(0)}}$ we have that $K_n \ll 1$ implies $\log\left(\frac{f^{(0)} + K_n f^{(1)}}{f^{(0)}}\right) = K_n \frac{f^{(1)}}{f^{(0)}}$ and thus $\log(f^{(0)} + K_n f^{(1)}) = K_n f^{(1)}/f^{(0)} + \log(f^{(0)})$.

Thus we can write,

$$\rho\eta^{(1)} = \int (f^{(0)} + \mathrm{Kn} f^{(1)}) \log (f^{(0)} + \mathrm{Kn} f^{(1)})\, d\underline{v}$$

$$= \int (f^{(0)} + \mathrm{Kn} f^{(1)}) \left(\log (f^{(0)}) + \mathrm{Kn}\, f^{(1)}/f^{(0)}\right) d\underline{v}$$

$$= \eta^{(0)} + \mathrm{Kn} \int f^{(1)} \underbrace{(\log (f^{(0)}) + 1)}_{\text{VANISH BY SOLVABILITY CONDITION.}} + \mathcal{O}(\mathrm{Kn}^2)$$

$$= \eta^{(0)} + \mathcal{O}(\mathrm{Kn}^2).$$

$$= \frac{3}{2} \log \left(\frac{2}{3}\, e(\underline{x},t)\, \rho(\underline{x},t)^{-2/3} \right) \Rightarrow e = e(\eta, \rho).$$

$$\Phi^{(1)} = \int w \log (f^{(0)} + \mathrm{Kn} f^{(1)}) (f^{(0)} + \mathrm{Kn} f^{(1)})\, dv$$

$$= \underset{\substack{\vert\vert\vert \\ 0}}{\Phi^{(0)}} + \underbrace{\mathrm{Kn} \int w \log (f^{(0)}) f^{(1)}\, dv}_{Q^{(1)}/\frac{4}{3}e} + \mathcal{O}(\mathrm{Kn}^2)$$

Lastly we notice that,

$$\zeta^{(1)} = \int dv \log (f^{(0)} + \mathrm{Kn} f^{(1)}) \frac{1}{2} (f^{(0)} - f^{(0)} - \mathrm{Kn} f^{(1)})$$

$$= -\frac{\mathrm{Kn}}{2} \int d\underline{v} \left[\log (f^{(0)}) + \mathrm{Kn}\, f^{(1)}/f^{(0)}\right] f^{(1)}$$

$$= -\frac{\mathrm{Kn}^2}{2} \int d\underline{v}\; f^{(1)} \cdot f^{(1)}/f^{(0)} = 2\nu\, \mathbb{S} : \mathbb{S} + \overset{\overset{k = k(e)}{\downarrow}}{k} \frac{\nabla e \cdot \nabla e}{e}$$

Thus we are left with the fact that $\mathrm{Kn} \searrow 0$ is equivalent to maximising $|\zeta|$ subject to $2\nu\, \mathbb{S}:\mathbb{S} + k \frac{\nabla e \cdot \nabla e}{e} = -\nabla u : \Pi + \hat{p}\, \nabla \cdot u - Q \cdot \nabla e/e$ hence $\hat{p} = \frac{1}{2} \mathrm{tr}(\nabla u)$, $\mathrm{dev}(\sigma) = \mathbb{S}$ and $Q = k \nabla e$.