# Homework #2

**Problem 1:** (a) Starting with

$$\hat{\mathbf{g}}(x,t) = \sum_{n=1}^{N} p_n(t)\,\delta^3(x - r_n(t)))$$

we get that

$$\partial_t \hat{\mathbf{g}}(x,t) = \sum_{n=1}^{N} \dot{p}_n(t)\,\delta^3(x - r_n(t)) \;\Big\}(\mathrm{I})$$

$$+ \sum_{n=1}^{N} p_n(t)\,(-\dot{r}_n(t)\cdot\nabla_x)\,\delta^3(x - r_n(t))\,)\Big\}(\mathrm{II})$$

by the product rule and the chain rule.

Since $\dot{r}_n(t) = p_n(t)/m$, the second term (II) becomes

$$(\mathrm{II}) = -\sum_{n=1}^{N} \frac{p_n(t)\,p_n(t)}{m}\cdot\nabla_x\,\delta^3(x - r_n(t))\,)$$

$$= -\nabla_x\cdot\left[\sum_{n=1}^{N} \frac{p_n(t)\,p_n(t)}{m}\,\delta^3(x - r_n(t))\,)\right]$$

Since $\dot{p}_n(t) = \sum_{m\neq n} F_{nm}$, the first term (I) becomes

$$(\mathrm{I}) = \sum_{\substack{n,m\\ n\neq m}} F_{n,m}\,\delta^3(x - r_n(t))\,).$$

By Newton's third law,

$$F_{n,m} = -F_{n,m}.$$

Thus, we may write by symmetrization

$$(I) = -\frac{1}{2} \sum_{\substack{n,m \\ n\neq m}} F_{n,m} \left[ \delta^3(x - r_m(t)) - \delta^3(x - r_n(t)) \right].$$

Note next by the fundamental theorem of calculus that

$$\delta^3(x - r_m) - \delta^3(x - r_n) = \int_0^1 ds \, \frac{d}{ds} \delta^3(x - r_n + s r_{nm})$$

w/ $r_{nm} = r_n - r_m$

$$= (r_{nm} \cdot \nabla_x) \int_0^1 ds \, \delta^3(x - r_n + s r_{nm})$$

by the chain rule.

Substituting gives

$$(I) = -\nabla_x \cdot \left[ \frac{1}{2} \sum_{\substack{n,m \\ n\neq m}} F_{n,m} r_{n,m} \int_0^1 ds \, \delta^3(x - r_n + s r_{nm}) \right].$$

Combining the two results gives $\partial_t j(x,t) + \nabla \cdot T(x,t) = 0$, with

$$\hat{T}(x,t) = \sum_{n=1}^{N} \frac{p_n(t) p_n(t)}{m} \delta^3(x - r_n(t)))$$

$$+ \frac{1}{2} \sum_{\substack{n,m \\ n\neq m}} F_{n,m} r_{nm} \int_0^1 ds \, \delta^3(x - r_n + s r_{nm}).$$

(b) We now make a similar argument for energy conservation, starting with

$$\hat{e}(x,t) = \sum_{n=1}^{N} \left( \frac{p_n^2(t)}{2m} + \frac{1}{2} \sum_{m \neq n} U(r_{nm}(t)) \right) \delta^3(x - r_n(t))$$

so that

$$\partial_t \hat{e}(x,t) = \left.\sum_{n=1}^{N} \frac{d}{dt} \left( \frac{p_n^2(t)}{2m} + \frac{1}{2} \sum_{m \neq n} U(r_{nm}(t)) \right) \delta^3(x - r_n(t)) \right\} (\text{II})$$

$$\left. + \sum_{n=1}^{N} \left( \frac{p_n^2}{2m} + \frac{1}{2} \sum_{m \neq n} U(r_{nm}(t)) \right) \frac{d}{dt} \delta^3(x - r_n(t)) \right\} (\text{I})$$

by the product rule.

For the term (I), we use as before that $\frac{d}{dt} \delta^3(x - r_n(t)) = -\frac{p_n(t)}{m} \cdot \nabla_x \delta^3(x - r_n(t))$, which gives

$$(\text{I}) = -\nabla_x \cdot \left[ \sum_{n=1}^{N} \left( \frac{p_n^2}{2m} + \frac{1}{2} \sum_{m \neq n} U(r_{nm}) \right) \frac{p_n}{m} \delta^3(x - r_n) \right].$$

The time-derivative of the second term (II) gives two contributions:

$$(\mathrm{II}) = \sum_{n=1}^{N} \frac{p_n(t)\cdot \dot{p}_n(t)}{m}\,\delta^3(x-r_n(t)) + \frac{1}{2}\sum_{\substack{n,m\\n\neq m}} \dot{r}_{nm}(t)\cdot \overbrace{\nabla U(r_{nm})}^{-F_{nm}}\,\delta^3(x-r_{nm}(t))$$

by the product & chain rule

$$= \sum_n \frac{p_n}{m}\Big(\sum_{m\neq n} F_{nm}\Big)\delta^3(x-r_n) - \frac{1}{2m}\sum_{\substack{n,m\\n\neq m}} (p_n - p_m)\cdot F_{nm}\,\delta^3(x-r_n)$$

by the equations of motion

$$= \sum_{\substack{n,m\\n\neq m}} \frac{1}{2m}(p_n + p_m)\cdot F_{nm}\,\delta^3(x-r_n) \qquad \text{by combining the terms}$$

$$= \sum_{\substack{n,m\\n\neq m}} \frac{1}{4m}(p_n+p_m)\cdot F_{n,m}\left[\delta^3(x-r_n) - \delta^3(x-r_m)\right] \qquad \text{using } F_{nm} = -F_{mn}$$

$$= -\nabla_x\cdot\left[\sum_{\substack{n,m\\n\neq m}} \frac{1}{4m}\Big((p_n+p_m)\cdot F_{nm}\Big) r_{nm}\int_0^1 ds\,\delta^3(x-r_n+s r_{nm})\right]$$

using the same identity for the difference of delta functions as before. Finally, we obtain $\partial_t \hat{e}(x,t) + \nabla\cdot\hat{s}(x,t) = 0$, with

$$\hat{s}(x,t) = \sum_{n=1}^{N}\Big(\frac{p_n^2}{2m} + \frac{1}{2}\sum_{m\neq n} U(r_{nm})\Big)\frac{p_n}{m}\,\delta^3(x-r_n)$$

$$+ \sum_{\substack{n,m\\n\neq m}} \frac{1}{4m}\Big((p_n+p_m)\cdot F_{nm}\Big) r_{nm}\int_0^1 ds\,\delta^3(x-r_n+s r_{nm})$$

Problem 2 (a) Multiplying the volume of the collision cylinder by the particle density gives the mean number of particles in the cylinder, which should be set equal to 1. This gives

$$1 = nV_{cyl} = n \times \pi d^2 \bar{v}\, \tau_{mf}$$

$$\Longrightarrow \quad \tau_{mf} = \frac{1}{n\pi d^2 \bar{v}} .$$

(b) Note that

$$v_{rel}^2 = \int d^3v \int d^3v' \, |\mathbf{v}-\mathbf{v}'|^2 \, p(\mathbf{v})\, p(\mathbf{v}')$$

$$= \int d^3v \int d^3v' \, (v^2 + v'^2 - 2\mathbf{v}\cdot\mathbf{v}')\, p(\mathbf{v})\, p(\mathbf{v}')$$

$$= 2\left(\int d^3v \, v^2 p(\mathbf{v})\right)\left(\cancelto{1}{\int d^3v' \, p(\mathbf{v}')}\right) - 2\left(\cancelto{0}{\int d^3v \, \mathbf{v}\, p(\mathbf{v})}\right)^2$$

$$= 2 v_{rms}^2 \quad \Longrightarrow \quad v_{rel} = \sqrt{2}\, v_{rms}$$

Thus,

$$\tau_{mf} = \frac{1}{n\pi d^2 v_{rel}} = \frac{1}{n\sqrt{2}\pi d^2 v_{rms}}$$

and

$$\lambda_{mf} = \tau_{mf} v_{rms} = \frac{1}{n\sqrt{2}\pi d^2}$$

(c) The number density is

$$n = \frac{P}{k_B T} = \frac{1.013 \times 10^{5}\ \mathrm{Pa}}{\left(1.38 \times 10^{-23}\ \frac{\mathrm{J}}{\mathrm{K}}\right)(300\,\mathrm{K})}$$

$$= 2.5 \times 10^{25}\ \mathrm{m}^{-3}$$

and the mean-free-path length

$$\lambda_{mf} = \frac{1}{\sqrt{2}\,\pi d^2 n}$$

$$= \frac{1}{\sqrt{2}\,\pi\,(3.1 \times 10^{-10}\,\mathrm{m})^2\,(2.5 \times 10^{25}\,\mathrm{m}^{-3})}$$

$$= 9.4 \times 10^{-8}\ \mathrm{m} \sim 98\ \mathrm{nm}$$

The ratio $\epsilon = \frac{R}{\lambda_{mf}}$ is calculated to be

$$\epsilon = \frac{1.55 \times 10^{-10}\ \mathrm{m}}{9.4 \times 10^{-8}\ \mathrm{m}} = 1.6 \times 10^{-3}.$$

Since $\epsilon \ll 1$, the Boltzmann equation is a reasonably accurate equation for the dynamics of air.

Problem 3. (a) We start with

$$\partial_t \rho + \nabla\cdot(\rho \mathbf{v}) = 0$$

$$\partial_t(\rho\mathbf{v}) + \nabla\cdot(\rho\mathbf{v}\mathbf{v} + \mathbf{T}^{(1)}) = -\nabla P.$$

The second equation may be written as

$$[\partial_t \rho + \nabla\cdot(\rho\mathbf{v})]\mathbf{v} + \rho(\partial_t + \mathbf{v}\cdot\nabla)\mathbf{v} + \nabla\cdot\mathbf{T}^{(1)} + \nabla P = 0$$

by the product rule. Thus, the first equation gives

$$\rho D_t \mathbf{v} = -\nabla\cdot\mathbf{T}^{(1)} - \nabla P$$

with $D_t = \partial_t + \mathbf{v}\cdot\nabla$. Now, write

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

$$= \frac{1}{2}\left[\partial_t(\rho\mathbf{v})\cdot\mathbf{v} + \rho\mathbf{v}\,\partial_t\mathbf{v}\right]$$

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

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

$$= -\frac{1}{2}\nabla\cdot\underbrace{(\rho\mathbf{v}\mathbf{v}\cdot\mathbf{v})}_{\rho|\mathbf{v}|^2\mathbf{v}.} - (\nabla\cdot\mathbf{T}^{(1)})\cdot\mathbf{v} - (\nabla P)\cdot\mathbf{v}$$

Note that

$$(\nabla\cdot\mathbf{T}^{(1)})\cdot\mathbf{v} = \nabla\cdot(\mathbf{T}^{(1)}\cdot\mathbf{v}) - \mathbf{T}^{(1)}:\nabla\mathbf{v}$$

and likewise

$$\nabla P \cdot \mathbf{v} = \nabla \cdot (P\mathbf{v}) - P(\nabla \cdot \mathbf{v})$$

so that

$$\boxed{\begin{aligned}\partial_t\left(\tfrac{1}{2}\rho v^2\right) = & -\nabla \cdot \left[\left(\tfrac{1}{2}\rho v^2 + P\right)\mathbf{v} + \mathbf{T}^{(1)} \cdot \mathbf{v}\right] \\ & - Q + P(\nabla \cdot \mathbf{v})\end{aligned}}$$

with

$$Q = -\mathbf{T}^{(1)} : \nabla \mathbf{v}$$

$$= \left[\eta\left(\nabla \mathbf{v} + (\nabla \mathbf{v})^T - \frac{2}{3}(\nabla \cdot \mathbf{v})\mathbf{I}\right) + \zeta(\nabla \cdot \mathbf{v})\mathbf{I}\right] : \nabla \mathbf{v}.$$

If we now write

$$\nabla \mathbf{v} = \mathbf{S} + \mathbf{\Omega} + \frac{1}{3} D\,\mathbf{I}$$

with

$$\mathbf{S} = \frac{1}{2}\left[(\nabla \mathbf{v}) + (\nabla \mathbf{v})^T - \frac{2}{3}(\nabla \cdot \mathbf{v})\mathbf{I}\right] \quad \text{symmetric, traceless}$$

$$\mathbf{\Omega} = \frac{1}{2}\left[(\nabla \mathbf{v}) - (\nabla \mathbf{v})^T\right] \quad \text{anti-symmetric}$$

$$D = \nabla \cdot \mathbf{v},$$

then

$$Q = 2\eta S^2 + \zeta D^2$$

for $S^2 = \mathbf{S} : \mathbf{S} = \sum_{ij} S_{ij}^2$.

(b) Starting with conservation of total energy

$$\partial_t\left(u+\tfrac{1}{2}\rho v^2\right)+\nabla\cdot\left[\left(u+\tfrac{1}{2}\rho v^2+P\right)\mathbf{v}+\mathbf{T}^{(1)}\cdot\mathbf{v}+\mathbf{q}\right]=0$$

and subtracting the result of (a) gives

$$\boxed{\partial_t u+\nabla\cdot(u\mathbf{v}+\mathbf{q})=Q-P(\nabla\cdot\mathbf{v})}$$

Using the product rule

$$\nabla\cdot(u\mathbf{v})=(\mathbf{v}\cdot\nabla)u+u(\nabla\cdot\mathbf{v}),$$

the above equation can be rewritten as

$$D_t u+u(\nabla\cdot\mathbf{v})+\nabla\cdot\mathbf{q}=Q-P(\nabla\cdot\mathbf{v})$$

(c) Again using the product rule

$$\nabla\cdot(\rho\mathbf{v})=(\mathbf{v}\cdot\nabla)\rho+\rho(\nabla\cdot\mathbf{v}),$$

the mass conservation equation

$$\partial_t\rho+\nabla\cdot(\rho\mathbf{v})=0$$

can likewise be rewritten as

$$D_t\rho+\rho(\nabla\cdot\mathbf{v})=0.$$

Solving for $\nabla\cdot\mathbf{v}$ the yields

$$\nabla\cdot\mathbf{v} = -\frac{D_t\rho}{\rho}.$$

Since $\rho = mn = m/\mathcal{V}$, the above relation can be written as well as

$$\nabla\cdot\mathbf{v} = +\frac{D_t\mathcal{V}}{\mathcal{V}}.$$

Defining as

$$D_tW = -P D_t\mathcal{V}$$

the rate of work performed by the fluid (following an element of the fluid), we obtain

$$P(\nabla\cdot\mathbf{v}) = -D_tW/\mathcal{V}.$$

Note that $P(\nabla\cdot\mathbf{v}) < 0$ when positive work is performed ($D_tW > 0$), so that kinetic energy is decreased while internal energy is increased. The opposite occurs when $D_tW < 0$. These energy exchanges are reversible. Not only can they have either sign, but they involve no irreversible increase of entropy.

(d) Following the hint, we get from the first law of thermodynamics

$$D_t s = \frac{1}{T} D_t u - \frac{\mu}{T} D_t \rho$$

$$= \frac{1}{T}\left[-u(\nabla\cdot\mathbf{v}) - \nabla\cdot\mathbf{q} + Q - P(\nabla\cdot\mathbf{v})\right]$$

$$- \frac{\mu}{T}\left[-\rho(\nabla\cdot\mathbf{v})\right]$$

$$= -\frac{(u + P - \mu\rho)}{T}(\nabla\cdot\mathbf{v}) - \frac{\nabla\cdot\mathbf{q}}{T} + \frac{Q}{T}$$

$$= -s(\nabla\cdot\mathbf{v}) - \frac{\nabla\cdot\mathbf{q}}{T} + \frac{Q}{T},$$

or, equivalently,

$$\partial_t s + \nabla\cdot(s\mathbf{v}) = -\frac{\nabla\cdot\mathbf{q}}{T} + \frac{Q}{T}.$$

Now, by the product rule

$$\nabla\cdot\left(\frac{\mathbf{q}}{T}\right) = \frac{\nabla\cdot\mathbf{q}}{T} + \mathbf{q}\cdot\nabla\left(\frac{1}{T}\right)$$

$$= \frac{\nabla\cdot\mathbf{q}}{T} - \frac{\mathbf{q}\cdot\nabla T}{T^2},$$

from which we obtain by addition to the previous equation that

$$\partial_t s + \nabla\cdot\left(s\mathbf{v} + q/T\right) = \frac{-q\cdot\nabla T}{T^2} + \frac{Q}{T}$$

or

$$\boxed{\partial_t s + \nabla\cdot\left(s\mathbf{v} + q/T\right) = \frac{\kappa|\nabla T|^2}{T^2} + \frac{Q}{T}}$$

with the Fourier law $q = -\kappa\nabla T$.

Remark: Note that $Q = \rho\varepsilon$ where $\varepsilon$ is the kinetic energy dissipation rate per unit mass. We have seen experimental evidence that turbulent flows lead to hugely enhanced values of $\varepsilon$, becoming independent of viscosity. By the above result, we see that turbulence should lead as well to a very greatly enhanced rate of entropy production. This is a signature of the strongly irreversible nature of turbulent fluid flows.

Problem 4 (a) With $\nu \doteq 1.5 \times 10^{-5}\ m^2/sec$ and with $\varepsilon \doteq 4 \times 10^{-2}\ m^2/sec^3$, one readily obtains

$$\eta = \left(\nu^3/\varepsilon\right)^{1/4} \doteq 5.4 \times 10^{-4}\ m \quad \text{or} \quad 0.54\ mm$$

$$v_\eta = (\nu\varepsilon)^{1/4} \doteq 2.78 \times 10^{-2}\ m/sec \quad \text{or} \quad 2.78\ cm/sec$$

(b) Consider N particles whose velocities $\mathbf{v}_n$, $n = 1, \ldots, N$ are independent and identically distributed, with

$$\mathbb{E}[\mathbf{v}_n] = \mathbf{u}, \quad \mathbb{E}\left[|\mathbf{v}_n - \mathbf{u}|^2\right] = c_s^2, \quad n = 1, \ldots, N$$

Setting

$$\overline{\mathbf{v}}_N = \frac{1}{N} \sum_{n=1}^{N} \mathbf{v}_n,$$

one then obtains

$$\mathbb{E}[\overline{\mathbf{v}}_N] = \frac{1}{N} \cdot N\mathbf{u} = \mathbf{u}$$

and

$$\mathbb{E}\left[|\overline{\mathbf{v}}_N - \mathbf{u}|^2\right] = \mathbb{E}\left[\left|\frac{1}{N}\sum_{n=1}^{N}(\mathbf{v}_n - \mathbf{u})\right|^2\right]$$

$$= \frac{1}{N^2}\sum_{n=1}^{N} \mathbb{E}\left[|\mathbf{v}_n - \mathbf{u}|^2\right]$$

by statistical independence

$$= \frac{1}{N^2} \cdot N c_s^2 = c_s^2/N$$

Thus, for $N_\ell = n \cdot \frac{4}{3}\pi \ell^3$ in a sphere of radius $\ell$, one obtains

$$v_\ell^\theta = \sqrt{\frac{c_s^2}{N_\ell}} = \frac{c_s}{\sqrt{N_\ell}}.$$

As expected by the central limit theorem, the r.m.s. velocity fluctuation decreases $\propto 1/\sqrt{N_\ell}$. Thus, the locally-averaged velocity becomes more nearly deterministic, with value $\doteq u$, for $N_\ell \gg 1$.

(c) Using $n \doteq 2.5 \times 10^{25}\ m^{-3}$ from Problem 2(d) and with $\eta \doteq 5.4 \times 10^{-4}\ m$, one obtains

$$N_\eta = n \cdot \frac{4}{3}\pi\eta^3 \doteq 1.64 \times 10^{16}$$

In that case,

$$v_\eta^\theta \doteq \frac{347\ m/sec}{\sqrt{1.64 \times 10^{16}}} = 2.71 \times 10^{-6}\ m/sec$$

$$\text{or} \quad 2.71 \times 10^{-4}\ cm/sec$$

We see that the magnitude of typical thermal velocity fluctuations at scale $\ell = \eta$ in the ABL is about <u>four orders of magnitude smaller</u> than $v_\eta$, the turbulent velocity fluctuation at the same scale!