Objectives

1. Derivation of mass, momentum and energy conservation using Boltzmann's equation.

Rewritting again for the Boltzmann's Equation, we get:

$$\frac{\partial f_j}{\partial t}+\mathbf{v_j}\cdot\nabla_{\mathbf{r}} f_j+\frac{\mathbf{F_j}}{m_j}\cdot\nabla_{\mathbf{v_j}} f_j = 2\pi\sum_i\int_{-\infty}^{\infty}\int_0^{\infty}\left(f_i' f_j' - f_i f_j\right) v_r b db d\mathbf{v_i} \tag{1}$$

Consider a property of a particle ϕ_j. ϕ_j can be either m_j, $m_j\mathbf{v_j}$ or $\frac{mv_j^2}{2}$. Let us first multiply both sides of this equation by ϕ_j and then integrate with respective to $\mathbf{v_j}$ and then sum over all j. For right hand side, we have:

$$2\pi\sum_j\sum_i\int_{-\infty}^{\infty}\int_{-\infty}^{\infty}\int_0^{\infty}\phi_j(f_i' f_j' - f_i f_j) v_r b db d\mathbf{v_i} d\mathbf{v_j}$$

By inspection, we can know that:

$$\int_{-\infty}^{\infty}\int_{-\infty}^{\infty}\int_{0}^{\infty} \phi_j(f_i'f_j' - f_if_j)v_r bdbd\mathbf{v_i}d\mathbf{v_j}$$

$$= -\int_{-\infty}^{\infty}\int_{-\infty}^{\infty}\int_{0}^{\infty} \phi_j'(f_i'f_j' - f_if_j)v_r bdbd\mathbf{v_i}d\mathbf{v_j}$$

$$= \frac{1}{2}\int_{-\infty}^{\infty}\int_{-\infty}^{\infty}\int_{0}^{\infty} (\phi_j - \phi_j')(f_i'f_j' - f_if_j)v_r bdbd\mathbf{v_i}d\mathbf{v_j}$$

$$\sum_i\sum_j\int_{-\infty}^{\infty}\int_{-\infty}^{\infty}\int_{0}^{\infty} (\phi_j - \phi_j')(f_i'f_j' - f_if_j)v_r bdbd\mathbf{v_i}d\mathbf{v_j}$$

The double sum operators allow us to exchange the indices i and j, and thus allowing us to write:

$$\sum_i\sum_j\int_{-\infty}^{\infty}\int_{-\infty}^{\infty}\int_{0}^{\infty} (\phi_j - \phi_j')(f_i'f_j' - f_if_j)v_r bdbd\mathbf{v_i}d\mathbf{v_j}$$

$$= \sum_i\sum_j\int_{-\infty}^{\infty}\int_{-\infty}^{\infty}\int_{0}^{\infty} (\phi_i - \phi_i')(f_i'f_j' - f_if_j)v_r bdbd\mathbf{v_i}d\mathbf{v_j}$$

$$\sum_i \sum_j \int_{-\infty}^{\infty} \int_{-\infty}^{\infty} \int_0^{\infty} \phi_j (f_i' f_j' - f_i f_j) v_r b db d\mathbf{v_i} d\mathbf{v_j}$$

$$= \frac{1}{4} \sum_i \sum_j \int_{-\infty}^{\infty} \int_{-\infty}^{\infty} \int_0^{\infty} (\phi_j + \phi_i - \phi_j' - \phi_i')(f_i' f_j' - f_i f_j) v_r b db d\mathbf{v_i} d\mathbf{v_j}$$

$$= 0$$

This is because $\phi_j + \phi_i - \phi_j' - \phi_i' = 0$. Before any more derivation, bear in mind that:

$$\mathbf{v_0} = \frac{\sum_j \rho_j m_j \langle \mathbf{v_j} \rangle}{\sum_j \rho_j m_j} \tag{2}$$

which means:

$$\rho_m \mathbf{v_0} = \sum_j \rho_j m_j \langle \mathbf{v_j} \rangle$$

$\rho_m = \sum_j \rho_j m_j$.

For the left hand side, if we neglect the force term, we have:

$$\sum_j \int_{-\infty}^{\infty} \phi_j \frac{\partial f_j}{\partial t} d\mathbf{v_j} + \sum_j \int_{-\infty}^{\infty} \phi_j \mathbf{v_j} \cdot \nabla_{\mathbf{r}} f_j d\mathbf{v_j}$$

Bear in mind that ϕ_j is a function of the coordinate $\mathbf{v_j}$, which is independent of $\mathbf{r}$ and t. Therefore, we can write:

$$\sum_j \int_{-\infty}^{\infty} \frac{\partial}{\partial t}(\phi_j f_j) d\mathbf{v_j} + \sum_j \int_{-\infty}^{\infty} \nabla_{\mathbf{r}} \cdot (\mathbf{v_j} f_j \phi_j) d\mathbf{v_j}$$

Putting all these together, we have:

$$\sum_j \int_{-\infty}^{\infty} \frac{\partial}{\partial t}(\phi_j f_j) d\mathbf{v_j} + \sum_j \int_{-\infty}^{\infty} \nabla_{\mathbf{r}} \cdot (\mathbf{v_j} f_j \phi_j) d\mathbf{v_j} = 0$$

The easiest case is that when $\phi_j = m_j$.

$$\begin{aligned}
\frac{\partial}{\partial t}\sum_j m_j \int_{-\infty}^{\infty} f_j d\mathbf{v_j} + \nabla_{\mathbf{r}} \cdot \sum_j \int_{-\infty}^{\infty} m_j(\mathbf{v_j} f_j) d\mathbf{v_j} = 0 \\
\frac{\partial}{\partial t}\sum_j \rho_j m_j + \nabla_{\mathbf{r}} \cdot \sum_j \rho_j m_j \langle \mathbf{v_j} \rangle = 0 \\
\frac{\partial \rho_m}{\partial t} + \nabla_{\mathbf{r}} \cdot (\rho_m \mathbf{v_0}) = 0
\end{aligned}$$

If we have $\phi_j = m_j \mathbf{v_j}$. Let us neglect the summation operator.

$$\begin{aligned}
\int_{-\infty}^{\infty} m_j \mathbf{v_j} \frac{\partial f_j}{\partial t} d\mathbf{v_j} + \int_{-\infty}^{\infty} m_j \mathbf{v_j} \mathbf{v_j} \cdot \nabla_{\mathbf{r}} f_j d\mathbf{v_j} = 0 \\
\frac{\partial}{\partial t} m_j \int_{-\infty}^{\infty} \mathbf{v_j} f_j d\mathbf{v_j} + \nabla_{\mathbf{r}} \cdot m_j \int_{-\infty}^{\infty} \mathbf{v_j} \mathbf{v_j} f_j d\mathbf{v_j} = 0
\end{aligned}$$

Attention must be drawn to the second term:

$$\mathbf{v_j}\mathbf{v_j} = (\mathbf{v_j} - \mathbf{v_0})(\mathbf{v_j} - \mathbf{v_0}) + 2\mathbf{v_j}\mathbf{v_0} - \mathbf{v_0}\mathbf{v_0}$$

The pressure tensor is defined as:

$$\mathsf{P}_j = m_j \int_{-\infty}^{\infty} (\mathbf{v_j} - \mathbf{v_0})(\mathbf{v_j} - \mathbf{v_0}) f_j d\mathbf{v_j}$$

Then we get:

$$\frac{\partial}{\partial t}(\rho_j m_j \langle \mathbf{v_j} \rangle) + \nabla_{\mathbf{r}} \cdot \mathsf{P}_j + \nabla_{\mathbf{r}} \cdot 2\rho_j m_j \langle \mathbf{v_j} \rangle \mathbf{v_0} - \nabla_{\mathbf{r}} \cdot (\rho_j m_j \mathbf{v_0}\mathbf{v_0}) = 0$$

Sum over all j.

$$\frac{\partial}{\partial t}(\rho_m \mathbf{v_0}) + \nabla_{\mathbf{r}} \cdot \mathsf{P} + \nabla_{\mathbf{r}} \cdot 2\rho_m \mathbf{v_0}\mathbf{v_0} - \nabla_{\mathbf{r}} \cdot (\rho_m \mathbf{v_0}\mathbf{v_0}) = 0$$

$$\nabla_{\mathbf{r}} \cdot (\rho_m \mathbf{v_0} \mathbf{v_0}) = \frac{\partial}{\partial k} \rho_m v_{0,k} v_{0,l} = \rho_m v_{0,k} \frac{\partial}{\partial k} v_{0,l} + v_{0,l} \frac{\partial}{\partial k} \rho_m v_{0,k}$$
$$= \rho_m \mathbf{v_0} \cdot \nabla_{\mathbf{r}} \mathbf{v_0} + \mathbf{v_0} \nabla_{\mathbf{r}} \cdot (\rho_m \mathbf{v_0})$$

$$\mathbf{v_0} \left[\frac{\partial \rho_m}{\partial t} + \nabla_{\mathbf{r}} \cdot (\rho_m \mathbf{v_0}) \right] + \rho_m \left[\frac{\partial \mathbf{v_0}}{\partial t} + \mathbf{v_0} \cdot \nabla_{\mathbf{r}} \mathbf{v_0} \right] + \nabla_{\mathbf{r}} \cdot \mathsf{P} = 0$$
$$\rho_m \left[\frac{\partial \mathbf{v_0}}{\partial t} + \mathbf{v_0} \cdot \nabla_{\mathbf{r}} \mathbf{v_0} \right] + \nabla_{\mathbf{r}} \cdot \mathsf{P} = 0$$

Finally, to derive the energy balance equation, the property $\frac{1}{2}m_jv_j^2$ has to be considered. Without any integration and summation operator,

$$\frac{1}{2}m_jv_j^2\frac{\partial f_j}{\partial t}+\frac{1}{2}m_jv_j^2\mathbf{v_j}\cdot\nabla_{\mathbf{r}}f_j=0$$

which can be rewritten as:

$$\frac{\partial}{\partial t}\Big[\frac{1}{2}f_jm_j(v_j-v_0)^2+\frac{1}{2}f_jm_jv_0^2\Big]+\nabla_{\mathbf{r}}\cdot f_j\mathbf{v_j}\frac{1}{2}m_jv_j^2=0 \quad (3)$$

Looking at the second term:

$$v_j^2\mathbf{v_j}=(v_j-v_0)^2(\mathbf{v_j}-\mathbf{v_0})+(v_j-v_0)^2\mathbf{v_0}+2(\mathbf{v_j}\cdot\mathbf{v_0})\mathbf{v_j}-v_0^2\mathbf{v_j} \quad (4)$$

Tackle them one by one: We know that:

$$\mathbf{q_j}=\frac{m_j}{2}\int_{-\infty}^{\infty}(v_j-v_0)^2(\mathbf{v_j}-\mathbf{v_0})f_jd\mathbf{v_j}$$

$$\rho_j \mathbf{v_0} \tilde{E}_j = \frac{\mathbf{v_0}}{2} \int_{-\infty}^{\infty} (v_j - v_0)^2 f_j d\mathbf{v_j}$$

Then, after applying integration over all $\mathbf{v_j}$:

$$\frac{\partial}{\partial t}\left[\rho_j m_j \tilde{E}_j + \frac{\rho_j m_j v_0^2}{2}\right] + \nabla_{\mathbf{r}} \cdot \left[\mathbf{q_j} + \rho_j m_j \tilde{E}_j \mathbf{v_0} - \frac{1}{2}\rho_j m_j \langle \mathbf{v_j} \rangle v_0^2 \right.$$
$$\left. + m_j \int f_j (\mathbf{v_j} \cdot \mathbf{v_0}) \mathbf{v_j} d\mathbf{v_j}\right] = 0$$

That integral has to be taken care of. Thinking in terms of index notation:

$$\sum_{k=x,y,z} v_{0,k}(v_{j,k} - v_{0,k})(v_{j,l} - v_{0,l})$$
$$= v_{0,k}(v_{j,k}v_{j,l} - v_{j,k}v_{0,l} - v_{0,k}v_{j,l} + v_{0,k}v_{0,l})$$

This gives us that:

$$\mathbf{v_0} \cdot (\mathbf{v_j} - \mathbf{v_0})(\mathbf{v_j} - \mathbf{v_0}) = (\mathbf{v_j} \cdot \mathbf{v_0})\mathbf{v_j} - (\mathbf{v_j} \cdot \mathbf{v_0})\mathbf{v_0} - v_0^2 \mathbf{v_j} + v_0^2 \mathbf{v_0}$$

We obtain the relation:

$$(\mathbf{v_j} \cdot \mathbf{v_0})\mathbf{v_j} = (\mathbf{v_j} \cdot \mathbf{v_0})\mathbf{v_0} + \mathbf{v_0} \cdot (\mathbf{v_j} - \mathbf{v_0})(\mathbf{v_j} - \mathbf{v_0}) + v_0^2 \mathbf{v_j} - v_0^2 \mathbf{v_0} \tag{5}$$

$$m_j \left[\int f_j \mathbf{v_j} d\mathbf{v_j} \right] \cdot \mathbf{v_0}\mathbf{v_0} = \rho_j m_j \langle \mathbf{v_j} \rangle \cdot \mathbf{v_0}\mathbf{v_0}$$

$$\mathbf{v_0} \cdot m_j \int f_j (\mathbf{v_j} - \mathbf{v_0})(\mathbf{v_j} - \mathbf{v_0}) d\mathbf{v_j} = \mathbf{v_0} \cdot \mathsf{P}_j$$

$$m_j v_0^2 \int f_j \mathbf{v_j} d\mathbf{v_j} = \rho_j m_j \langle \mathbf{v_j} \rangle v_0^2$$

$$m_j v_0^2 \mathbf{v_0} \int f_j d\mathbf{v_j} = \rho_j m_j v_0^2 \mathbf{v_0}$$

Now sum over all these terms over j, we obtain:

$$\sum_j \left[\rho_j m_j \langle \mathbf{v_j} \rangle \cdot \mathbf{v_0 v_0} + \mathbf{v_0} \cdot \mathsf{P}_j + \rho_j m_j \langle \mathbf{v_j} \rangle v_0^2 - \rho_j m_j v_0^2 \mathbf{v_0}\right]$$
$$= \rho_m v_0^2 \mathbf{v_0} + \mathbf{v_0} \cdot \mathsf{P}$$

The entire equation becomes:

$$\frac{\partial \rho_m \tilde{E}}{\partial t} + \frac{1}{2}\frac{\partial \rho_m v_0^2}{\partial t} + \nabla_{\mathbf{r}} \cdot \left[\mathbf{q} + \rho_m \tilde{E} \mathbf{v_0} - \frac{\rho_m v_0^2}{2}\mathbf{v_0} + \rho_m v_0^2 \mathbf{v_0} + \mathbf{v_0} \cdot \mathsf{P}\right]$$
$$= 0$$

Look for mass balance relation and material derivative:

$$\tilde{E}\frac{\partial \rho_m}{\partial t} + \tilde{E}\nabla_{\mathbf{r}} \cdot (\rho_m \mathbf{v_0}) = 0$$

$$\rho_m \frac{\partial \tilde{E}}{\partial t} + \rho_m \mathbf{v_0} \cdot \nabla_{\mathbf{r}} \tilde{E} = \rho_m \frac{D\tilde{E}}{Dt}$$

$$\frac{1}{2}\left[v_0^2 \frac{\partial \rho_m}{\partial t} + v_0^2 \nabla_{\mathbf{r}} \cdot \rho_m \mathbf{v_0}\right] = 0$$

$$\rho_m \frac{D\tilde{E}}{Dt} + \frac{\rho_m}{2}\frac{\partial v_0^2}{\partial t} + \nabla_{\mathbf{r}} \cdot \mathbf{q} + \frac{\rho_m \mathbf{v_0}}{2} \cdot \nabla_{\mathbf{r}} v_0^2 + \nabla_{\mathbf{r}} \cdot \mathbf{v_0} \cdot \mathsf{P} = 0$$

$$\rho_m \frac{D\tilde{E}}{Dt} + \rho_m \mathbf{v_0} \cdot \frac{\partial \mathbf{v_0}}{\partial t} + \nabla_{\mathbf{r}} \cdot \mathbf{q} + \rho_m \mathbf{v_0}\mathbf{v_0} : \nabla_{\mathbf{r}} \mathbf{v_0} + \nabla_{\mathbf{r}} \cdot \mathbf{v_0} \cdot \mathsf{P} = 0$$

Multiply both sides of the momentum balance by $\mathbf{v_0}$.

$$\rho_m \mathbf{v_0} \cdot \frac{\partial \mathbf{v_0}}{\partial t} + \rho_m \mathbf{v_0}\mathbf{v_0} : \nabla_{\mathbf{r}} \mathbf{v_0} + \mathbf{v_0} \cdot \nabla_{\mathbf{r}} \cdot \mathsf{P} = 0$$

Then, we get:

$$\rho_m \frac{D\tilde{E}}{Dt} + \nabla_{\mathbf{r}} \cdot \mathbf{q} + \mathsf{P} : \nabla_{\mathbf{r}} \mathbf{v_0} = 0$$