

From
Newton's law
to
hydrodynamic equations

18.354 - L14

Goal: derive

$$\frac{\partial \rho}{\partial t} + \nabla \cdot (\rho \mathbf{u}) = 0.$$

$$\frac{D\mathbf{u}}{Dt} = \frac{-\nabla p}{\rho} + \mathbf{g}.$$

$$\frac{D}{Dt} = \frac{\partial}{\partial t} + (\mathbf{u} \cdot \nabla)$$

13.2 From Newton's laws to hydrodynamic equations

$$\frac{d\mathbf{x}_i}{dt} = \mathbf{v}_i, \quad m \frac{d\mathbf{v}}{dt} = \mathbf{F}_i,$$

$$\mathbf{F}(\mathbf{x}_1, \dots, \mathbf{x}_n) = \mathbf{G}(\mathbf{x}_i) + \sum_{j \neq i} \mathbf{H}(\mathbf{x}_i - \mathbf{x}_j) = -\nabla_{\mathbf{x}_i} \Phi(\mathbf{x}_1, \dots, \mathbf{x}_n)$$

$$\mathbf{H}(\mathbf{r}) = -\mathbf{H}(-\mathbf{r})$$

We define the fine-grained phase-space density

$$f(t, \mathbf{x}, \mathbf{v}) = \sum_{i=1}^N \delta(\mathbf{x} - \mathbf{x}_i(t)) \delta(\mathbf{v} - \mathbf{v}_i(t))$$

where $\delta(\mathbf{x} - \mathbf{x}_i) = \delta(x - x_i) \delta(y - y_i) \delta(z - z_i)$

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$$\begin{aligned} \frac{\partial}{\partial t} f &= \sum_{i=1}^N \frac{d}{dt} [\delta(\mathbf{x} - \mathbf{x}_i) \delta(\mathbf{v} - \mathbf{v}_i)] \\ &= \sum_i^N \{ \delta(\mathbf{v} - \mathbf{v}_i) \nabla_{\mathbf{x}_i} \delta(\mathbf{x} - \mathbf{x}_i) \cdot \dot{\mathbf{x}}_i + \delta(\mathbf{x} - \mathbf{x}_i) \nabla_{\mathbf{v}_i} \delta(\mathbf{v} - \mathbf{v}_i) \cdot \dot{\mathbf{v}}_i \} \\ &= -\nabla_{\mathbf{x}} \sum_{i=1}^N \delta(\mathbf{v} - \mathbf{v}_i) \delta(\mathbf{x} - \mathbf{x}_i) \cdot \mathbf{v}_i - \nabla_{\mathbf{v}} \sum_{i=1}^N \delta(\mathbf{x} - \mathbf{x}_i) \delta(\mathbf{v} - \mathbf{v}_i) \cdot \frac{\mathbf{F}_i}{m} \end{aligned}$$

where, in the last step, we inserted Newton's equations and used that

$$\frac{\partial}{\partial x_i} \delta(x - x_i) = -\frac{\partial}{\partial x} \delta(x - x_i)$$

$$\begin{aligned}
\frac{\partial}{\partial t} f &= -\mathbf{v} \cdot \nabla_{\mathbf{x}} \sum_{i=1}^N \delta(\mathbf{v} - \mathbf{v}_i) \delta(\mathbf{x} - \mathbf{x}_i) - \nabla_{\mathbf{v}} \sum_{i=1}^N \delta(\mathbf{x} - \mathbf{x}_i) \delta(\mathbf{v} - \mathbf{v}_i) \cdot \frac{\mathbf{F}_i}{m} \\
&= -\mathbf{v} \cdot \nabla_{\mathbf{x}} f - \frac{1}{m} \nabla_{\mathbf{v}} \sum_{i=1}^N \delta(\mathbf{x} - \mathbf{x}_i) \delta(\mathbf{v} - \mathbf{v}_i) \cdot \mathbf{F}_i.
\end{aligned} \tag{313}$$

Writing $\nabla = \nabla_{\mathbf{x}}$ and inserting (309) for the forces, we may rewrite

$$\begin{aligned}
m \left(\frac{\partial}{\partial t} + \mathbf{v} \cdot \nabla \right) f &= -\nabla_{\mathbf{v}} \sum_{i=1}^N \delta(\mathbf{x} - \mathbf{x}_i) \delta(\mathbf{v} - \mathbf{v}_i) \cdot \left[\mathbf{G}(\mathbf{x}_i) + \sum_{j \neq i} \mathbf{H}(\mathbf{x}_i - \mathbf{x}_j) \right] \\
&= -\nabla_{\mathbf{v}} \sum_{i=1}^N \delta(\mathbf{x} - \mathbf{x}_i) \delta(\mathbf{v} - \mathbf{v}_i) \cdot \left[\mathbf{G}(\mathbf{x}) + \sum_{\mathbf{x}_j \neq \mathbf{x}} \mathbf{H}(\mathbf{x} - \mathbf{x}_j) \right] \\
&= - \left[\mathbf{G}(\mathbf{x}) + \sum_{\mathbf{x}_j \neq \mathbf{x}} \mathbf{H}(\mathbf{x} - \mathbf{x}_j) \right] \cdot \nabla_{\mathbf{v}} f
\end{aligned}$$

$$m \left(\frac{\partial}{\partial t} + \mathbf{v} \cdot \nabla \right) f = - \left[\mathbf{G}(\mathbf{x}) + \sum_{\mathbf{x}_j \neq \mathbf{x}} \mathbf{H}(\mathbf{x} - \mathbf{x}_j) \right] \cdot \nabla_{\mathbf{v}} f \quad (314)$$

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

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

$$\{\mathbf{x}_1(t), \dots, \mathbf{x}_N(t)\}$$

$$\{\mathbf{x}_1(0), \dots, \mathbf{x}_N(0); \mathbf{v}_1(0), \dots, \mathbf{v}_N(0)\} =: \Gamma_0$$

$$\langle f(t, \mathbf{x}, \mathbf{v}) \rangle = \int d\mathbb{P}(\Gamma_0) f(t, \mathbf{x}, \mathbf{v}). \quad (315)$$

$$m \left(\frac{\partial}{\partial t} + \mathbf{v} \cdot \nabla \right) \langle f \rangle = -\nabla_{\mathbf{v}} \cdot [\mathbf{G}(\mathbf{x}) \langle f \rangle + \mathbf{C}] \quad (316)$$

where the collision-term

$$C(t, \mathbf{x}, \mathbf{v}) := \sum_{\mathbf{x}_j \neq \mathbf{x}} \langle \mathbf{H}(\mathbf{x} - \mathbf{x}_j) f(t, \mathbf{x}, \mathbf{v}) \rangle \quad (317)$$

We now define the mass density ρ , the velocity field \mathbf{u} , and the specific kinetic energy tensor Σ by

$$\rho(t, \mathbf{x}) = m \int d^3v \langle f(t, \mathbf{x}, \mathbf{v}) \rangle, \quad (318a)$$

$$\rho(t, \mathbf{x}) \mathbf{u}(t, \mathbf{x}) = m \int d^3v \langle f(t, \mathbf{x}, \mathbf{v}) \rangle \mathbf{v}. \quad (318b)$$

$$\rho(t, \mathbf{x}) \Sigma(t, \mathbf{x}) = m \int d^3v \langle f(t, \mathbf{x}, \mathbf{v}) \rangle \mathbf{v} \mathbf{v}. \quad (318c)$$

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$$\rho(t, \mathbf{x}) \Sigma(t, \mathbf{x}) = m \int d^3v \langle f(t, \mathbf{x}, \mathbf{v}) \rangle \mathbf{v}\mathbf{v}. \quad (318c)$$

The tensor Σ is, by construction, symmetric as can be seen from the definition of its individual components

$$\rho(t, \mathbf{x}) \Sigma_{ij}(t, \mathbf{x}) = m \int d^3v \langle f(t, \mathbf{x}, \mathbf{v}) \rangle v_i v_j,$$

and the trace of Σ defines the local *kinetic energy density*

$$\epsilon(t, \mathbf{x}) := \frac{1}{2} \text{Tr}(\rho \Sigma) = \frac{m}{2} \int d^3v \langle f(t, \mathbf{x}, \mathbf{v}) \rangle |\mathbf{v}|^2. \quad (319)$$

Mass conservation

$$m \left(\frac{\partial}{\partial t} + \mathbf{v} \cdot \nabla \right) \langle f \rangle = -\nabla_{\mathbf{v}} \cdot [\mathbf{G}(\mathbf{x}) \langle f \rangle + \mathbf{C}] \quad (316)$$

Integrating Eq. (316) over \mathbf{v} , we get

$$\frac{\partial}{\partial t} \rho + \nabla \cdot (\rho \mathbf{u}) = - \int dv^3 \nabla_{\mathbf{v}} \cdot [\mathbf{G}(\mathbf{x}) \langle f \rangle + \mathbf{C}], \quad (320)$$

but the rhs. can be transformed into a surface integral (in velocity space) that vanishes since for physically reasonable interactions $[\mathbf{G}(\mathbf{x}) \langle f \rangle + \mathbf{C}] \rightarrow \mathbf{0}$ as $|\mathbf{v}| \rightarrow \infty$. We thus recover the mass conservation equation

$$\frac{\partial}{\partial t} \rho + \nabla \cdot (\rho \mathbf{u}) = 0. \quad (321)$$

Momentum conservation

$$m \left(\frac{\partial}{\partial t} + \mathbf{v} \cdot \nabla \right) \langle f \rangle = -\nabla_{\mathbf{v}} \cdot [\mathbf{G}(\mathbf{x}) \langle f \rangle + \mathbf{C}] \quad (316)$$

To obtain the momentum conservation law, let's multiply (316) by \mathbf{v} and subsequently integrate over \mathbf{v} ,

$$\int dv^3 m \left(\frac{\partial}{\partial t} + \mathbf{v} \cdot \nabla \right) \langle f \rangle \mathbf{v} = - \int dv^3 \mathbf{v} \nabla_{\mathbf{v}} \cdot [\mathbf{G}(\mathbf{x}) \langle f \rangle + \mathbf{C}]. \quad (322)$$

$$\int dv^3 m \left(\frac{\partial}{\partial t} + \mathbf{v} \cdot \nabla \right) \langle f \rangle \mathbf{v} = - \int dv^3 \mathbf{v} \nabla_{\mathbf{v}} \cdot [\mathbf{G}(\mathbf{x}) \langle f \rangle + \mathbf{C}]. \quad (322)$$

The lhs. can be rewritten as

$$\begin{aligned} \int dv^3 m \left(\frac{\partial}{\partial t} + \mathbf{v} \cdot \nabla \right) \langle f \rangle \mathbf{v} &= \frac{\partial}{\partial t}(\rho \mathbf{u}) + \nabla \cdot \int dv^3 m \langle f \rangle \mathbf{v} \mathbf{v} \\ &= \frac{\partial}{\partial t}(\rho \mathbf{u}) + \nabla \cdot (\rho \boldsymbol{\Sigma}) \\ &= \frac{\partial}{\partial t}(\rho \mathbf{u}) + \nabla \cdot (\rho \mathbf{u} \mathbf{u}) + \nabla \cdot [\rho(\boldsymbol{\Sigma} - \mathbf{u} \mathbf{u})] \\ &= \rho \frac{\partial}{\partial t} \mathbf{u} + \mathbf{u} \frac{\partial}{\partial t} \rho + \mathbf{u} \nabla \cdot (\rho \mathbf{u}) + \rho \mathbf{u} \cdot \nabla \mathbf{u} + \nabla \cdot [\rho(\boldsymbol{\Sigma} - \mathbf{u} \mathbf{u})] \\ &\stackrel{(321)}{=} \rho \left(\frac{\partial}{\partial t} + \mathbf{u} \cdot \nabla \right) \mathbf{u} + \nabla \cdot [\rho(\boldsymbol{\Sigma} - \mathbf{u} \mathbf{u})] \end{aligned} \quad (323)$$

The rhs. of (322) can be computed by partial integration, yielding

$$\begin{aligned} - \int dv^3 \mathbf{v} \nabla_{\mathbf{v}} \cdot [\mathbf{G}(\mathbf{x}) \langle f \rangle + \mathbf{C}] &= \int dv^3 \cdot [\mathbf{G}(\mathbf{x}) \langle f \rangle + \mathbf{C}] \\ &= \rho \mathbf{g} + \mathbf{c}(t, \mathbf{x}), \end{aligned} \quad (324)$$

where $\mathbf{g}(\mathbf{x}) := \mathbf{G}(\mathbf{x})/m$ is the force per unit mass (acceleration) and the last term

$$\mathbf{c}(t, \mathbf{x}) = \int dv^3 \mathbf{C} = \int dv^3 \sum_{\mathbf{x}_j \neq \mathbf{x}} \langle \mathbf{H}(\mathbf{x} - \mathbf{x}_j) f(t, \mathbf{x}, \mathbf{v}) \rangle \quad (325)$$

encodes the mean pair interactions. Combining (323) and (324), we find

$$\rho \left(\frac{\partial}{\partial t} + \mathbf{u} \cdot \nabla \right) \mathbf{u} = -\nabla \cdot [\rho(\boldsymbol{\Sigma} - \mathbf{u}\mathbf{u})] + \rho \mathbf{g}(\mathbf{x}) + \mathbf{c}(t, \mathbf{x}). \quad (326)$$

The symmetric tensor

$$\boldsymbol{\Pi} := \boldsymbol{\Sigma} - \mathbf{u}\mathbf{u} \quad (327)$$

measures the covariance of the local velocity fluctuations of the molecules

related to their temperature. To estimate \mathbf{c} , let us assume that the pair interaction force \mathbf{H} can be derived from a pair potential φ , which means that $\mathbf{H}(\mathbf{r}) = -\nabla_{\mathbf{r}}\varphi(\mathbf{r})$. Assuming further that $\mathbf{H}(\mathbf{0}) = \mathbf{0}$, we may write

$$\mathbf{c}(t, \mathbf{x}) = - \int dv^3 \sum_{\mathbf{x}_j(t)} \langle [\nabla_{\mathbf{x}}\varphi(\mathbf{x} - \mathbf{x}_j)] f(t, \mathbf{x}, \mathbf{v}) \rangle \quad (328)$$

Replacing for some function $\zeta(\mathbf{x})$ the sum over all particles by the integral

$$\sum_{\mathbf{x}_j} \zeta(\mathbf{x}_j) \simeq \frac{1}{m} \int d^3y \rho(t, \mathbf{y}) \zeta(\mathbf{y}) \quad (329)$$

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we have

$$\begin{aligned} \mathbf{c}(t, \mathbf{x}) &\simeq -\frac{1}{m} \int dv^3 \int d^3y \rho(t, \mathbf{y}) \langle [\nabla_{\mathbf{x}} \varphi(\mathbf{x} - \mathbf{y})] f(t, \mathbf{x}, \mathbf{v}) \rangle \\ &= -\frac{1}{m} \int dv^3 \int d^3y \rho(t, \mathbf{y}) \langle [-\nabla_{\mathbf{y}} \varphi(\mathbf{x} - \mathbf{y})] f(t, \mathbf{x}, \mathbf{v}) \rangle \\ &= -\frac{1}{m} \int dv^3 \int d^3y [\nabla \rho(t, \mathbf{y})] \langle \varphi(\mathbf{x} - \mathbf{y}) f(t, \mathbf{x}, \mathbf{v}) \rangle \end{aligned} \quad (330)$$

$$\mathbf{c}(t, \mathbf{x}) \simeq -\frac{1}{m} \int dv^3 \int d^3y [\nabla \rho(t, \mathbf{y})] \langle \varphi(\mathbf{x} - \mathbf{y}) f(t, \mathbf{x}, \mathbf{v}) \rangle$$

In general, it is impossible to simplify this further without some explicit assumptions about initial distribution \mathbb{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,

$$\varphi(\mathbf{r}) = \phi_0 a^3 \delta(\mathbf{r}), \quad (331)$$

where φ_0 is the interaction energy and a^3 the effective particle volume. In this case,

$$\begin{aligned} \mathbf{c}(t, \mathbf{x}) &= -\frac{\varphi_0 a^3}{m} \int dv^3 \int d^3y [\nabla \rho(t, \mathbf{y})] \langle \delta(\mathbf{x} - \mathbf{y}) f(t, \mathbf{x}, \mathbf{v}) \rangle \\ &= -\frac{\varphi_0 a^3}{m} [\nabla \rho(t, \mathbf{x})] \int dv^3 \langle f(t, \mathbf{x}, \mathbf{v}) \rangle \\ &= -\frac{\varphi_0 a^3}{m^2} [\nabla \rho(t, \mathbf{x})] \rho(t, \mathbf{x}) \\ &= -\frac{\varphi_0 a^3}{2m^2} \nabla \rho(t, \mathbf{x})^2 \end{aligned} \quad (332)$$

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

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

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

where

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

is the *stress tensor* with \mathbf{I} denoting unit matrix.

Closure problem

a commonly adopted closure condition is the ideal isotropic gas approximation

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

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

$$\Xi := - \left[\rho(\Sigma - \mathbf{u}\mathbf{u}) + \frac{\varphi_0 a^3}{2m^2} \rho^2 \mathbf{I} \right] \quad \Sigma - \mathbf{u}\mathbf{u} = \frac{kT}{m} \mathbf{I},$$

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

$$\Xi = -p\mathbf{I} + \mu(\nabla^\top \mathbf{u} + \nabla \mathbf{u}^\top) - \frac{2\mu}{3}(\nabla \cdot \mathbf{u}), \quad (335)$$

where $p(t, \mathbf{x})$ is the pressure field and μ 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

$$\mathbf{E} = \frac{1}{2}(\nabla^\top \mathbf{u} + \nabla \mathbf{u}^\top) \quad (336)$$

and $(\nabla \cdot \mathbf{u})$ is the *rate-of-expansion* of the flow.

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

$$\nabla \cdot \mathbf{u} = 0 \quad (337a)$$

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

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

14 The Navier-Stokes Equations

$$\begin{aligned}\rho \frac{Du_i}{Dt} &= -\frac{\partial p}{\partial x_i} + 2\mu \sum \frac{\partial}{\partial x_j} \frac{1}{2} \left(\frac{\partial u_j}{\partial x_i} + \frac{\partial u_i}{\partial x_j} \right) \\ &= -\nabla_i p + \mu \nabla_i (\nabla \cdot \mathbf{u}) + \mu \nabla^2 u_i.\end{aligned}$$

When the fluid density doesn't change very much we have seen that $\nabla \cdot \mathbf{u} = 0$, and under these conditions the *Navier-Stokes equations* for fluid motion are

$$\rho \frac{D\mathbf{u}}{Dt} = -\nabla p + \mu \nabla^2 \mathbf{u}. \quad (347)$$

14.2 The Reynolds number

For an incompressible flow, we have established that the equations of motion are

$$\rho \frac{\partial \mathbf{u}}{\partial t} + \rho \mathbf{u} \cdot \nabla \mathbf{u} = -\nabla p + \mu \nabla^2 \mathbf{u} + \mathbf{f}_{ext}, \quad (348)$$

An important parameter that indicates the relative importance of viscous and inertial forces in a given situation is the *Reynolds number*. Suppose we are looking at a problem where the characteristic velocity scale is U_0 , and the characteristic length scale for variation of the velocity is L . Then the size of the terms in the equation are

$$\frac{\partial \mathbf{u}}{\partial t} \sim \frac{U_0^2}{L}, \quad \mathbf{u} \cdot \nabla \mathbf{u} \sim \frac{U_0^2}{L}, \quad \mu \nabla^2 \mathbf{u} \sim \frac{\mu U_0}{L^2}. \quad (349)$$

The ratio of the inertial terms to the viscous term is

$$\frac{\rho U_0^2 / L}{\mu U_0 / L^2} = \frac{\rho U_0 L}{\mu} = Re, \quad (350)$$