12 Towards hydrodynamic equations

The previous classes focussed on the continuum description of static (time-independent) elastic systems. We become more ambitious now and look to derive the hydrodynamic equations for a system of particles obeying Newton’s laws. There are two ways we can go about this: by going from the microscopic to the macroscopic scale, or by adopting a continuum approximation and deriving the macro-equations from general considerations.

The general principle underlying this subject is that the macroscopic variables are quantities that are microscopically conserved. The reason for this is simply that the entire notion of a macroscopic equation relies on scale separation with the microscopic scale. Any quantity which is not conserved microscopically necessarily varies on a macroscopic scale. The only quantities that are candidate hydrodynamic variables are therefore those which are
conserved. This simple argument shows that what we really need to do is figure out how to generalise our random walkers to something that conserves momentum and energy.

To rigorously justify the macroscopic equations of motion for a fluid (i.e., a collection of particles interacting with each other by Newton’s laws) it is necessary to find a way of passing in detail from the microscopic (quantum) mechanical description, to the macroscopic description. The ideas behind this are highly related to what we have already done for the random walker, albeit with another level of complexity.

12.1 Euler equations

Instead of obtaining macroscopic equations of fluid motion from microscopic principles (this will be done in Sec. 12.2 below), we shall first derive the equations of inviscid (frictionless) hydrodynamics purely from macro-considerations alone. This requires us to adopt a continuum approximation, which assumes a macroscopic scale large compared with the distance between molecules. We assume that the fluid is continuous in structure, and physical quantities such as the mass and momentum are spread uniformly over small volume elements.

The validity of the continuum hypothesis under everyday conditions is clear, as two of the more common fluids, air and water, are so obviously continuous and smoothly varying that no different hypothesis would seem natural. One or two numbers readily show the great difference between the lengthscale representative of the fluid as a whole and that representative of the particle structure. For most laboratory experiments, a characteristic linear dimension of the region occupied by the fluid is at least 1cm, and very little variation of the physical and dynamical properties of the fluid occurs over a distance of $10^{-3}$ cm. Thus an instrument with a sensitive volume of $10^{-9}$ cm$^3$ would give a local measurement. Small though this volume is, it contains about $10^{10}$ molecules of air at normal temperature and pressure (and an even larger number of molecules of water), which is large enough for an average of all the molecules to be independent of their number.

The continuum hypothesis implies that it is possible to attach a definite meaning to the notion of value ‘at a point’ of the various fluid properties such as density, velocity and temperature, and that in general values of these quantities are continuous functions of position and time. There is ample observational evidence that common real fluids move as if they were continuous, under normal conditions and indeed for considerable departures from normal conditions. However, some of the properties of the equivalent continuous media need to be determined empirically, and cannot be derived directly from microscopic principles.

12.1.1 The continuity equation

Let’s suppose the fluid density is described by a function $\rho(r, t)$. The total mass enclosed in a fixed volume $V$ is

$$\int_V \rho dV. \quad (297)$$

The mass flux leaving this volume through the bounding surface $S = \partial V$ is

$$\int_S \rho \mathbf{u} \cdot n dS, \quad (298)$$
where \( u(\mathbf{x}, t) \) is the velocity of the fluid and \( n \) is the outward normal. Hence we have

\[
\int_V \frac{\partial \rho}{\partial t} dV = -\int_S \rho \mathbf{u} \cdot n dS = -\int_V \nabla \cdot (\rho \mathbf{u}) dV. \tag{299}
\]

This must hold for any arbitrary fluid element \( dV \), thus

\[
\frac{\partial \rho}{\partial t} + \nabla \cdot (\rho \mathbf{u}) = 0. \tag{300}
\]

This is called the \textit{continuity equation}.

For fluids like water, the density does not change very much and we will often be tempted to neglect the density variations. If we make this approximation the continuity equation reduces to the \textit{incompressibility condition}

\[
\nabla \cdot \mathbf{u} = 0. \tag{301}
\]

Like all approximations, this one is sometimes very good and sometimes not so good. We will have to figure out where it fails.

### 12.1.2 Momentum equations

So far we have more unknowns than equations (three velocity components but only one equation). We now consider the conservation of linear momentum and, adopting an alternative viewpoint to that used in deriving the continuity equation, consider Newton’s laws for a particular \textit{moving} element of fluid:

\[
\frac{d}{dt} \int_{V(t)} \rho u dV = -\int_{S(t)} \rho \mathbf{u} \cdot n dS + \int_{V(t)} f dV, \tag{302}
\]

where \( V(t) \) is the volume of the element enclosed by the surface \( S(t) \), \( f \) is the density of body forces, such as gravity \( \rho g \), and \( p \) is a pressure force. The pressure force is a normal force per unit area (usually compressive) exerted across the surface of a fluid element, and is related to both intermolecular forces and momentum transfer across an interface. For any volume, the pressure force is

\[
-\int p n dS = -\int \nabla p dV. \tag{303}
\]

Both \( V(t) \) and \( S(t) \) are being deformed by the motion of the fluid, so if we want to take the \( d/dt \) inside the integral sign we must take account of this. The \textit{Reynolds transport theorem} does so, and it can be shown that for a deforming, \textit{incompressible} fluid element

\[
\frac{d}{dt} \int_{V(t)} \rho u dV = \int_{V(t)} p \frac{D\mathbf{u}}{Dt} dV \tag{304}
\]

Here

\[
\frac{D}{Dt} = \frac{\partial}{\partial t} + (\mathbf{u} \cdot \nabla) \tag{305}
\]
is called the \textit{convective derivative}, and we shall discuss its significance in a moment. Hence, assuming that \( f \) is solely given by gravity, \( f = \rho g \), we find
\[
\int_{V(t)} \rho \frac{Du}{Dt} dV = \int_{V(t)} (-\nabla p + \rho g) dV
\]  
(306)

Since this must hold for any arbitrary fluid element we arrive at
\[
\frac{Du}{Dt} = -\nabla p + \rho g.
\]  
(307)

This, combined with the continuity equation (300), constitutes the \textit{Euler equations}. Things can be tidied up a little if we realise that the gravitational force, being conservative, can be written as the gradient of a scalar potential \( \nabla \psi \). It is therefore usual to redefine pressure as \( p + \psi \rightarrow p \). This implies that gravity simply modifies the pressure distribution in the fluid and does nothing to change the velocity. However, we cannot do this if \( \rho \) is not constant or if we have a free surface (as we shall see later with water waves).

Assuming the density is constant means we now have four equations in four unknowns: three components of \( u \) and \( p \). Note that if we do not demand constant density then the equations (continuity+momentum) only close with another relation, an equation of state \( p(\rho) \).

12.2 From Newton’s laws to hydrodynamic equations

To complement the purely macroscopic considerations from the previous section, we will now discuss how one can obtain hydrodynamic equations from the microscopic dynamics. To this end, we consider a many-particle system governed by Newton’s equations
\[
\frac{dx_i}{dt} = v_i, \quad m \frac{dv_i}{dt} = F_i,
\]  
(308)

assuming that all particles have the same mass \( m \), and that the forces \( F_i \) can be split into an external contribution \( G \) and pair interactions \( H(r) = -H(-r) \)
\[
F(x_1, \ldots, x_n) = G(x_i) + \sum_{j \neq i} H(x_i - x_j) = -\nabla x_i \Phi(x_1, \ldots, x_n)
\]  
(309)

We define the fine-grained phase-space density
\[
f(t, x, v) = \sum_{i=1}^{N} \delta(x - x_i(t)) \delta(v - v_i(t))
\]  
(310)

where \( \delta(x - x_i) = \delta(x - x_i) \delta(y - y_i) \delta(z - z_i) \) in three dimensions. Intuitively, the density \( f \) counts the number of particles that at time \( t \) are in the small volume \([x, x + dx]\) while having velocities in \([v, v + dv]\). By chain and product rule
\[
\frac{\partial}{\partial t} f = \sum_{i=1}^{N} \frac{d}{dt} \left[ \delta(x - x_i) \delta(v - v_i) \right]
\]
\[
= \sum_{i=1}^{N} \left\{ \delta(v - v_i) \nabla x_i \delta(x - x_i) \cdot \dot{x}_i + \delta(x - x_i) \nabla v_i \delta(v - v_i) \cdot \dot{v}_i \right\}
\]
\[
= -\nabla x \sum_{i=1}^{N} \delta(v - v_i) \delta(x - x_i) \cdot \dot{x}_i - \nabla v \sum_{i=1}^{N} \delta(x - x_i) \delta(v - v_i) \cdot \frac{F_i}{m}
\]  
(311)
where, in the last step, we inserted Newton’s equations and used that
\[
\frac{\partial}{\partial x_i} \delta(x - x_i) = - \frac{\partial}{\partial x} \delta(x - x_i) \tag{312}
\]
Furthermore, making use of the defining properties of the delta-function
\[
\frac{\partial}{\partial t} f = - v \cdot \nabla_x \sum_{i=1}^{N} \delta(v - v_i) \delta(x - x_i) - \nabla_v \sum_{i=1}^{N} \delta(x - x_i) \delta(v - v_i) \cdot \frac{F_i}{m} \\
= - v \cdot \nabla_x f - \frac{1}{m} \nabla_v \sum_{i=1}^{N} \delta(x - x_i) \delta(v - v_i) \cdot F_i. \tag{313}
\]
Writing \( \nabla = \nabla_x \) and inserting (309) for the forces, we may rewrite
\[
m \left( \frac{\partial}{\partial t} + v \cdot \nabla \right) f = - \nabla_v \sum_{i=1}^{N} \delta(v - v_i) \delta(x - x_i) \cdot \left[ G(x_i) + \sum_{j \neq i} H(x_i - x_j) \right] \\
= - \nabla_v \sum_{i=1}^{N} \delta(v - v_i) \delta(x - x_i) \cdot \left[ G(x) + \sum_{x_j \neq x} H(x - x_j) \right] \\
= - \left[ G(x) + \sum_{x_j \neq x} H(x - x_j) \right] \cdot \nabla_v f \tag{314}
\]
In the second line, we have again exploited the properties of the delta function which allow us to replace \( x_i \) by \( x \). Also note the appearance of the convective derivative on the lhs.; the above derivation shows that it results from Newton’s first equation.

To obtain the hydrodynamic equations from (314), two additional reductions will be necessary:

- We need to replace the fine-grained density \( f(t, x, v) \), which still depends implicitly on the (unknown) solutions \( x_j(t) \), by a coarse-grained density \( \langle f(t, x, v) \rangle \).
- We have to construct the relevant field variables, the mass density \( \rho(t, r) \) and velocity field \( u \), from the coarse-grained density \( f \).

To motivate the coarse-graining procedure, let us recall that the Newton equations (308) form a system of deterministic ODEs whose solutions are \( \{ x_1(t), \ldots, x_N(t) \} \) are uniquely determined by the initial conditions \( \{ x_1(0), \ldots, x_N(0); v_1(0), \ldots, v_N(0) \} =: \Gamma_0 \). However, for any experimental realization of a macroscopic system (say, a glass of water), it is practically impossible to determine the initial conditions exactly. To account for this lack of knowledge, we may assume that the initial conditions are drawn from some probability distribution \( \mathbb{P}(\Gamma_0) \). Without specifying the exact details of this distribution at this point, we may define the coarse-grained density \( \langle f \rangle \) by averaging the fine-grained density \( f \) with respect to \( \mathbb{P}(\Gamma_0) \), formally expressed as
\[
\langle f(t, x, v) \rangle = \int d\mathbb{P}(\Gamma_0) f(t, x, v). \tag{315}
\]
Averaging Eq. (314) and using the fact that integration over initial conditions commutes with the partial differentiations, we have
\[
m \left( \frac{\partial}{\partial t} + v \cdot \nabla \right) \langle f \rangle = -\nabla v \cdot [G(x)\langle f \rangle + C] \tag{316}
\]
where the collision-term
\[
C(t, x, v) := \sum_{x_j \neq x} \langle H(x - x_j) f(t, x, v) \rangle \tag{317}
\]
represents the average effect of the pair interactions on a fluid particle at position \(x\).

We now define the mass density \(\rho\), the velocity field \(u\), and the specific kinetic energy tensor \(\Sigma\) by
\[
\begin{align*}
\rho(t, x) &= m \int d^3v \langle f(t, x, v) \rangle, \tag{318a} \\
\rho(t, x) u(t, x) &= m \int d^3v \langle f(t, x, v) \rangle v. \tag{318b} \\
\rho(t, x) \Sigma(t, x) &= m \int d^3v \langle f(t, x, v) \rangle vv. \tag{318c}
\end{align*}
\]

The tensor \(\Sigma\) is, by construction, symmetric as can be seen from the definition of its individual components
\[
\rho(t, x) \Sigma_{ij}(t, x) = m \int d^3v \langle f(t, x, v) \rangle v_i v_j,
\]
and the trace of \(\Sigma\) defines the local kinetic energy density
\[
\epsilon(t, x) := \frac{1}{2} \text{Tr}(\rho \Sigma) = \frac{m}{2} \int d^3v \langle f(t, x, v) \rangle |v|^2. \tag{319}
\]

Integrating Eq. (316) over \(v\), we get
\[
\frac{\partial}{\partial t} \rho + \nabla \cdot (\rho u) = -\int dv^3 \nabla_v \cdot [G(x)\langle f \rangle + C], \tag{320}
\]
but the rhs. can be transformed into a surface integral (in velocity space) that vanishes since for physically reasonable interactions \([G(x)\langle f \rangle + C] \to 0\) as \(|v| \to \infty\). We thus recover the mass conservation equation
\[
\frac{\partial}{\partial t} \rho + \nabla \cdot (\rho u) = 0. \tag{321}
\]

To obtain the momentum conservation law, let's multiply (316) by \(v\) and subsequently integrate over \(v\),
\[
\int dv^3 \ m \left( \frac{\partial}{\partial t} + v \cdot \nabla \right) \langle f \rangle v = -\int dv^3 v \nabla_v \cdot [G(x)\langle f \rangle + C]. \tag{322}
\]
The lhs. can be rewritten as
\[
\int dv^3 m\left(\frac{\partial}{\partial t} + v \cdot \nabla\right)\langle f \rangle v = \frac{\partial}{\partial t}(\rho u) + \nabla \cdot \int dv^3 m\langle f \rangle vv
\]
\[
= \frac{\partial}{\partial t}(\rho u) + \nabla \cdot (\rho \Sigma)
\]
\[
= \frac{\partial}{\partial t}(\rho u) + \nabla \cdot (\rho \Sigma) + \rho u \cdot \nabla (\rho u) + \rho u \cdot \nabla \cdot [\rho(\Sigma - uu)]
\]
\[
= \rho\left(\frac{\partial}{\partial t} + u \cdot \nabla\right)u + \nabla \cdot [\rho(\Sigma - uu)] \quad (321)
\]

The rhs. of (322) can be computed by partial integration, yielding
\[
- \int dv^3 u \nabla v \cdot \left[G(x)\langle f \rangle + C\right] = \int dv^3 \cdot [G(x)\langle f \rangle + C]
\]
\[
= \rho g + c(t, x), \quad (324)
\]
where \(g(x) := G(x)/m\) is the force per unit mass (acceleration) and the last term
\[
c(t, x) = \int dv^3 C = \int dv^3 \sum x_j \langle H(x - x_j)f(t, x, v)\rangle
\]
(325)
encodes the mean pair interactions. Combining (323) and (324), we find
\[
\rho\left(\frac{\partial}{\partial t} + u \cdot \nabla\right)u = -\nabla \cdot [\rho(\Sigma - uu)] + \rho g(x) + c(t, x). \quad (326)
\]
The symmetric tensor
\[
\Pi := \Sigma - uu \quad (327)
\]
measures the covariance of the local velocity fluctuations of the molecules which can be related to their temperature. To estimate \(c\), let us assume that the pair interaction force \(H\) can be derived from a pair potential \(\varphi\), which means that \(H(r) = -\nabla_r \varphi(r)\). Assuming further that \(H(0) = 0\), we may write
\[
c(t, x) = -\int dv^3 \sum x_j \langle [\nabla_x \varphi(x - x_j)]f(t, x, v)\rangle \quad (328)
\]
Replacing for some function \(\zeta(x)\) the sum over all particles by the integral
\[
\sum x_j \zeta(x_j) \simeq \frac{1}{m} \int d^3 y \rho(t, y) \zeta(y) \quad (329)
\]
we have
\[
c(t, x) \simeq -\frac{1}{m} \int dv^3 \int d^3 y \rho(t, y) \langle [\nabla_x \varphi(x - y)]f(t, x, v)\rangle
\]
\[
= -\frac{1}{m} \int dv^3 \int d^3 y \rho(t, y) \langle [-\nabla_y \varphi(x - y)]f(t, x, v)\rangle
\]
\[
= -\frac{1}{m} \int dv^3 \int d^3 y \left[\nabla \rho(t, y)\right] \langle \varphi(x - y)f(t, x, v)\rangle \quad (330)
\]

The symmetric tensor
\[
\Pi := \Sigma - uu
\]
measures the covariance of the local velocity fluctuations of the molecules which can be related to their temperature. To estimate \(c\), let us assume that the pair interaction force \(H\) can be derived from a pair potential \(\varphi\), which means that \(H(r) = -\nabla_r \varphi(r)\). Assuming further that \(H(0) = 0\), we may write
\[
c(t, x) = -\int dv^3 \sum x_j \langle [\nabla_x \varphi(x - x_j)]f(t, x, v)\rangle \quad (328)
\]
Replacing for some function \(\zeta(x)\) the sum over all particles by the integral
\[
\sum x_j \zeta(x_j) \simeq \frac{1}{m} \int d^3 y \rho(t, y) \zeta(y) \quad (329)
\]
we have
\[
c(t, x) \simeq -\frac{1}{m} \int dv^3 \int d^3 y \rho(t, y) \langle [\nabla_x \varphi(x - y)]f(t, x, v)\rangle
\]
\[
= -\frac{1}{m} \int dv^3 \int d^3 y \rho(t, y) \langle [-\nabla_y \varphi(x - y)]f(t, x, v)\rangle
\]
\[
= -\frac{1}{m} \int dv^3 \int d^3 y \left[\nabla \rho(t, y)\right] \langle \varphi(x - y)f(t, x, v)\rangle \quad (330)
\]

62
In general, it is impossible to simplify this further without some explicit assumptions about initial distribution $P$ that determines the average $\langle \cdot \rangle$. There is however one exception, namely, the case when interactions are very short-range so that we can approximate the potential by a delta-function,

$$\varphi(r) = \varphi_0 a^3 \delta(r), \quad (331)$$

where $\varphi_0$ is the interaction energy and $a^3$ the effective particle volume. In this case,

$$c(t, x) = -\frac{\varphi_0 a^3}{m} \int dv \int d^3y \left[ \nabla \rho(t, y) \right] \langle \delta(x - y) f(t, x, v) \rangle$$

$$= -\frac{\varphi_0 a^3}{m} \left[ \nabla \rho(t, x) \right] \int dv \langle f(t, x, v) \rangle$$

$$= -\frac{\varphi_0 a^3}{m^2} \left[ \nabla \rho(t, x) \right] \rho(t, x)$$

$$= -\frac{\varphi_0 a^3}{2m^2} \nabla \rho(t, x)^2 \quad (332)$$

Inserting this into (326), we have thus derived the following hydrodynamic equations

$$\frac{\partial}{\partial t} \rho + \nabla \cdot (\rho u) = 0 \quad (333a)$$

$$\rho \left( \frac{\partial}{\partial t} + u \cdot \nabla \right) u = \nabla \cdot \Xi + \rho g(x), \quad (333b)$$

where

$$\Xi := -\left[ \rho(\Sigma - uu) + \frac{\varphi_0 a^3}{2m^2} \rho^2 I \right] \quad (333c)$$

is the stress tensor with $I$ denoting unit matrix.

Note that Eqs. (333) do not yet form a closed system, due to the appearance of the second-moment tensor $\Sigma$. This is a manifestation of the well-known hierarchy problem, encountered in all attempts to derive hydrodynamic equations from microscopic models. More precisely, the hierarchy problem means that the time evolution of the $n$th-moment depends on that of the higher moments. The standard approach to overcoming this obstacle is to postulate (guess) reasonable ad-hoc closure conditions, which essentially means that one tries to express higher moments, such as $\Sigma$, in terms of the lower moments. For example, a commonly adopted closure condition is the ideal isotropic gas approximation

$$\Sigma - uu = \frac{kT}{m} I, \quad (334)$$

where $T$ is the temperature and $k$ the Boltzmann constant. For this closure condition, Eqs. (333a) and (333b) become to a closed system for $\rho$ and $u$.

Traditionally, and in most practical applications, one does not bother with microscopic derivations of $\Xi$; instead one merely postulates that

$$\Xi = -pI + \mu(\nabla^T u + \nabla u^T) - \frac{2\mu}{3}(\nabla \cdot u), \quad (335)$$

$^{14}$Except, perhaps for very trivial examples.
where \( p(t, x) \) is the pressure field and \( \mu \) the dynamic viscosity, which can be a function of pressure, temperature etc. depending on the fluid. Equations (333a) and (333b) combined with the empirical ansatz (335) are the famous Navier-Stokes equations. The second summand in Eq. (335) contains the rate-of-strain tensor

\[
E = \frac{1}{2}(\nabla^\top u + \nabla u^\top)
\]

and \((\nabla \cdot u)\) is the rate-of-expansion of the flow.

For incompressible flow, defined by \( \rho = \text{const.} \), the Navier-Stokes equations simplify to

\[
\nabla \cdot u = 0 \tag{337a}
\]

\[
\rho \left( \frac{\partial}{\partial t} + u \cdot \nabla \right) u = -\nabla p + \mu \nabla^2 u + \rho g. \tag{337b}
\]

In this case, one has to solve for \((p, u)\).