

## §5. From Local To Global Equilibrium (Transport Equations)

### 5.1 Inhomogeneous distributions

We have so far discussed a very simple situation in which the gas is homogeneous so the velocity pdf  $f(\vec{v})$  described the situation at any point in space and quantities s.t.  $n, p, T$  were constants and there were no flows.

This need not be the case in general: thus, we know from experience that if we open the door or a window from a warm room onto cold Oxford autumn, it will be colder near the door than far away from it, there may be a draft (mean flow of air) etc.

Clearly this must correspond to the distribution of molecules being different in different places.

So we introduce the particle distribution both in position and velocity space:

$F(t, \vec{r}, \vec{v}) d^3\vec{r} d^3\vec{v} =$  avg # of particles with velocities in the cube ~~position~~  $[v_x, v_x + dv_x] \times [v_y, v_y + dv_y, v_z + dv_z]$  finding themselves in  $[x, x + dx] \times [y, y + dy, z + dz]$  at time  $t$

Note that it is conventional to normalise

$$\int d^3\vec{r} \int d^3\vec{v} F(t, \vec{r}, \vec{v}) = N \quad \text{\# of particles} \quad (1)$$

(rather than 1)

$$\text{Clearly, } \int d^3\vec{v} F(t, \vec{r}, \vec{v}) = n(\vec{r}) \quad \text{particle density} \quad (2)$$

at position  $\vec{r}$

$$\text{and } \int d^3\vec{r} n(\vec{r}) = N \quad (3)$$

↑  
Cover the system volume

[In a homogeneous system,

$$F(\vec{r}, \vec{v}) = F(\vec{v}) = n f(\vec{v}) \quad (4)$$

$\uparrow$  not a f-n of  $\vec{r}$ !       $\uparrow$  our old pdf,  $\int d^3v f(\vec{v}) = 1$

If we know  $F(\vec{r}, \vec{v})$ , we can calculate other bulk properties of the gas, besides its local density  $n(\vec{r})$ :

$$\int d^3v \vec{v} F(\vec{r}, \vec{v}) = n(\vec{r}) \underbrace{\vec{u}(\vec{r})}_{\substack{\text{mean velocity} \\ \text{of the gas flow}}} \quad (5)$$

It is interesting to look at what is particle energy now (cf. p.7): particle motion consists of mean  $\vec{u}$  and chaotic  $\vec{w} = \vec{v} - \vec{u}$  (peculiar velocity), so the total energy per unit volume at position  $\vec{r}$  is

$$\int d^3v \frac{mv^2}{2} F(t, \vec{r}, \vec{v}) = \int d^3w \frac{m(\vec{u} + \vec{w})^2}{2} F(t, \vec{r}, \vec{v})$$

$$= \frac{mu^2}{2} \underbrace{\int d^3w F}_{n(t, \vec{r})} + m\vec{u} \cdot \underbrace{\int d^3w \vec{w} F}_{0 \text{ by def. of } \vec{w}} + \int d^3w \frac{mw^2}{2} F$$

$$= \frac{mn u^2}{2} + \underbrace{\left\langle \frac{mw^2}{2} \right\rangle}_{\substack{\text{mean internal energy} \\ \text{per particle}}} n \quad (6)$$

energy density of the mean motions

internal energy density (motions around the mean)  $\equiv \mathcal{E}(t, \vec{r})$

NB: everything now a function  $\vec{r}$

Total "ordered" energy  $K = \int d^3r \frac{mn u^2}{2}$

Total internal energy  $U = \int d^3r \mathcal{E} = \int d^3r n \left\langle \frac{mw^2}{2} \right\rangle$

5.2 Local Maxwellian equilibrium

So what is  $F(t, \vec{r}, \vec{v})$ ? Recall that its dependence on  $\vec{r}$  and  $t$  is attributed to certain macroscopic inhomogeneities in the system (open window etc.) It is reasonable to assume then that the spatial and temporal scales on which these inhomogeneities exist/change are much longer than  $\lambda_{mfp}$  or  $\tau_c$  in our gas:

$$L \gg \lambda_{mfp}, T \gg \tau_c \leftarrow \text{not temperature!}$$

Then we could break up our gas into "fluid elements" of size  $l$  and consider them for time  $t$  s.t.

$$L \gg l \gg \lambda_{mfp}, T \gg t \gg \tau_c$$

Clearly they will behave as little homogeneous systems, with locally constant  $n$  and moving at some locally constant  $\vec{u}$ . We can then go to a locally moving frame (with velocity  $\vec{u}$ ) and expect all our old results for homogeneous static gas to apply, - in particular, we would expect ~~then~~ our gas to attain (on the collisional time scale) local Maxwellian equilibrium:

$$F_M(t, \vec{r}, \vec{v}) = \frac{n(t, \vec{r})}{[2\pi k_B T(t, \vec{r})/m]^{3/2}} e^{-\frac{|\vec{v} - \vec{u}(t, \vec{r})|^2}{2k_B T(t, \vec{r})/m}} \quad (7)$$

$$= \frac{n}{(\pi v_{th}^2)^{3/2}} e^{-w^2/v_{th}^2}, \text{ where } n \text{ and } v_{th} = \sqrt{\frac{2k_B T}{m}} \text{ are functions of } t \text{ and } \vec{r}$$

and everything is as before, except locally, e.g. pressure is

$$p(t, \vec{r}) = n(t, \vec{r}) k_B T(t, \vec{r}) = \frac{2}{3} \epsilon(t, \vec{r}) \quad (8)$$

So how then do we determine  $n, \vec{u}, T$ ?

(it is progress to learn that these three functions in 3D completely describe the particle distribution in 6D but it is still unclear what they are!)  $\uparrow$   $(\vec{v}, \vec{r})$

Thermodynamics gives us a hint ~~about~~ as to how they will evolve in time: we know that if we put in contact two systems with different  $T$ , the temperatures will tend to equalize - thus temperature gradients ~~are~~ tend to relax (still by collisions because that is how contact between particles of different energy is made).

Same is true about velocity gradients (we will prove this thermodynamically later, it also follows from the 2nd law as it turns out: see Landau and Lifshitz vol. 5 §10 if you are impatient).

But thermodynamics just tells us that everything must tend to this global equilibrium (no gradients) - not how fast that happens or what the intermediate stages look like. Kinetic theory will allow us to determine this route to equilibrium.

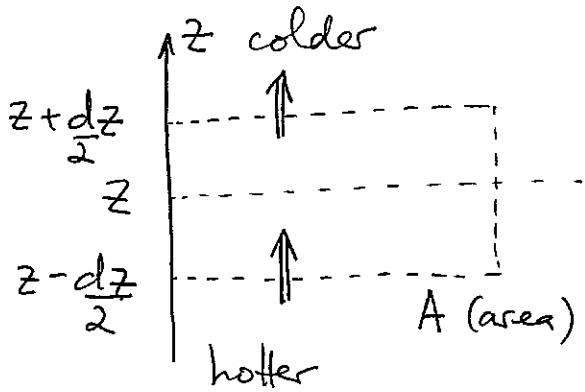


So all the energy is internal energy  $\epsilon = \frac{3}{2} n k_B T(t, \vec{r})$  and only temperature is inhomogeneous.

To simplify even further, let us consider a 1D problem:

$$T = T(t, z)$$

↑ direction of variation



Internal energy (heat) will flow from hot to cold regions

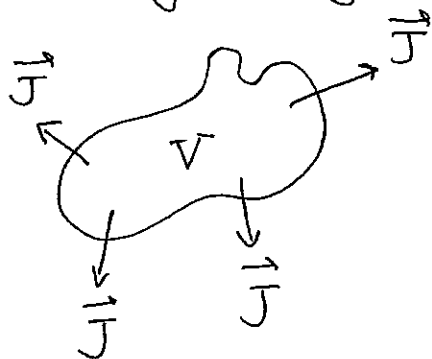
$$\frac{\partial}{\partial t} \underbrace{\frac{3}{2} n k_B T \cdot A dz}_{\text{energy inside the box } A \times dz} = \underbrace{J_z(z - \frac{dz}{2}) \cdot A}_{\text{energy flow in}} - \underbrace{J_z(z + \frac{dz}{2}) \cdot A}_{\text{energy flow out}}$$

where  $J_z(z) = \underline{\text{heat flux}} = \frac{\text{energy}}{\text{unit area} \cdot \text{unit time}}$  (about  $z$ )

$$\frac{\partial}{\partial t} \frac{3}{2} n k_B T = - \frac{J_z(z + \frac{dz}{2}) - J_z(z - \frac{dz}{2})}{dz} = - \frac{\partial J_z}{\partial z} \quad (12)$$

Thus, to calculate the evolution of  $T$ , we need to know the heat flux.

More generally, in 3D,



$$\frac{\partial}{\partial t} \int_V d^3\vec{r} \frac{3}{2} n k_B T = - \int_{\partial V} d^2\vec{S} \cdot \vec{J}$$

flux out through boundary (can be negative, means in)

$$= - \int_V d^3\vec{r} \nabla \cdot \vec{J}$$

Gauss theorem

Since  $V$  can be chosen completely arbitrarily,

$$\boxed{\frac{\partial}{\partial t} \frac{3}{2} n k_B T = -\nabla \cdot \vec{J}} \quad (B)$$

This is simply a local statement of energy conservation

Ex. Prove (from Maxwell's equations)

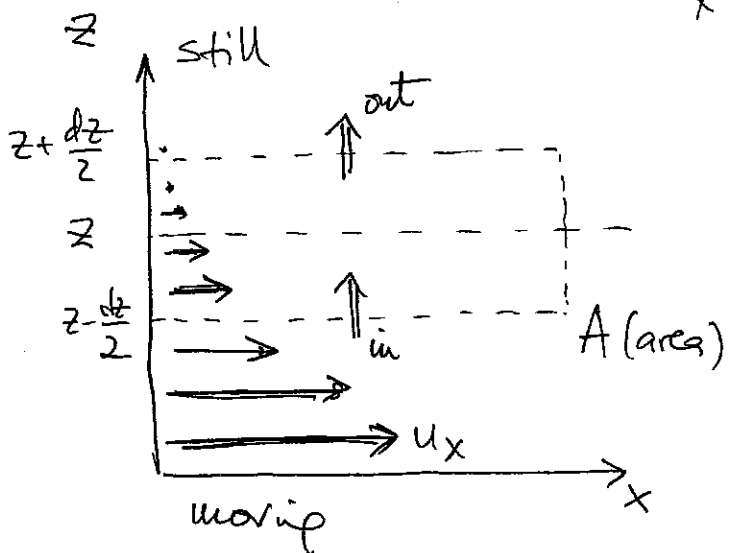
$$\frac{\partial \rho}{\partial t} = -\nabla \cdot \vec{J}$$

$\uparrow$  charge density       $\nwarrow$  current density (flux of charge)

We can handle momentum conservation

similarly: still assume  $n = \text{const}$  but now

let  $\vec{u} = u_x(z) \hat{x}$   $z$ -dependent velocity in the  $x$  direction "shear flow"



Momentum will flow up (from moving to still) because layers of fluid experience friction with each other (particles collide)

$$\frac{\partial}{\partial t} \underbrace{mn u_x \cdot A dz}_{\text{momentum inside the box } A \times dz} = \underbrace{\Pi_{zx} \left(z - \frac{dz}{2}\right) \cdot A}_{\text{momentum flow in}} - \underbrace{\Pi_{zx} \left(z + \frac{dz}{2}\right) \cdot A}_{\text{momentum flow out}}$$

where  $\Pi_{zx} = \underline{\text{momentum flux}} = \frac{\text{momentum in } x \text{ direction}}{\text{unit area} \cdot \text{unit time}} \perp z$

Just as we did for energy,

$$\boxed{\frac{\partial}{\partial t} \rho n u_x = - \frac{\partial \Pi_{zx}}{\partial z}} \quad (14)$$

|| Thus, to calculate the evolution of  $u_x$ , we need to know the momentum flux

Ex. 1) Figure out how to generalise this to a 3D situation where  $\vec{u} = \vec{u}(t, \vec{r})$ .

NB: Momentum flux is now a tensor:

$\Pi_{ij}$  = flux of  $j$ -velocity in the  $i$ -direction

- 2) The momentum flux consists of three parts
- one due to the fact that the boundary of a fluid element containing the same particles itself moves with velocity  $\vec{u}$
  - one due to the fact that temperature - and, therefore, pressure - varies with  $\vec{r}$  and pressure ~~gradients~~ differences (gradients) produce forces, which change momentum of a fluid element
  - one due to friction between layers of fluid moving at different velocities - we have not yet worked out how to calculate this part of the flux. Leave this part as an unknown, show that

$$\rho n \frac{\partial \vec{u}}{\partial t} = - \rho n \vec{u} \cdot \nabla \vec{u} - \nabla p - \nabla \cdot \hat{\Pi}^{\text{(frictional)}} \quad (15)$$

bit due to mean motion
pressure
unknown frictional contribution

[this is quite hard - but you can look it up in any book on fluid dynamics]





Similarly,  $\Pi_{zx} \neq 0$  only if  $\frac{\partial u_x}{\partial z} \neq 0$  and has opposite sign.

It is then tempting to conjecture that fluxes will be simply  $\propto$  gradients — in fact, this is more or less inevitable if the gradients are in some (tbd) sense not very large because we can simply ~~expand~~

Taylor-expand <sup>a</sup> flux in the value of the gradient:

$$J_z\left(\frac{\partial T}{\partial z}\right) = J_z(0) + J_z'(0) \frac{\partial T}{\partial z} + \dots$$

"  
0 no flux w/o a gradient

So, we expect

$$J_z = -\kappa \frac{\partial T}{\partial z} \quad (17)$$

NB: In 3D,

$$\vec{J} = -\kappa \nabla T$$

$\hat{\Pi}$  (tensor)

is complicated

(look it up!)

$$\Pi_{zx} = -\eta \frac{\partial u_x}{\partial z} \quad (18)$$

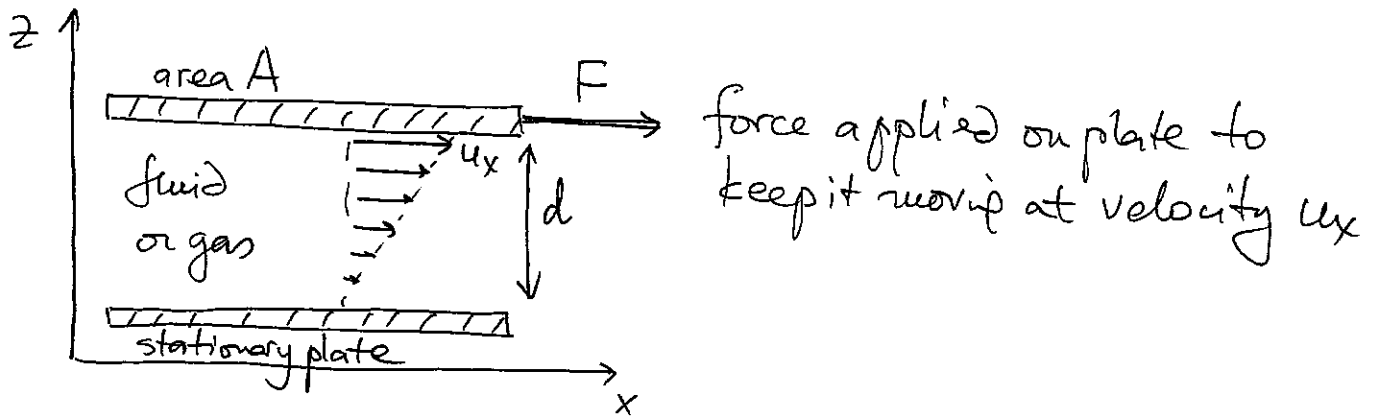
↑  
dynamical viscosity

These proportionalities do indeed hold experimentally in a good range of physical parameters ( $n, T$ , type of gas or other substance) and ~~mean~~  $\kappa$  and  $\eta$  can be just experimentally measured and tabulated even if we know nothing of kinetics or microphysics

(thus physics — and certainly engineering! — often progresses)

~ ~~These~~ NB: These relationships are valid much more broadly than will be our expressions for  $\kappa$  and  $\eta$  that we'll derive for ideal gas! Eg. we can talk about viscosity of water or th. conductivity of metal, although neither obviously consists of non-interacting billiard-ball particles on any level of simplification!

For example, viscosity can be introduced/measured so



It turns out that for small enough  $d$ ,

$$\frac{F}{A} = \eta \frac{u_x}{d} \approx \eta \frac{\partial u_x}{\partial z}$$

↑  
const. of proportionality

$$\frac{\text{force}}{\text{area}} = \frac{\text{momentum/time}}{\text{area}} = \text{momentum flux} = -\Pi_{zx} \Rightarrow \text{eq. (18)}$$

Physics: upper plate moves, molecules collide with it, get some mean momentum, then collide with lower layer, pass some mean momentum to it etc.

### 5.5 Transport equations

Sub. (17) and (18)  $\rightarrow$  (12) & (14)

$$\left\{ \begin{array}{l} \frac{\partial}{\partial t} \frac{3}{2} n k_B T = \alpha \frac{\partial^2 T}{\partial z^2} \quad (19) \\ \frac{\partial}{\partial t} m n u_x = \eta \frac{\partial^2 u_x}{\partial z^2} \quad (20) \end{array} \right. \quad \text{transport equations}$$

(assume  $\alpha$  and  $\eta$  are approx. independent of  $z$  - to be verified)

transport  
These equations have the same mathematical structure: diffusion equation

(21)  $\left\{ \begin{array}{l} \frac{\partial T}{\partial t} = D_T \frac{\partial^2 T}{\partial z^2} \quad D_T = \frac{\kappa}{n c_v} \text{ thermal diffusivity} \\ c_v = \frac{3}{2} k_B \text{ heat capacity per molecule} \end{array} \right.$

(22)  $\left\{ \begin{array}{l} \frac{\partial u_x}{\partial t} = \nu \frac{\partial^2 u_x}{\partial z^2} \quad \nu = \frac{\eta}{m n} \text{ kinematic viscosity} \end{array} \right.$

In the spirit of continuum to guess the answers w/o doing a proper calculation (yet), what can  $D_T$  and  $\nu$  possibly be equal to?

Dimensional analysis:  $[D_T] = [\nu] = \frac{cm^2}{sec}$

and they are microscopic properties to do with collisions, so must depend on  $\lambda_{mfp}$  and  $\tau_c$

To wit,  $D_T \sim \nu \sim \frac{\lambda_{mfp}^2}{\tau_c} \sim v_{th}^2 \tau_c \sim v_{th} \lambda_{mfp}$

NB:  
 $\kappa = n \frac{3}{2} k_B D_T$   
 $\sim n k_B v_{th} \frac{1}{n \sigma}$   
 $= k_B v_{th} / \sigma$   
 $\eta = m n \nu \sim \frac{m v_{th}}{\sigma}$   
 independent of density!  
 (23)

This is actually true, although of course we can't calculate numerical prefactors this way.

The following (also non-rigorous) calculation gives another angle on this problem and perhaps sheds some qualitative light on how particle motion leads to the diffusion equation.

Suppose at time  $t$  the momentum density at point  $z$  is  $m n u_x(t, z)$ .

What is it after a (short) time  $\Delta t$ ?

$$\langle u_x(t+\Delta t, z) \rangle = \langle u_x(t, z-\Delta z) \rangle$$

average over all particles - i.e., over the (random) displacements  $\Delta z$

Suppose we take  $\Delta t$  small enough that  $\Delta z$  is smaller

whatever it was at  $t$  at positions  $z-\Delta z$  where particles that are at  $z$  at  $t+\Delta t$  were at  $t$

than the scale of variation of  $u_x$ , i.e.  $\Delta z \ll \left(\frac{\partial \ln u_x}{\partial z}\right)^{-1}$ .

Then we can Taylor-expand:

$$u_x(t+\Delta t, z) = \left\langle u_x(t, z) - \Delta z \frac{\partial u_x}{\partial z} + \frac{\Delta z^2}{2} \frac{\partial^2 u_x}{\partial z^2} + \dots \right\rangle$$

$$= u_x(t, z) - \underbrace{\langle \Delta z \rangle}_{=0} \frac{\partial u_x}{\partial z} + \frac{\langle \Delta z^2 \rangle}{2} \frac{\partial^2 u_x}{\partial z^2} + \dots$$

can neglect because  $\Delta z$  is small

Therefore,

assump no mean motion in  $z$

(if there is, look at what happens and recall the exercise on p. 38)

$$\frac{u_x(t+\Delta t, z) - u_x(t, z)}{\Delta t} = \frac{\langle \Delta z^2 \rangle}{2\Delta t} \frac{\partial^2 u_x}{\partial z^2}$$

$$\boxed{\frac{\partial u_x}{\partial t} = \nu \frac{\partial^2 u_x}{\partial z^2}}$$

the diffusion equation!

$$\text{assump } \nu = \frac{\langle \Delta z^2 \rangle}{2\Delta t}$$

(24)

mean square particle displacement over time  $\Delta t$

is finite for  $\Delta t \rightarrow 0$

(i.e.  $\Delta t \ll \left(\frac{\partial \ln u_x}{\partial t}\right)^{-1}$ )

It is then natural to estimate  $\langle \Delta z^2 \rangle \sim \lambda_{\text{diff}}^2$  if  $\Delta t \sim \tau_c$ ,

$$\text{so } \nu \sim \frac{\lambda_{\text{diff}}^2}{\tau_c} \text{ as in eq. (23)}$$

The same argument works for energy density ( $\frac{3}{2}nk_B T$ ) or for any ~~transported~~ other property of the particles that they carry with them.

E.g. if we label some particles (e.g. radioactive isotopes), then the concentration  $n^*$  of this admixture will, by the same arguments, satisfy the same equation:

$$\frac{\partial n^*}{\partial t} = D \frac{\partial^2 n^*}{\partial z^2}, \quad D \sim v_{th} \lambda_{mfp} \quad \text{diff. coefficient (or diffusivity)}$$

"Fick's law" (25) coll. mfp of the labelled species

Note that diffusion is directly related to the famous "Brownian motion" - a random meandering of a particle being bombarded by other particles in a gas or fluid and for which it is possible to prove that the mean square displacement  $\langle \Delta z^2 \rangle \propto t$  and so  $D = \frac{\langle \Delta z^2 \rangle}{2\Delta t}$  is a well defined constant (this basically follows from the Central Limit Theorem as  $\Delta z$  is a sum of a sequence of independent kicks)  
This will be studied in more detail in B-I.

### 5.7 Relaxation to global equilibrium

Recall that the ~~basic~~ motivation of this whole line of inquiry was that the gas would get to local Maxwellian equilibrium over a few collision times and then will slowly evolve towards global Maxwellian equilibrium (no gradients in anything).

Let us convince ourselves that the transport eqns we have derived (or, rather, anticipated) do indeed

result in such a slow evolution.

The time scale for evolution:

$$\frac{\partial}{\partial t} \sim D \frac{\partial^2}{\partial z^2}$$

So  $\frac{1}{t} \sim \frac{\lambda_{mfp}^2}{\tau_c} \frac{1}{l^2}$

time to relax to global equilibrium

$$\frac{t}{\tau_c} \sim \left( \frac{l}{\lambda_{mfp}} \right)^2 \gg 1 \quad (26)$$

scale on which mean quantities are inhomogeneous

q.e.d.

Does the diffusion equation really lead to relaxation of gradients (and not steepening)?

The solutions are studied in Math. Methods: we know the Laplacian is a negative definite operator.

Simplest way to see this is by consider the evolution

~~of an initial condition decomposed into a Fourier series:~~

~~of an initial condition decomposed into a Fourier series:~~

of an initial condition decomposed into a Fourier series:

$$T(t=0, z) = \sum_k \hat{T}_0(k) e^{ikz}$$

or sin's or cos's depending on boundary conditions

Then the solution

$$T(t, z) = \sum_k \hat{T}(t, k) e^{ikz}$$

Satisfies

$$\frac{\partial \hat{T}}{\partial t} = -D_T k^2 \hat{T}$$

$$\hat{T}(t, k) = \hat{T}_0(k) e^{-D_T k^2 t}$$

So gradients (k) relax exp'ly fast in time

with characteristic time scale  $t \sim 1/D_T k^2$  [see (26)].

(27)

NB: longest wavelengths decay the slowest!

**5.8 Sources and Sinks**

So far we have only discussed the situation where some initial non-equilibrium state relaxes (diffusively) towards a global equilibrium.

However, in the real world there can be external circumstances that mathematically amount to sources or sinks in the transport equation, which keep the system out of equilibrium even as it ever strives towards it. These are easy to include.

- In the momentum equation, there can be

(body) forces:

(28)  $\frac{\partial}{\partial t} m n u_x = \eta \frac{\partial^2 u_x}{\partial z^2} + f_x$

← density of force in the x direction, e.g.

}

→

although strictly speaking none of these can be there if velocity is in x direction only and variation of anything in z only (Ex. Why?)

pressure grad. =  $-\frac{\partial p}{\partial x}$

gravity =  $mng_x$

Coriolis

centrifugal } rotating

Lorentz (for conducting media)

...

- In the heat diffusion equation, there can be heating or cooling terms

(29)  $\frac{\partial}{\partial t} \frac{3}{2} n k_B T = \kappa \frac{\partial^2 T}{\partial z^2} + H - C$

↑

heat density

e.g. viscous (see later)

Ohmic (When current flows)

compressional

↑

cooling density

e.g. radiative

Newton

( $\propto (T - T_0)$ )



Sources or sinks of heat or momentum can also come via boundary conditions : e.g.

- keeping a surface at a given temperature
- pumping a particular heat flux through a surface
- keeping a surface at a given velocity etc.

### 5.9 Steady States

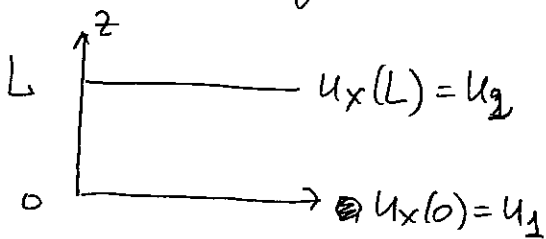
If sources/sinks are present or boundaries are maintained ~~at~~ under some fixed conditions, transport equations can have steady state solutions ( $\frac{\partial}{\partial t} = 0$ ) other than a global uniform equilibrium. Such non-equilibrium states are possible because energy/momentum are constantly supplied from the "outside"

For example, force balance :

$$\eta \frac{\partial^2 u_x}{\partial z^2} + f_x = 0 \Rightarrow \text{solve for } u_x \quad (30)$$

analogously,  $\kappa \frac{\partial^2 T}{\partial z^2} + H = 0$

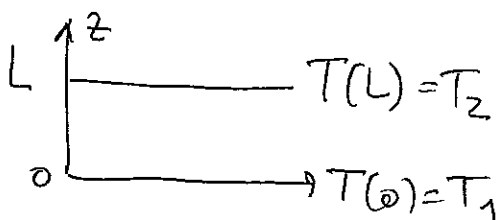
or, if a particular velocity is imposed on boundary :



$$\frac{\partial^2 u_x}{\partial z^2} = 0 \text{ subject to } \begin{cases} u_x(L) = u_2 \\ u_x(0) = u_1 \end{cases}$$

$$u_x(z) = u_1 + (u_2 - u_1) \frac{z}{L} \quad \text{solution shear flow}$$

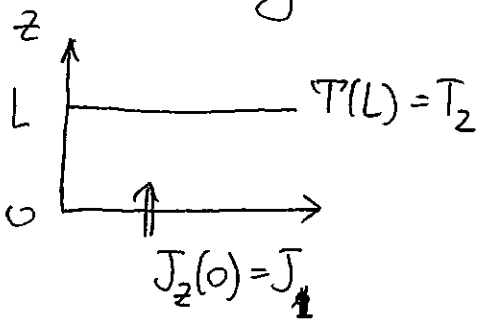
Similarly,



$$\frac{\partial^2 T}{\partial z^2} = 0 \text{ subject to } \begin{cases} T(L) = T_2 \\ T(0) = T_1 \end{cases}$$

$$T(z) = T_1 + (T_2 - T_1) \frac{z}{L}$$

Alternatively, we might know the heat flux through a boundary:



$$\frac{\partial J_z}{\partial z} = 0 \quad \text{or}$$

$$J_z = \text{const} = J_1$$

"

$$-\kappa \frac{\partial T}{\partial z}$$

⇓

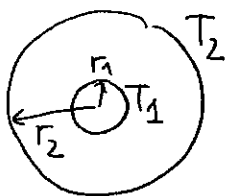
$$T = \frac{J_1}{\kappa} (L-z) + T_2$$

and we learn  $T(0) = \frac{J_1}{\kappa} L + T_2$

(e.g. we are heating with known power at the bottom and cooling at the top by fixing the temperature in contact with fixed-T environment)

Note that such steady-state solutions are not necessarily stable: time-dependent motions can develop as a result of small perturbations of the steady state growth (e.g. for convection with large enough temperature contrasts). Indeed, it is very commonplace for nature to find such ways of relaxing gradients via instabilities and resulting motions/turbulence when collisional transport is too slow to do the job! (Nature is impatient!)

Ex.



Work out temperature profile  $T(r)$

NB:  $\frac{\partial T}{\partial t} = D_T \nabla^2 T$

↑ need this in cylindrical geometry