Fundamentals of Continuum Mechanics

(Draft)

I-Liang Chern

Department of Mathematics

National Taiwan University

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Contents

Part I

Fluid Mechanics

Chapter 1

Thermodynamics of Fluids

Thermodynamics is a branch of physics which studies the energy exchange of homogeneous materials at equilibrium. These materials can be gases, liquids, solids, plasma, metals, concrete, soil, and more. The properties of these materials are described by state variables. Homogeneity in materials refers to the absence of spatial variations at a macroscopic scale. Examples of homogeneous materials are gases confined in a cylinder, parcels of fluids, or pieces of metal. The energies considered include the internal energy of the systems, mechanical work, heat, and so on.

1.1 The Thermodynamics of Gases

Goal: We will study the thermodynamics of *single-component* gases confined in a cylinder. The cylinder is equipped with a movable piston on one end, allowing for the exchange of mechanical work with the external world (see Figure 3.1). Additionally, we can introduce or extract heat from the system. The theory of thermodynamics for gases aims to describe the exchange of energy between *heat, work*, and the *internal energy* of the system.

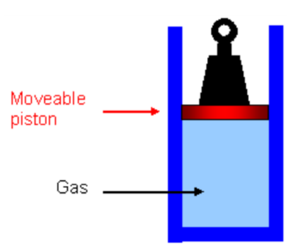

Figure 1.1: Gas in a cylinder with piston. Copied from `http://galileo.phys.virginia.edu/classes/152.mf1i.spring02/Boyle.htm`

1.1.1 Basic concepts

- **Closed system**: A closed system is defined as one that does not interchange energy with the external environment.

- **Macroscopic scales**: The macroscopic scale refers to conditions where:

  (i) The time scale dt is much larger than the time scale of particle motion τ, which is typically defined as the "mean time of free particle motion."

  (ii) The spatial scales dx^1, dx^2, and dx^3 are much larger than the "mean distance of free particle motion."

  For example, on the Earth's surface, the actual dx is approximately 68 nm for a container with 2.7×10^{25} molecules per square meter and experiencing a pressure of 759.8 Torr. Further information can be found in the Mean Free Path article on Wikipedia. For the mean time of free motion, which is the inverse of collision frequency, you can consult the Collision Frequency article on Wikipedia.

- **Equilibrium**: A thermodynamic system is considered to be in equilibrium if it remains unchanged at the macroscopic scale.

- **Thermodynamic parameters** A simple thermodynamic system consists of gases confined in a cylinder. Several measurable quantities characterize this system at equilibrium, including:

  (i) V (specific volume), representing the volume of gas per unit mass,

  (ii) p (pressure),

  (iii) T (temperature).

  The volume is a geometric quantity, while pressure is a response of the system to changes in volume. The term "thermodynamic parameters" refers to these quantities. More parameters such as entropy, internal energy, etc., will be introduced later.

- **Equation of state** The thermodynamic parameters T, V, and V associated with equilibrium are not independent. Experimental observations lead to an equation $f(T,p,V)=0$, known as the equation of state. This relation is substance-dependent; for ideal gases, $f(T,p,V)=pV-RT$. Generally, we postulate that such a thermodynamic system has only 2 degrees of freedom. It forms a surface in the p-V-T space, and its projection on the p-V plane is termed a p-V diagram. Isotherms, representing curves with constant temperatures, can be observed on the p-V plane, see subfigure (a) in Figure 1.2.

1.1.2 Works

1. Doing work to/by the system We can alter the state of the system through various physical processes. Let us introduce the following terminologies.

- **Quasi-Static Process**: A quasi-static process is characterized by its slow occurrence, ensuring the system remains in equilibrium at every instant during the process. In a continuous quasi-static process, the system is represented by a curve on the p-V plane.

- **Adiabatic Process**: An adiabatic process is a type of quasi-static process where there is no exchange of energy with the external environment except for the work done.

- **Adiabatically reachable**: Two states (p_1, V_1) and (p_2, V_2) are considered adiabatically reachable if there exists an adiabatic process connecting them. We denote the work for such an adiabatic process moving from (p_1, V_1) to (p_2, V_2) as $W(p_1, V_1; p_2, V_2)$. Please refer to Figure 1.2.

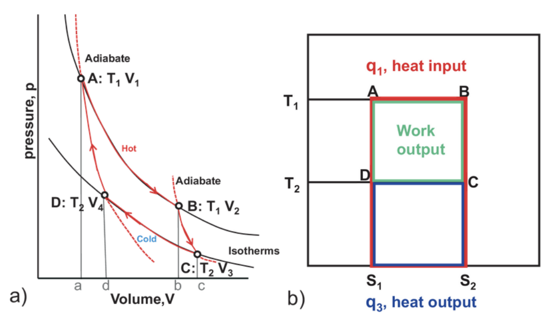

Figure 1.2: Carnot cycle on the thermodynamic plane. The left figure represents the p-V plane, while the right figure represents the T-S plane. Image source: `https://www.tf.uni-kiel.de/matwis/amat/td_kin_i/kap_1/backbone/r_se31.html`

2. First Law of Thermodynamics *The first law of thermodynamics states that the work amount $W(p_1, V_1; p_2, V_2)$ satisfies the equation*

$$W(p_1, V_1; p_2, V_2) = W(p_1, V_1; p', V') + W(p', V'; p_2, V_2),$$

for any (p', V') that can be reached from (p_1, V_1) through an adiabatic process.

- **Internal energy** From the first law, we can infer that there exists a function $U(p,V)$ called the internal energy such that

$$U(p_2,V_2) - U(p_1,V_1) = W(p_1,V_1;p_2,V_2)$$

for any pair of adiabatically reachable states (p_1,V_1) and (p_2,V_2). The function U is well-defined up to a constant. Physically, it represents the sum of all energies in the system, including translation energy, vibration energy, rotation energy, radiation energy, etc. The internal energy can be measured through the work added from outside through an adiabatic process.

- **Unit of energy** The SI unit of energy is joule (J):

$$1\,J = 1\,kg\frac{m^2}{s^2} = 10^7 ergs.$$

A practical unit is the calorie:

$$1\,cal = 4.1858\,J.$$

- **Kinetic equation of state** We shall call the relation: $U = U(p,V)$ the kinetic equation of state. An example is the ideal gas relation:

$$U(p,V) = \frac{c_v}{R}pV,$$

where c_v is the specific heat capacity at constant volume and R is the gas constant.

3. Stability assumption of the kinetic equation of state The stability assumption of the internal energy is given by

$$\boxed{\frac{\partial U}{\partial p} > 0, \quad \frac{\partial U}{\partial V} > 0.} \tag{1.1}$$

- When p is fixed, an increase in V means that we have more particles with the same momentum. As a result, the internal energy also increases, i.e., $\partial U/\partial V > 0$.

- When the size of the cylinder is fixed (i.e., the volume V is fixed), a higher pressure indicates that the particles inside the cylinder have higher momentum. This results in a higher internal energy U, implying $\partial U/\partial p > 0$.

- The assumption $\partial U/\partial p > 0$ allows us to invert the function $U = U(p,V)$ to $p = p(U,V)$. This is another form of the kinetic equation of state.

- The ideal gas relation naturally satisfies the stability assumption.

1.1.3 Characterizing adiabatic processes

In this subsection, we aim to characterize adiabatic processes by the level sets of a function on the *P*-*V* plane.

Infinitesimal Work along an adiabatic process Let us consider a gas cylinder containing a unit mass of gases. The cylinder has a piston on one end, allowing its volume to change by pushing or pulling the piston. The cylinder's wall is assumed to be thermally isolated, enabling the piston to move through an adiabatic process with no energy exchange between the gases inside the cylinder and its environment except for the work done by the piston.

For an infinitesimal pushing of the piston, the work done by the piston to the system is $dW = -p\,dV$. Here, the volume change is $-dV = -dx \cdot A$, where A is the area of the cross-section of the cylinder. The term pA represents the force F exerted on the piston per unit area A by the gas particles, and $-F\,dx$ is the work done by the piston on the gas particles in the cylinder. The first law of thermodynamics gives

$$dU = -p\,dV \tag{1.2}$$

along an adiabatic process.

Existence of the entropy function We will now demonstrate that the relationship $U = U(p,V)$ and equation (1.2) lead to the existence of a function called entropy, denoted by σ. This entropy is another thermodynamic parameter that characterizes various adiabatic processes. In other words, the level sets of σ represent adiabatic processes. This derivation, attributed to Carathéodory, establishes the mathematical foundation of thermodynamics. [1] Here are the steps for the existence of an entropy function σ:

1. Let us plug $U = U(p,V)$ into (1.2) to get

   $$U_p dp + (U_V + p)dV = 0.$$

   This is called a *Pfaffian equation*. It is equivalent to the ODE:

   $$\frac{dp}{dV} = -\frac{U_V(p,V) + p}{U_p(p,V)}. \tag{1.3}$$

   Note that from (1.1), the right-hand side of (1.3) is always less than 0 in the region $(p > 0, V > 0)$. Thus, (1.3) is always solvable in this region.

[1] Lionello Pogliani and Mario N. Berberan-Santos, "Constantin Carathéodory and the axiomatic thermodynamics" (2000)

2. A curve in the p-V plane is called an integral curve of (1.2) (or (1.3)) if it satisfies (1.2). A function $\sigma(p,V)$ is called an integral of (1.2) if its level set ($\sigma(p,V) =$ constant) is an integral curve of (1.3), that is:
$$d\sigma = 0 \quad \Leftrightarrow \quad dU + pdV = 0. \tag{1.4}$$
The solutions of (1.3) form a one-parameter family of curves: $\sigma(p,V) = C$, where C is the parameter. Each curve $\sigma(p,V) = C$ represents a specific adiabatic process. An integral of (1.2) is termed an *entropy function* of the system.

3. From (1.4), there exists a function $\mu(p,V) \neq 0$ (referred to as the integration factor) such that
$$d\sigma = \sigma_p dp + \sigma_V dV = \mu \cdot (dU + pdV). \tag{1.5}$$
We shall choose $\mu > 0$. This gives $\sigma_p > 0$ and $\sigma_V > 0$ in the region $(p > 0, V > 0)$.

4. The solutions of μ and σ are not unique. In fact, suppose σ is a solution, we can easily construct a new integration factor $\bar{\mu} := \nu(\sigma)\mu$, where $\nu(\sigma)$ is an arbitrary chosen function. In fact, by multiplying (1.5) by $\nu(\sigma)$:
$$\nu(\sigma)d\sigma = \nu(\sigma)\mu \cdot (dU + pdV),$$
we see that $\bar{\sigma}$ with $d\bar{\sigma} = \nu(\sigma)d\sigma$ is a new entropy function.

Characterizing heat

1. **Entropy Function Discovery:** From the preceding paragraph, we have
$$dU = \frac{1}{\mu} d\sigma - pdV.$$
This suggests that (σ, V) is a natural independent variable for the internal energy. For this purpose, we make a change of variable:
$$(p,V) \mapsto (\sigma, V)$$
using the formula
$$\sigma = \sigma(p,V).$$
This inversion $p = p(\sigma, V)$ is always possible in the region $(p > 0, V > 0)$ because $\sigma_p > 0$ there. Using (σ, V) as the new state variables, we express equation (1.5) as:
$$dU = \tau d\sigma - pdV, \tag{1.6}$$
where $\tau = 1/\mu = U_\sigma$.

2. **Interpretation of Formula (1.6):** This formula has a meaningful interpretation: When $d\sigma = 0$ (i.e., adiabatic process), the change in internal energy is attributed to the work exerted from outside, represented by $-pdV$. When $dV = 0$ (i.e., no exerted work), the change in U is due to $\tau d\sigma$, denoting the heat added from outside to the system.

3. **Uniqueness of Integration Factor and Entropy Function:** As previously mentioned, the integration factor $1/\tau$ and the integral (entropy function) σ lack uniqueness. Later on, we will introduce the concepts of intensive variables and extensive variables. By selecting τ as an intensive variable (termed the absolute temperature), the corresponding σ becomes the physical entropy S.

1.1.4 Heats

Intensive and extensive variables There are two kinds of thermodynamic state variables, the intensive and extensive variables. A variable is considered intensive if it is independent of the system's size. In other words, for the combined system of two subsystems I and II, an intensive variable x remains unchanged ($x_{I+II} = x_I = x_{II}$), while an extensive variable x adds up ($x_{I+II} = x_I + x_{II}$). Examples of extensive variables include volume (V) and internal energy (U), while temperature (T) and pressure (p) are intensive. Notably, if x and y are extensive variables, then $\partial y/\partial x$ is intensive.

In the first law of thermodynamics

$$dU = \tau d\sigma - pdV$$

U, V are extensive, while p is intensive. Choosing τ to be intensive makes σ extensive. A natural choice of τ is the temperature, the corresponding σ becomes the entropy. The temperature is further characterized below.

Equilibrium and empirical temperature

- **Thermo equilibrium** When two systems $\mathscr{S}_1$ and $\mathscr{S}_2$ are in contact, allowing energy transfer but not with the outside, they reach a steady state on the macroscopic scale, signifying thermo equilibrium ($\mathscr{S}_1 \sim \mathscr{S}_2$).

- **The zeroth law of thermodynamics:**

  $$\text{If } \mathscr{S}_1 \sim \mathscr{S}_2 \text{ and } \mathscr{S}_2 \sim \mathscr{S}_3, \text{ then } \mathscr{S}_1 \sim \mathscr{S}_3.$$

  This law establishes an equivalence relation among all states, represented by the temperature.

- **Ideal gas thermometer** The ideal gas is postulated to satisfy $pV = constant$ in an equilibrium equivalent class. The temperature label for this class is

$$\theta = pV/R,$$

where R is the gas constant.

- **Heat bed and empirical temperature** By merging a small system $\mathscr{S}$ into a heat bed filled with ideal gases, we measure its temperature. The empirical temperature of the heat bed represents the temperature of $\mathscr{S}$. Thus, each state of $\mathscr{S}(p,V)$ is associated with an empirical temperature $\theta(p,V)$.

Caloric equation of state

- **Existence Postulate** The zeroth law of thermodynamics can be postulated by the *existence of a state function $\theta(p,V)$, characterizing thermo equilibrium states.* characterizing thermo equilibrium states. Two states (p_1,V_1) and (p_2,V_2) are in thermo equilibrium if $\theta(p_1,V_1) = \theta(p_2,V_2)$.

- **Stability assumption:** The state function $\theta(p,V)$ is postulated to satisfy stability conditions:

$$\frac{\partial\theta}{\partial p} > 0, \quad \frac{\partial\theta}{\partial V} > 0. \tag{1.7}$$

Absolute temperature T and the entropy S Let us revisit the solution of the Pfaffin equation (1.2). Let σ be one of its solution and $1/\tau$ be the corresponding integration factor. We relate τ and the empirical temperature θ by the following steps.

1. We divide the system $\mathscr{S}$ into two subsystems $\mathscr{S}_1$ and $\mathscr{S}_2$, which are in thermodynamic equilibrium with a common empirical temperature θ.

2. We shall use (σ,θ) as our new state variables instead of (σ,V). It can be verified that $\theta = \theta(\sigma,V)$ satisfies $\left(\frac{\partial\theta}{\partial V}\right)_\sigma \neq 0$, allowing us to invert θ and V in the formula $\theta = \theta(\sigma,V)$.

3. At thermodynamic equilibrium, $\mathscr{S} = (\sigma,\theta)$, $\mathscr{S}_1 = (\sigma_1,\theta)$, $\mathscr{S}_2 = (\sigma_2,\theta)$, and by adding heat to $\mathscr{S}$ without doing work, equation (1.6) gives:

$$\tau(\theta,\sigma)d\sigma = \tau_1(\theta,\sigma_1)d\sigma_1 + \tau_2(\theta,\sigma_2)d\sigma_2. \tag{1.8}$$

   This implies that the entropy function σ of the combined system $\mathscr{S}$, originally a function of $(\theta,\sigma_1,\sigma_2)$, is independent of θ.

4. Therefore, $\sigma = \sigma(\sigma_1, \sigma_2)$ and

$$\frac{\tau_1(\theta,\sigma_1)}{\tau(\theta,\sigma)} = \left(\frac{\partial\sigma}{\partial\sigma_1}\right)_{\sigma_2} = \phi(\sigma_1,\sigma_2),$$
$$\frac{\tau_2(\theta,\sigma_2)}{\tau(\theta,\sigma)} = \left(\frac{\partial\sigma}{\partial\sigma_2}\right)_{\sigma_1} = \psi(\sigma_1,\sigma_2),$$

   are independent of θ.

5. This implies the existence of functions $T(\theta)$, $\nu_1(\sigma_1)$, $\nu_2(\sigma_2)$, $\nu(\sigma)$ such that

$$\tau_1(\theta,\sigma_1) = T(\theta)\nu_1(\sigma_1),$$
$$\tau_2(\theta,\sigma_2) = T(\theta)\nu_2(\sigma_2),$$
$$\tau(\theta,\sigma) = T(\theta)\nu(\sigma).$$

   Equation (1.8) becomes

$$T\nu(\sigma)d\sigma = T\nu_1(\sigma_1)d\sigma_1 + T\nu_2(\sigma_2)d\sigma_2. \tag{1.9}$$

6. If we define

$$S_i(\sigma_i) := \int^{\sigma_i} \nu_i(\sigma_i)\, d\sigma_i, \quad , i = 1,2,$$

   then (1.9) implies

$$dS = dS_1 + dS_2. \tag{1.10}$$

7. The function $T(\theta)$ defined above is called the *absolute temperature* of the system. Note that $T \neq 0$. So, we choose

$$T > 0.$$

   Choosing the integration factor $\mu := 1/T$ implies that the corresponding entropy function has the property (1.10). If $\mathscr{S}$ is divided into m subsystems, then

$$dS = \sum_{i=1}^{m} dS_i.$$

   Since S can be determined uniquely up to an integration constant, we can choose S so that

$$S = \sum_{i=1}^{m} S_i. \tag{1.11}$$

Measuring system's entropy On the thermo p-V plan , we can draw isothermal curves (Figure 1.2). Along an isothermal curve, the line integral

$$S_2 - S_1 = \int_{S_1}^{S_2} \frac{dQ}{T}$$

gives entropy the difference. This can be used to measure the entropy of a state (p,V).

Gibbs relation: The first law of thermodynamics now reads

$$\boxed{dU = TdS - pdV.} \tag{1.12}$$

The term dU represents the change in the internal energy of the system, the first term on the right TdS is the heat added to the system, and the second term $-pdV$ is the mechanical work done from outside to the system. Formula (1.12) is called the *Gibbs relation*.

Constitutive Law Using (S,V) as the independent variable, the internal energy can be expressed as

$$\boxed{U = U(S,V).} \tag{1.13}$$

This is called the constitutive law of the gas system. The temperature T and the pressure p are derived parameters:

$$T = \left(\frac{\partial U}{\partial S}\right)_V, \quad p = -\left(\frac{\partial U}{\partial V}\right)_S.$$

Summary: Complete characterization of the gas thermosystem The thermodynamics of a gas system is completely characterized by the constitutive relation

$$U = U(S,V).$$

The first law of thermodynamics

$$dU = TdS - pdV,$$

leads to

$$T = \left(\frac{\partial U}{\partial S}\right)_V, \quad p = -\left(\frac{\partial U}{\partial V}\right)_S.$$

Conversely, one can use the first law of thermodynamics together with two equations of states:

- kinetic equation of state: $U = U(p,V)$,
- caloric equation of state: $T = \theta(p,V)$,

to obtain the constitutive law $U = U(S,V)$.

1.1.5 Ideal Gases and Polytropic Gases

In a gas thermodynamic system, we deal with five thermodynamic variables (V, p, S, T, U), with only two of them being independent. The first law of thermodynamics (11.3), and two equations of states: kinetic and calorie, govern these variables, deriving from either measurements or statistical mechanics. Here, we illustrate a specific examples of a gas thermodynamic system, known as the ideal gases and the polytropic gases. [2]

Ideal gas law

- **Kinetic equation of state - Ideal gas law:** The ideal gas law, representing Boyle's and Gay-Lussac's laws, is given by:

$$pV = RT, \tag{1.14}$$

where R is the universal gas constant (approximately $8.314462618\ \mathrm{J}\cdot\mathrm{K}^{-1}\cdot\mathrm{mol}^{-1}$), see Gas Constant, Wiki. Under a mild assumption (stated below), the ideal gas law and the Gibbs relation imply that U is solely a function of T.

- **Theorem:** *Under a mild assumption (1.16) below, the ideal gas law and the Gibbs relation imply that U is only a function of T.* [3]
Derivation:

  1. From the first law of thermodynamics (1.12), treating (S, V) as the independent variables, we obtain:

  $$p = -\left(\frac{\partial U}{\partial V}\right)_S \quad \text{and} \quad T = \left(\frac{\partial U}{\partial S}\right)_V.$$

  Plugging these into the ideal gas law (1.14), we get a partial differential equation (PDE) for U in (S, V):

  $$R\frac{\partial U}{\partial S} + V\frac{\partial U}{\partial V} = 0.$$

  This linear first-order equation can be solved by the method of characteristics as shown below.

  2. Let us rewrite this equation as a directional differentiation:

  $$\left(R\frac{\partial}{\partial S} + V\frac{\partial}{\partial V}\right)U = 0. \tag{1.15}$$

[2] Courant and Friedrichs, Supersonic Flows and Shock Waves
[3] This derivation is referred to in Courant-Friedrichs' book.

It means that U is unchanged along the direction: $(dS, dV) \parallel (R, V)$. The integral curves of these directions are the solutions of the differential equation

$$\frac{dV}{dS} = \frac{V}{R}.$$

They are called the characteristic curves. This equation can be integrated as

$$\frac{dV}{V} - \frac{dS}{R} = 0 \quad \Rightarrow \quad \ln V - \frac{S}{R} = C \quad \Rightarrow \quad V \exp(-S/R) = e^C.$$

Here, C is an integration constant. Thus, (1.15) implies that $U(V,S)$ is constant whenever $\phi := V \exp(-S/R)$ is a constant. This means that U and ϕ are functionally dependent, which implies that there exists a function $h : \mathbb{R}^+ \to \mathbb{R}$ such that

$$U = h(\phi).$$

3. We claim that U is a function of T only. This can be derived by the following arguments. First, we note that $h' < 0$ because

$$p = -(\frac{\partial U}{\partial V})_S = -\exp(-S/R)h'(V \exp(-S/R)) > 0.$$

Next, from

$$T = (\frac{\partial U}{\partial S})_V = h'(\phi)\left(\frac{\partial \phi}{\partial S}\right)_V = h'(\phi)\left(-\frac{V}{R}e^{-S/R}\right) = -\frac{1}{R}h'(\phi)\cdot\phi,$$

we see that T is a function of ϕ.

4. We shall make an assumption that this function is invertible. That is, the derivative

$$\left(h'(\phi)\phi\right)' > 0 \text{ for } \phi > 0. \tag{1.16}$$

We get that T is a decreasing function of ϕ. With this, we can invert the relation between T and ϕ and treat ϕ as a decreasing function of T. By inverting U and ϕ, and T and ϕ, we get that U is an increasing function of T:

$$\boxed{U = U(T).}$$

We shall make this our second constitutive relation.

The heat capacities

- **Specific heat capacities** Let us denote by $dQ = TdS$ the heat added to the system. From Gibbs' relation, $dQ = dU + pdV$. Using $RT = pV$, we have

$$\begin{aligned} dQ &= dU + pdV \\ &= U'(T)dT + pdV \\ &= U'(T)dT + RdT - Vdp. \end{aligned}$$

  The first and the third equalities lead to the following derived quantities:

$$\begin{aligned} c_v &:= \left(\frac{\partial Q}{\partial T}\right)_V = U'(T), \\ c_p &:= \left(\frac{\partial Q}{\partial T}\right)_p = U'(T) + R, \end{aligned}$$

  called the *specific heat capacities at constant volume and constant pressure*, respectively. Since $R > 0$, we have $c_p > c_v$. Recall that c_p is the amount of heat added to a system per unit mass at constant pressure. When we heat the system at constant pressure, the volume has to expand to maintain constant pressure, the extra amount of work for expansion is supplied by the extra amount of heat, which is R per unit mass.

- **Heat capacity ratio** $\gamma := c_p/c_v$

  1. Let γ be the ratio between c_p and c_v:

  $$\gamma = \frac{c_p}{c_v} = \frac{c_v + R}{c_v}.$$

     This heat capacity ratio is also called the adiabatic index.

  2. For a monatomic gas molecule (like helium or argon), there are three translational degrees of freedom. Every atom has an average kinetic energy of $\frac{3}{2}k_B T$ in thermal equilibrium, where k_B is the Boltzmann constant. For 1 mole of gas, this becomes $U = \frac{3}{2}RT$. Thus, $c_v = U'(T) = \frac{3}{2}R$. Note that the number 3 comes from the three translational degrees of freedom. Each degree of freedom contribute $RT/2$ amount of energy.

  3. For ideal gas with f degrees of freedom, $U = \frac{f}{2}RT$, and the corresponding

  $$c_v = \frac{f}{2}R.$$

This is a consequence of the equipartition theorem in statistical mechanics. For a diatomic molecule (like oxygen or nitrogen), in addition to translational motion (in $\mathbb{R}^3$), there are two rotational degrees of freedom (in S^2). This totals to $f = 5$ degrees of freedom.

4. Thus, we have

$$\gamma = \frac{c_v + R}{c_v} = \frac{f+2}{f}, \quad 1 < \gamma \leq \frac{5}{3} \tag{1.17}$$

for ideal gases. When γ is closer to $5/3$, the gas is harder to compress because all work input is reacted by the translation of the mono-atoms. On the other hand, when γ is closer to 1, the gas is easily compressed as the input energy is transferred to other modes of molecular energies. For further discussion about γ, we refer to wiki: Heat Capacity Ratio.

Polytropic gases

- **Caloric equation of state:** If $U(T) = c_v T$, the energy we add to the system is proportional to the temperature, we call such gases the *polytropic gases.* The ratio c_v is called the specific heat capacity at constant volume.

- **Algebraic relations of the polytropic gases**

1. We have five thermodynamic variables p, V, U, S, T, and three relations:

$$\begin{cases} pV &= RT \\ U &= c_v T \\ dU &= T dS - p dV \end{cases}.$$

2. Plugging the two constitutive relations

$$pV = RT \text{ and } U = c_v T \tag{1.18}$$

into the first law of thermodynamics (1.12), we obtain

$$
\begin{aligned}
& dU = T\,dS - p\,dV \\
& \frac{c_v}{R} d(pV) = \frac{pV}{R} dS - p\,dV \\
& c_v \frac{d(pV)}{pV} = dS - R\frac{dV}{V} \\
& dS = d\ln\left((pV)^{c_v}\right) + d\ln\left(V^R\right) \\
& \quad\;\; = d\ln\left(p^{c_v}\cdot V^{c_v+R}\right) \\
& S - S_0 = \ln\left(p^{c_v}\cdot V^{c_v+R}\right) \\
& e^{S-S_0} = \left(pV^{(c_v+R)/c_v}\right)^{c_v} \\
& e^{(S-S_0)/c_v} = pV^{(c_v+R)/c_v}.
\end{aligned}
$$

3. Define

$$\gamma := 1 + R/c_v, \quad A(S) := \exp((S-S_0)/c_v),$$

then, the algebraic relations of the thermodynamic variables in terms of (S,V) are

$$
\begin{cases}
p = A(S)V^{-\gamma} \\
T = \frac{A(S)}{R} V^{-\gamma+1} \\
U = \frac{c_v A(S)}{R} V^{-\gamma+1}.
\end{cases}
\tag{1.19}
$$

Summary of algebraic relations of state variables For ideal gases, these two equations of states are the ideal gas law: $pV = RT$ and $U = c_v T$. The algebraic relations of the state variables are listed below.

- In terms of (ρ, U):

$$p = (\gamma-1)\rho U, \quad T = \frac{\gamma-1}{R} U,$$

$$S - S_0 = \frac{R}{\gamma-1} \ln\left(U\rho^{-\gamma+1}\right).$$

- In terms of (V, S):

$$U = (\gamma-1)^{-1} A(S) V^{-\gamma+1}, \quad A(S) = \exp\left(\frac{\gamma-1}{R}(S-S_0)\right),$$

$$p = A(S)V^{-\gamma}, \quad T = \frac{1}{R} A(S) V^{-\gamma+1}.$$

- In terms of (ρ, p):

$$U = \frac{1}{\gamma - 1} p\rho^{-1}, \quad T = \frac{1}{R} p\rho^{-1},$$
$$S - S_0 = \frac{R}{\gamma - 1} \ln\left(\frac{1}{\gamma - 1} p\rho^{-\gamma}\right).$$

Homeworks

1. Prove that adiabats (lines of constant entropy) have a steeper slope than isotherms (lines of constant temperature) for an ideal gas on a p-V diagram, where the pressure p is the ordinate and the volume per unit mass V the abscissa. Again, carefully draw a diagram of a Carnot cycle, and compute the slopes of the isotherms and adiabats in terms of p and V.

2. Write a short report on Carnot cycle for an ideal gas.

1.2 Other energy forms, Legendre transform

1.2.1 Enthalpy, Helmholtz, Gibbs free energies

- **Enthalpy:** In the Gibbs relation

$$dU = TdS - pdV,$$

the system's energy U can be varied by changing the volume at constant entropy, or by adding heat at constant volume. The relative changes give

$$-p = \left(\frac{\partial U}{\partial V}\right)_S \quad \text{and} \quad T = \left(\frac{\partial U}{\partial S}\right)_V,$$

respectively. We say that (S,V) are the natural independent variables for U.

Alternatively, we can analyze system's energy change with respect to p at constant entropy. This suggests the following change of variable:

$$(S,V) \mapsto (S,p) \text{ through } -p = \left(\frac{\partial U}{\partial V}\right)_S.$$

By adding $d(PV)$ in the Gibbs relation:

$$dU + d(pV) = TdS - pdV + d(pV) = TdS + Vdp,$$

the natural independent variables become (S,p). The corresponding energy, $H(S,p) := U + pV$, is termed the *enthalpy*. Enthalpy comprises a system's internal energy and the work required to create the system by displacing its environment, establishing its volume and pressure.

- **Helmholtz Free Energy** Using the change-variable formula:

$$(S,V) \mapsto (T,V) \text{ through } T = \left(\frac{\partial U}{\partial S}\right)_T,$$

and noting

$$dU - d(TS) = TdS - pdV - TdS - SdT,$$

we define the Helmholtz free energy $\Psi(T,V) := U - TS$, and get

$$d\Psi = -SdT - pdV.$$

Note that

$$-p = \left(\frac{\partial \Psi}{\partial V}\right)_T = \left(\frac{\partial U}{\partial V}\right)_S,$$

meaning that the pressure can be obtained from the response of Ψ to the volume change at constant temperature, or the response of U to the volume change at constant entropy.

- **Gibbs Free Energy:** At last, we consider the change-of-variable:

$$(S,V) \mapsto (T,p)$$

through both

$$-p = \left(\frac{\partial U}{\partial V}\right)_S \text{ and } T = \left(\frac{\partial U}{\partial S}\right)_T$$

Define the Gibbs free energy

$$G(T,p) := U + pV - TS.$$

We have

$$dG = TdS - pdV + d(pV) - d(TS) = -SdT + Vdp.$$

- **Process's names with Fixed Thermo Variables:**

$$\text{Adiabatic: } dS = 0, \quad \text{Isochoric: } dV = 0,$$
$$\text{Isothermal: } dT = 0, \quad \text{Isobaric: } dp = 0.$$

1.2.2 Legendre Transformation

- The transformations from U to H, Ψ, and G are called Legendre transformations. Let us introduce it mathematically.

- Consider a convex function $f : \mathbb{R} \to \mathbb{R}$. The differential

$$df(x) = f'(x)dx.$$

Let us introduce a new variable $y = f'(x)$. Consider the change of variable

$$x \mapsto y = f'(x). \tag{1.20}$$

This mapping is invertible because f is convex and thus f' is an increasing function. We then define

$$f^*(y) := xy - f(x).$$

Here x is treated as a function of y from (1.20). We have

$$df^*(y) = d(xy) - f'(x)dx = d(xy) - ydx = xdy,$$

$$x = (f^*(y))'.$$

- Since f is a convex function, there is another equivalent expression for $f^*(y)$:

$$f^*(y) := \sup_x [x \cdot y - f(x)].$$

The maximum occurs at $y = f'(x)$. The pair (x, y) with $y = f'(x)$ is called a conjugate pair.

- **Lemma.** f^* is convex.

- **Lemma.** If f is convex, then $f^{**}(x) = f(x)$.

- $-H$, $-\Psi$ and $-G$ are the Legendre transformations of the internal energy U:

$$\begin{aligned}
-H(S,p) &= \sup_V [(-p)V - U(S,V)] \\
-\Psi(T,V) &= \sup_S [ST - U(S,V)] \\
-G(T,p) &= \sup_V \sup_S [(-p)V + ST - U(S,V)]
\end{aligned}$$

Or equivalently,

$$\begin{aligned} H(S,p) &= \min_V [U(S,V) + pV] \\ \Psi(T,V) &= \min_S [U(S,V) - TS] \\ G(T,p) &= \min_{V,S} [U(S,V) + pV - TS] \end{aligned}$$

To have a legitimate Legendre transformations, we require U to be convex in S and V, respectively.

- Both (p,V) and (T,S) are conjugate pairs.

1.2.3 Maxwell relations

Thermo relations The thermo relations are expressed in terms of two independent thermo variables.

- Using (S,V) as independent variables:

$$T = \left(\frac{\partial U}{\partial S}\right)_V, \quad -p = \left(\frac{\partial U}{\partial V}\right)_S,$$

- Using (S,p) as independent variables:

$$T = \left(\frac{\partial H}{\partial S}\right)_p, \quad V = \left(\frac{\partial H}{\partial p}\right)_S,$$

- Using (T,V) as independent variables:

$$-S = \left(\frac{\partial \Psi}{\partial T}\right)_V, \quad -p = \left(\frac{\partial \Psi}{\partial V}\right)_T$$

- Using (T,p) as independent variables:

$$-S = \left(\frac{\partial G}{\partial T}\right)_p, \quad V = \left(\frac{\partial G}{\partial p}\right)_T$$

Maxwell relations From

$$\frac{\partial^2 U}{\partial V \partial S} = \frac{\partial^2 U}{\partial S \partial V}, \quad T = \left(\frac{\partial U}{\partial S}\right)_V, \quad -p = \left(\frac{\partial U}{\partial V}\right)_S,$$

we get

$$\left(\frac{\partial T}{\partial V}\right)_S = -\left(\frac{\partial p}{\partial S}\right)_V.$$

In general, we have the following Maxwell relations:

$$\left(\frac{\partial T}{\partial V}\right)_S = -\left(\frac{\partial p}{\partial S}\right)_V = \frac{\partial^2 U}{\partial S \partial V} \tag{1.21}$$

$$\left(\frac{\partial T}{\partial p}\right)_S = \left(\frac{\partial V}{\partial S}\right)_p = \frac{\partial^2 H}{\partial S \partial p} \tag{1.22}$$

$$\left(\frac{\partial S}{\partial V}\right)_T = \left(\frac{\partial p}{\partial T}\right)_V = -\frac{\partial^2 \Psi}{\partial T \partial V} \tag{1.23}$$

$$-\left(\frac{\partial S}{\partial p}\right)_T = \left(\frac{\partial V}{\partial T}\right)_p = \frac{\partial^2 G}{\partial T \partial p}. \tag{1.24}$$

1.3 Thermodynamic Stability

Material properties can be characterized by its response to some external probs. For instance, we can measure how much heat to add to the system in order to increase its temperature by one degree. This is the heat capacity (dQ/dT). We can measure the volume change under increase of pressure. This is the compressibility (dV/dp). We can measure volume change under increase of temperature (dV/dT). This is the expansion rate.

Heat capacity Let us define $dQ = TdS$, the heat added to the system. Define heat capacity to be the heat added to the system per unit temperature, with either V or p fixed. That is,

$$c_v := \left(\frac{dQ}{dT}\right)_V, \quad c_p := \left(\frac{dQ}{dT}\right)_p.$$

From the Gibbs relations

$$dU = dQ - pdV, \quad dH = dQ + Vdp,$$

we get

$$c_v = \left(\frac{\partial U}{\partial T}\right)_V, \quad c_p = \left(\frac{\partial H}{\partial T}\right)_p,$$

and

$$c_v = \left(\frac{dQ}{dT}\right)_V = T\left(\frac{\partial S}{\partial T}\right)_V = -T\left(\frac{\partial^2 \Psi}{\partial T^2}\right)_V, \tag{1.25}$$

$$c_p = \left(\frac{dQ}{dT}\right)_p = T\left(\frac{\partial S}{\partial T}\right)_p = -T\left(\frac{\partial^2 G}{\partial T^2}\right)_p. \tag{1.26}$$

Compression rate The isentropic/isothermal compressibility rate are defined as

$$\kappa_S := -\frac{1}{V}\left(\frac{\partial V}{\partial p}\right)_S = -\frac{1}{V}\left(\frac{\partial^2 H}{\partial p^2}\right)_S, \tag{1.27}$$

$$\kappa_T := -\frac{1}{V}\left(\frac{\partial V}{\partial p}\right)_T = -\frac{1}{V}\left(\frac{\partial^2 G}{\partial p^2}\right)_T. \tag{1.28}$$

Expansion rate: The expansion rate is defined as

$$\alpha_p := \frac{1}{V}\left(\frac{\partial V}{\partial T}\right)_p = \frac{1}{V}\left(\frac{\partial}{\partial T}\right)_p\left(\frac{\partial G}{\partial p}\right)_T.$$

Proposition 1.1. *The heat capacities and compressibility rates satisfy*

$$\kappa_T(c_p - c_v) = TV\alpha_p^2 \tag{1.29}$$

$$c_p(\kappa_T - \kappa_S) = TV\alpha_p^2, \tag{1.30}$$

and

$$\frac{c_p}{c_v} = \frac{\kappa_T}{\kappa_S}.$$

Thus, there are five parameters with two independent relations.

Proof. 1. Differentiate $S(T, V(T,p))$ in T with fixed p:

$$\left(\frac{\partial S}{\partial T}\right)_p = \left(\frac{\partial S}{\partial T}\right)_V + \left(\frac{\partial S}{\partial V}\right)_T\left(\frac{\partial V}{\partial T}\right)_p,$$

then multiply it by T, we get

$$c_p = c_v + T\left(\frac{\partial S}{\partial V}\right)_T\left(\frac{\partial V}{\partial T}\right)_p.$$

Multiply this by $\kappa_T = -\frac{1}{V}\left(\frac{\partial V}{\partial p}\right)_T$, we get

$$\begin{aligned}
\kappa_T(c_p - c_v) &= -\frac{T}{V}\left(\frac{\partial V}{\partial p}\right)_T \left(\frac{\partial S}{\partial V}\right)_T \left(\frac{\partial V}{\partial T}\right)_p \\
&= -\frac{T}{V}\left(\frac{\partial S}{\partial p}\right)_T \left(\frac{\partial V}{\partial T}\right)_p && \because \text{chain rule} \\
&= +\frac{T}{V}\left(\frac{\partial V}{\partial T}\right)_p \left(\frac{\partial V}{\partial T}\right)_p && \because (1.24) \\
&= TV\left(\frac{1}{V}\left(\frac{\partial V}{\partial T}\right)_p\right)^2 \\
&= TV\alpha_p^2
\end{aligned}$$

2. Differentiate $V(p, S(p,T))$ in p with fixed T:

$$\left(\frac{\partial V}{\partial p}\right)_T = \left(\frac{\partial V}{\partial p}\right)_S + \left(\frac{\partial V}{\partial S}\right)_p \left(\frac{\partial S}{\partial p}\right)_T.$$

Multiply it by $-1/V$, we get

$$\kappa_T = \kappa_S - \frac{1}{V}\left(\frac{\partial V}{\partial S}\right)_p \left(\frac{\partial S}{\partial p}\right)_T.$$

Then multiply it by $c_p = T\left(\frac{\partial S}{\partial T}\right)_p$, we get

$$\begin{aligned}
c_p(\kappa_T - \kappa_S) &= -\frac{T}{V}\left(\frac{\partial S}{\partial T}\right)_p \left(\frac{\partial V}{\partial S}\right)_p \left(\frac{\partial S}{\partial p}\right)_T \\
&= -\frac{T}{V}\left(\frac{\partial V}{\partial T}\right)_p \left(\frac{\partial S}{\partial p}\right)_T && \because \text{chain rule} \\
&= \frac{T}{V}\left(\frac{\partial S}{\partial p}\right)_T \left(\frac{\partial S}{\partial p}\right)_T && \because (1.24) \\
&= \frac{T}{V}\left(\frac{\partial V}{\partial T}\right)_p^2 \\
&= TV\left(\frac{1}{V}\left(\frac{\partial V}{\partial T}\right)_p\right)^2 \\
&= TV\alpha_p^2.
\end{aligned}$$

$\square$

Theorem 1.1. *The following statements hold.*

(i) U *satisfies* $\left(\frac{\partial^2 U}{\partial S^2}\right)_V \geq 0, \quad \left(\frac{\partial^2 U}{\partial V^2}\right)_S \geq 0 \quad \Leftrightarrow \quad \kappa_S \geq 0,\ c_v \geq 0$

(ii) H *satisfies* $\left(\frac{\partial^2 H}{\partial S^2}\right)_p \geq 0, \quad \left(\frac{\partial^2 H}{\partial p^2}\right)_S \leq 0 \quad \Leftrightarrow \quad \kappa_S \geq 0,\ c_p \geq 0$

(iii) Ψ *satisfies* $\left(\frac{\partial^2 \Psi}{\partial T^2}\right)_V \leq 0, \quad \left(\frac{\partial^2 \Psi}{\partial V^2}\right)_T \geq 0 \quad \Leftrightarrow \quad \kappa_T \geq 0,\ c_v \geq 0$

(iv) G *satisfies* $\left(\frac{\partial^2 G}{\partial T^2}\right)_p \leq 0, \quad \left(\frac{\partial^2 G}{\partial p^2}\right)_T \leq 0 \quad \Leftrightarrow \quad \kappa_T \geq 0,\ c_p \geq 0$

Proof. The second derivatives of U, h, A, B are respectively

$$
\begin{aligned}
\left(\frac{\partial^2 U}{\partial S^2}\right)_V &= \left(\frac{\partial T}{\partial S}\right)_V = \frac{T}{T\left(\frac{\partial S}{\partial T}\right)_V} = \frac{T}{c_v} \\
\left(\frac{\partial^2 U}{\partial V^2}\right)_S &= \left(-\frac{\partial p}{\partial V}\right)_S = -\frac{\frac{1}{V}}{\frac{1}{V}\left(\frac{\partial V}{\partial p}\right)_S} = \frac{1}{V}\frac{1}{\kappa_S} \\
\left(\frac{\partial^2 H}{\partial S^2}\right)_p &= \left(\frac{\partial T}{\partial S}\right)_p = \frac{T}{T\left(\frac{\partial S}{\partial T}\right)_p} = \frac{T}{c_p} \\
\left(\frac{\partial^2 H}{\partial p^2}\right)_S &= \left(\frac{\partial V}{\partial p}\right)_S = -V\left(\frac{-1}{V}\left(\frac{\partial V}{\partial p}\right)_S\right) = -V\kappa_S \\
\left(\frac{\partial^2 \Psi}{\partial T^2}\right)_V &= -\frac{c_v}{T} \\
\left(\frac{\partial^2 \Psi}{\partial V^2}\right)_T &= -\left(\frac{\partial p}{\partial V}\right)_T = \frac{1}{V}\frac{1}{\kappa_T} \\
\left(\frac{\partial^2 G}{\partial T^2}\right)_p &= -\frac{c_p}{T} \\
\left(\frac{\partial^2 G}{\partial p^2}\right)_T &= -V\kappa_T.
\end{aligned}
$$

□

From Proposition 1.1, we only need three of the above four inequalities for stability.

Definition 1.1. *A gas thermodynamic system is called thermodynamic stable if* $U_{SS} \geq 0$ *and* $U_{VV} \geq 0$.

Note that ($U_{SS} \ge 0$, $U_{VV} \ge 0$) is equivalent to any one of the following three:

- $H_{SS} \ge 0$, $H_{pp} \le 0$,
- $\Psi_{TT} \le 0$, $\Psi_{VV} \ge 0$,
- $G_{TT} \le 0$, $G_{pp} \le 0$.

That is, *the energy is convex in extensive variable and concave in intensive variable*[Callen].

Corollary 1.1. *Assuming thermodynamic stability, then*

$$c_p \ge c_v, \quad \kappa_T \ge \kappa_S.$$

Remarks

- This stability condition $U_{VV} > 0$ is equivalent to the condition of finite sound speed. The sound speed is defined by
$$c^2 := \left(\frac{\partial p(\rho, S)}{\partial \rho}\right)_S,$$
which is also
$$c^2 = \left(\frac{\partial V}{\partial \rho}\right)_S \left(\frac{\partial}{\partial V}\right)_S \left(-\frac{\partial U}{\partial V}\right)_S = V^2 \left(\frac{\partial^2 U}{\partial V^2}\right)_S.$$
The positivity on the right-hand side of the above equation gives real value of sound speed. This property leads to finite speed propagation of signal in rest gases. Namely, the governing equation for the perturbed gas is
$$u_{tt} = c^2 u_{xx},$$
where $u = \delta\rho$ is the perturbed density. If initial data is e^{ikx}, then the solution has the form $e^{i(kx \pm \omega(k)t)}$, where $\omega(k)$ satisfies the dispersion relation: $\omega^2 = c^2 k^2$. If c is not real, then u will grow exponentially in time. This is unstable.

- For γ-law gases, the stability $\left(\frac{\partial p}{\partial \rho}\right)_S > 0$ is equivalent to $\gamma > 1$.

- The Hessian of G is
$$\begin{bmatrix} G_{TT} & G_{Tp} \\ G_{Tp} & G_{pp} \end{bmatrix} = \begin{bmatrix} -\frac{c_p}{T} & \alpha_p V \\ \alpha_p V & -V\kappa_T \end{bmatrix}$$
Its determinant
$$\Delta = \frac{V}{T}\kappa_T c_p - \alpha_p^2 V^2 = \frac{V}{T} c_v \kappa_T.$$
Here, we have used (1.29). The negative definiteness of the Hessian of G is referred to a stronger thermodynamic stability. We refer this to Callen's book.

Homework.

1. Find the Hessian of U.
   Hint: The transformation $(S,V) \mapsto (T,p)$ is the Legendre transformation associated with U. Its Jacobian is the Hessian of U. Its inverse map $(T,p) \mapsto (S,V)$ is the Legendre transformation associated with G.

Historial remarks

- The axiomatic approach in this chapter is mainly due to Gibbs and Carathéodory.
- Historical Note of Thermodynamics about Irreversibility and the Second Law of Thermodynamics.

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Chapter 2

Dynamics of Fluid Flows

There are two formulations of fluid dynamics: Eulerian and Lagrangian. The former is described from the observer's frame of reference, while the latter is described from the material frame (or reference frame), meaning that the fluid particles are initially labeled, and the description is from each labeled particle's point of view.

Suppose the fluid (the continuum object) occupies a region $\hat{M}$ initially and evolves to a domain M_t at time t. We will refer to M_t as the observer's domain, while $\hat{M}$ is the material (reference) domain.

- In the Lagrangian formulation, we assume $\hat{M} \subset \mathbb{R}^3$, and the coordinate of the reference domain $\hat{M}$ is called the Lagrangian coordinate, material coordinate, reference coordinate, or label coordinate. It will be denoted by X. Its components are denoted by X^α, $\alpha = 1, 2, 3$. The embedding $\hat{M} \subset \mathbb{R}^3$ induces a natural volume element $\hat{\mu} = dX = dX^1 \wedge dX^2 \wedge dX^3$ in $\hat{M}$.

- The coordinate of the observer's domain M_t is called the Eulerian coordinate or the observer's coordinate. It is denoted by $\mathbf{x}$. Its components are denoted by x^i, $i = 1, 2, 3$. The domain $M_t \subset \mathbb{R}^3$ has a natural volume form $\mu_t = d\mathbf{x} = dx^1 \wedge dx^2 \wedge dx^3$.

2.1 Dynamics of Fluid Flows in Eulerian Coordinates

The governing equations of fluid flows are derived based on three physical laws: conservation of mass, momentum, and energy. Initially derived by Leonhard Euler in 1755 without accounting for viscous effects and the energy law, the flow is considered adiabatic. The entropy equation was later added by Pierre-Simon Laplace in 1816. Subsequently, the effects of viscosity and thermal conductivity were introduced, and a theory was developed by Claude-Louis Navier (1822) and George Gabriel Stokes (1842-1850).

2.1.1 Conservation of mass, momentum and energy

The equations of fluid dynamics are derived based on three conservation laws: mass, momentum, and energy.

Conservation of mass Consider an arbitrary domain $\Omega \subset M_t$. The change of mass per unit time in Ω is given by

$$\frac{d}{dt}\int_\Omega \rho \, d\mathbf{x}.$$

This quantity is equal to the mass flowing into Ω through its boundary $\partial\Omega$ per unit time. To measure the mass flows through $\partial\Omega$, the concept of *mass flux* is introduced. For a small area dA on the surface $\partial\Omega$ with an outer normal ν, and flow velocity $\mathbf{v}$ in its vicinity, the mass flux is defined as $\rho\mathbf{v}\cdot(-\nu)$. [1] Here, $-\nu$ represents the inner normal, indicating the flow into Ω from outside. The mass flux is integrated over $\partial\Omega$ to obtain the total mass flow into Ω per unit time:

$$\int_{\partial\Omega} \rho\mathbf{v}\cdot(-\nu)\, dA.$$

The conservation of mass is expressed as

$$\frac{d}{dt}\int_\Omega \rho \, d\mathbf{x} = \int_{\partial\Omega} [-\rho\mathbf{v}\cdot\nu] dA = -\int_\Omega \nabla\cdot(\rho\,\mathbf{v})\, d\mathbf{x},$$

or

$$\int_\Omega \left(\frac{\partial\rho}{\partial t} + \nabla\cdot(\rho\mathbf{v})\right) d\mathbf{x} = 0.$$

This holds for arbitrary domain Ω. This leads to the *continuity equation:*

$$\boxed{\frac{\partial\rho}{\partial t} + \nabla\cdot(\rho\,\mathbf{v}) = 0.} \tag{2.1}$$

Conservation of Momentum The momentum change in Ω is given by

$$\frac{d}{dt}\int_\Omega \rho\mathbf{v}\, d\mathbf{x}.$$

This change results from:

(a) the momentum carried into Ω through the boundary $\partial\Omega$, given by $(\rho\mathbf{v})[\mathbf{v}\cdot(-\nu)]$,

[1] The mass in the parallelogram spanned by dA and the vector $\mathbf{v}\Delta t$ will flow into Ω through dA in the period Δt. The volume of this parallelogram is $(\mathbf{v}\Delta t\cdot\nu)dA$. The mass in this parallelogram is $\rho(\mathbf{v}\Delta t\cdot\nu)dA$. Thus the mass flows into Ω through dA per unit time, per unit area is $\rho\mathbf{v}\cdot(-\nu)$.

(b) a surface force (per unit area) $\mathbf{t}$ on the boundary $\partial\Omega$,

(c) a body force (per unit volume) $\mathbf{f}$ in Ω.

Here, the surface force $\mathbf{t}$ comes from the impacts of particles on the surface. It is assumed that

$$\mathbf{t} = \sigma \cdot \nu,$$

where σ is a rank-2 tensor: $\sigma = (\sigma_{ij})$, termed the Cauchy stress tensor. [2] Thus, there exists a rank 2 tensor σ, such that $\mathbf{t} = \sigma \cdot \nu$. This leads to the momentum conservation equation:

$$\begin{aligned}\frac{d}{dt}\int_\Omega \rho \mathbf{v}\, d\mathbf{x} &= \int_{\partial\Omega} \rho \mathbf{v}[\mathbf{v}\cdot(-\nu)]\, dA + \int_{\partial\Omega} \sigma \cdot \nu\, dA + \int_\Omega \mathbf{f}\, d\mathbf{x} \\ &= \int_\Omega [\nabla \cdot (-\rho \mathbf{v}\mathbf{v} + \sigma) + \mathbf{f}]\, d\mathbf{x}.\end{aligned}$$

This holds for arbitrary domain Ω. Thus, we obtain [3]

$$\boxed{\frac{\partial(\rho \mathbf{v})}{\partial t} + \nabla \cdot (\rho\, \mathbf{v}\mathbf{v}) = \nabla \cdot \sigma + \mathbf{f}.} \tag{2.2}$$

For each velocity component v^i, the momentum conservation equation is:

$$\begin{aligned}\frac{d}{dt}\int_\Omega \rho v^i\, d\mathbf{x} &= \int_{\partial\Omega} [-\rho v^i v^j + \sigma_{ij}]\nu^j\, dA + \int_\Omega f^i\, d\mathbf{x} \\ &= \int_\Omega \partial_j[-\rho v^i v^j + \sigma_{ij}] + f^i\, d\mathbf{x}.\end{aligned}$$

Inviscid assumption for gas flows In gas flows, the stress mainly comes from the impact of gas particles on the surface, which gives a stress of the form

$$\sigma = -pI,$$

where p is the pressure and I is the 3×3 identity matrix. The minus sign means that the surface force $\sigma \cdot \nu = -p\nu$ is inward to Ω. The stress has the form pI meaning that the gas is isotropic, i.e., the particle impacts at a point have no preference direction. Note that particles can also collide with each other or experience a random force from thermo noise, which is a secondary effect in gas flows. We will neglect it for the moment. With $\sigma = -pI$, the momentum equation now reads

$$\boxed{\frac{\partial(\rho \mathbf{v})}{\partial t} + \nabla \cdot (\rho\, \mathbf{v}\mathbf{v}) = -\nabla p + \mathbf{f}.} \tag{2.3}$$

[2] This will be proven that $\mathbf{t}$ is a linear function of the outer normal ν. See Cauchy's stress in the later chapter.

[3] The notation $\mathbf{vv}$ stands for a tensor: $\mathbf{vv} = (v^i v^j)$, and $\nabla \cdot (\rho \mathbf{vv})$ stands for a vector whose ith component is $\partial_j(\rho v^i v^j)$.

Conservation of energy The total energy per unit volume is

$$\rho E := \frac{1}{2}\rho |\mathbf{v}|^2 + \rho U,$$

the sum of kinetic energy and internal energy. The energy change in a region Ω per unit time is due to

(a) the energy carried in through the boundary $\partial\Omega$, which is $\rho E\mathbf{v}\cdot(-\nu)$ $\left(= -\rho E v^i \nu^i\right)$,

(b) the work done by the stress from the boundary, which is $\mathbf{v}\cdot\sigma\cdot\nu$ $\left(= v^i \sigma_{ij} \nu^j\right)$,

(c) the work done by the body force in Ω, which is $\mathbf{v}\cdot\mathbf{f}$ $\left(= v^i f^i\right)$,

(d) the heat transfer into Ω through boundary, which is $\mathbf{q}\cdot(-\nu)$. Here, $\mathbf{q}$, is the *heat flux*.

The conservation of energy reads

$$\frac{d}{dt}\int_\Omega \rho E\, d\mathbf{x} = \int_{\partial\Omega} [-\rho E\mathbf{v}\cdot\nu + \sigma\cdot\mathbf{v}\cdot\nu - \mathbf{q}\cdot\nu]\, dA + \int_\Omega \mathbf{f}\cdot\mathbf{v}\, d\mathbf{x}.$$

By applying the divergence theorem, we obtain the energy equation: [4]

$$\boxed{\frac{\partial(\rho E)}{\partial t} + \nabla\cdot[(\rho E\mathbf{I} - \sigma)\cdot\mathbf{v} + \mathbf{q}] = \mathbf{v}\cdot\mathbf{f}.} \tag{2.4}$$

Adiabatic assumption for gas flows We shall assume no heat conduction for inviscid gas flows. This means that $\mathbf{q} = 0$.

System (2.1),(2.3),(2.4) is called the (compressible) Euler equations. There are 5 equations (momentum equation has 3 equations) for 5 unknowns (ρ, U, v^1, v^2, v^3). The pressure p is given as $p(\rho, U)$ from the equation-of-state.

2.1.2 Initial conditions and boundary conditions

We consider the fluid flows in a fixed domain $M = \hat{M} = M_t$.

Initial conditions The Euler equation is first-order in time and thus requires initial condition

$$\rho(0,\mathbf{x}) = \rho_0(\mathbf{x}), \quad U(0,\mathbf{x}) = U_0(\mathbf{x}), \quad \mathbf{v}(0,\mathbf{x}) = \mathbf{v}_0(\mathbf{x}), \quad \mathbf{x}\in M.$$

[4] The notation $\nabla\cdot[\mathbf{v}\cdot\sigma]$ is $\partial_j(v^i\sigma^{ij})$.

Boundary conditions Typically, we consider a *closed system*, implying that there are no transported fluxes from outside the domain. In other words:

$$\rho\mathbf{v}\cdot\nu = 0, \quad \rho\mathbf{v}\mathbf{v}\cdot\nu = 0, \quad \rho E\mathbf{v}\cdot\nu = 0 \text{ on } \partial M.$$

This is equivalent to the following Neumann boundary condition:

$$\boxed{\mathbf{v}\cdot\nu = 0 \text{ on } \partial M.} \tag{2.5}$$

2.1.3 General conservation laws in Eulerian coordinate

The fluid dynamics can be expressed in the following abstract form:

$$\boxed{\partial_t \mathcal{U} + \nabla_{\mathbf{x}}\cdot\mathcal{F} = \mathcal{R}} \tag{2.6}$$

where

$$\mathcal{U} = \begin{bmatrix}\rho\\ \rho\mathbf{v}\\ \rho E\end{bmatrix}, \quad \mathcal{F} = \begin{bmatrix}\rho\mathbf{v}\\ \rho\mathbf{v}\mathbf{v}-\sigma\\ \mathbf{v}\cdot(\rho E\mathbf{I}-\sigma)+\mathbf{q}\end{bmatrix}, \quad \mathcal{R} = \begin{bmatrix}0\\ \mathbf{f}\\ \mathbf{v}\cdot\mathbf{f}\end{bmatrix}.$$

Here, $\mathcal{F}$ is an $m\times 3$ matrix. It can be expressed as $\mathcal{F} = (\mathcal{F}_1,\mathcal{F}_2,\mathcal{F}_3)$. $\nabla_{\mathbf{x}}\cdot\mathcal{F} := \partial_{x^i}\mathcal{F}_i$. By using the divergence theorem, the above equation can be expressed in the following integral form:

$$\int_\Omega \partial_t\mathcal{U}\,d\mathbf{x} + \int_{\partial\Omega}\mathcal{F}\cdot\nu\,dS_t = \int_\Omega \mathcal{R}\,d\mathbf{x}. \tag{2.7}$$

where $\Omega\subset M_t$ is an arbitrary subdomain and ν is its outer normal.

2.2 Equations of Inviscid Fluid Flows in Lagrangian Coordinates

2.2.1 Flow maps and velocity fields

Flow map and velocity field

- **Fluid parcel:** The fluid in a small box dX centered at X is a called a fluid parcel at X. Let $\mathbf{x}(\cdot,X)$ be the trajectory of the fluid parcel at X.

- **Velocity:** The time derivative $\dot{\mathbf{x}}(t,X)$ is the parcel's velocity, denoted by $\mathbf{V}$. In the Lagrangian coordinate system,

$$\mathbf{V}(t,X) := \dot{\mathbf{x}}(t,X).$$

In observer's coordinate, we use $\mathbf{v}(t,\mathbf{x})$ and it satisfies

$$\mathbf{v}(t,\mathbf{x}(t,X)) := \dot{\mathbf{x}}(t,X).$$

Sometimes, we denote $\mathbf{v}(t,\cdot)$ by $\mathbf{v}_t$ and treat it as a tangent vector in TM_t. Thus, given a flow field $\mathbf{v}_t \in TM_t$, the trajectory $\mathbf{x}(t,X)$ is the solution of the ODE:

$$\dot{\mathbf{x}}(t) = \mathbf{v}(t,\mathbf{x}), \quad \mathbf{x}(0,X) = X.$$

- **Flow map:** The mapping $\varphi_t : \hat{M} \to M_t$ which maps

$$X \mapsto \mathbf{x}(t,X)$$

  is called a *flow map*. Given a flow map φ_t is equivalent to giving a velocity field $\mathbf{v}_t$ on M_t.

- Physical quantities can be represented in Eulerian coordinate $f(t,\mathbf{x})$ or in Lagrange coordinate $f(t,X) := f(t,\mathbf{x}(t,X))$ (we abuse notation by using the same notation in both coordinates). The partial derivative $\partial/\partial t$ means the partial derivative in time with fixed $\mathbf{x}$, while $\frac{d}{dt}$ or simply the dot, means the time derivative with fixed Lagrangian coordinate X.

2.2.2 Deformation Gradients

- The deformation gradient of a flow map $\varphi_t(X) = \mathbf{x}(t,X)$ is defined as

$$F(t,X) := \frac{\partial \mathbf{x}}{\partial X}(t,X), \quad F^i_\alpha = \frac{\partial x^i}{\partial X^\alpha}. \tag{2.8}$$

  It is treated as a tensor that measures the deformation of a fluid parcel.

- Since fluid flows may have discontinuities (shocks, contact discontinuities), the velocity field $\mathbf{v}(t,\mathbf{x})$ is only piecewise smooth. Thus, the corresponding flow map φ_t can only be Lipschitz continuous, and the corresponding Lipschitz constant depends on time. Nevertheless, we fix t in our analysis, and the corresponding deformation gradient $\frac{\partial \mathbf{x}}{\partial X}$ is well-defined and bounded in a fixed finite time.

- We will need F^T, F^{-1} and F^{-T} in later sections. They are defined as
  - $(F^T)^\alpha_i := F^i_\alpha = \frac{\partial x^i}{\partial X^\alpha}$
  - $(F^{-1})^\alpha_i := \frac{\partial X^\alpha}{\partial x^i}, \quad \because (F \cdot F^{-1})^i_j = F^i_\alpha (F^{-1})^\alpha_j = \delta^i_j.$
  - $(F^{-T})^i_\alpha := (F^{-1})^\alpha_i = \frac{\partial X^\alpha}{\partial x^i}.$

- The Jacobian $J(t,X) := det(\frac{\partial \mathbf{x}}{\partial X})$. It satisfies

$$d\mathbf{x}(t,X) = J(t,X)dX.$$

It is required that

$$J(t,X) > 0.$$

Thus, the flow map φ_t is invertible.

2.2.3 Euler-Lagrange Transformation Formula

We aim to express the Euler equation (2.6) in the Lagrangian coordinate system. This transformation relies on the following two propositions.

Proposition 2.2 (Renolds transportation Theorem)**.** *Let $\mathbf{v}(t,\mathbf{x})$ be a vector field, and φ_t be the flow map from $\hat{M}$ to M_t generated by $\mathbf{v}$. Suppose Ω_0 is a subdomain in $\hat{M}$ and $\Omega(t) := \varphi_t(\Omega_0)$. Then, for any function $f(t,\mathbf{x})$, we have*

$$\boxed{\frac{d}{dt}\int_{\Omega(t)} f(t,\mathbf{x})\,d\mathbf{x} = \int_{\Omega(t)} \frac{\partial}{\partial t} f(t,\mathbf{x})\,d\mathbf{x} + \int_{\partial\Omega(t)} f(t,\mathbf{x})\mathbf{v}\cdot\nu\,dS_t,} \tag{2.9}$$

where ν is the outer normal on $\partial\Omega(t)$.

Proof. We have

$$\frac{d}{dt}\int_{\Omega(t)} f(t,\mathbf{x})\,d\mathbf{x} = \int_{\Omega(t)} \frac{\partial}{\partial t} f(t,\mathbf{x})\,d\mathbf{x} + \lim_{\Delta t\to 0}\frac{1}{\Delta t}\int_{\Omega(t+\Delta t)-\Omega(t)} f(t,\mathbf{x})\,d\mathbf{x}$$

and

$$\lim_{\Delta t\to 0}\frac{1}{\Delta t}\int_{\Omega(t+\Delta)-\Omega(t)} f(t,\mathbf{x})\,d\mathbf{x} = \lim_{\Delta t\to 0}\frac{1}{\Delta t}\int_{\partial\Omega(t)} f(t,\mathbf{x})(\mathbf{v}\Delta t)\cdot\nu\,dS_t$$

we get the result. □

Proposition 2.3. *Let φ_t be the flow map from $\hat{M}$ to M_t. Then the normal surface area elements νdS_t on ∂M_t and $\mathbf{n}dS_0$ on $\partial\hat{M}$ satisfy the following transformation formula*

$$\boxed{\nu dS_t = JF^{-T}\mathbf{n}\,dS_0,} \tag{2.10}$$

where ν and $\mathbf{n}$ are respectively the outer normals of ∂M_t and $\partial\hat{M}$, $F = \partial\varphi_t/\partial X$, and $J = det\,F$.

Proof. Let dX_1 and dX_2 be a pair of two infinitesimal vectors such that [5]

$$\mathbf{n}\, dS_0 = dX_1 \times dX_2.$$

Suppose dX_i is deformed to $d\mathbf{x}_i$ at time t, then

$$\begin{aligned} \nu dS_t &= d\mathbf{x}_1 \times d\mathbf{x}_2 \\ &= F dX_1 \times F dX_2. \end{aligned}$$

Multiplying both sides by F^T gives

$$F^T \cdot \nu dS_t = F^T \cdot F dX_1 \times F dX_2.$$

In coordinate form, it reads

$$\begin{aligned} F^i_\gamma \nu^i dS_t &= F^i_\gamma \left(\varepsilon_{ijk} F^j_\alpha dX_1^\alpha F^k_\beta dX_2^\beta \right) \\ &= \varepsilon_{ijk} F^i_\gamma F^j_\alpha F^k_\beta dX_1^\alpha dX_2^\beta \\ &= J \varepsilon_{\gamma\alpha\beta} dX_1^\alpha dX_2^\beta \\ &= J n^\gamma dS_0 \end{aligned}$$

Here, ε_{ijk} stands for Kronecker delta symbol, [6] and we have used the determinant expression:

$$\varepsilon_{ijk} F^i_1 F^j_2 F^k_3 = det(F) = J.$$

Thus, we get

$$F^T \cdot \nu dS_t = ((F^T)^\gamma_i \nu^i dS_t = F^i_\gamma \nu^i dS_t = J n^\gamma dS_0 = J\mathbf{n}\, dS_0.$$

□

[5] We can parameterize $\hat{M}$ by (u_1, u_2) through a map $(u_1, u_2) \mapsto X(u_1, u_2)$. Then $dX_i = \frac{\partial X}{\partial u_i} du_i$, $i = 1, 2$.

$$dX_1 \times dX_2 = \left(\frac{\partial X}{\partial u_1} \times \frac{\partial X}{\partial u_2} \right) du_1 \wedge du_2 = \left(\frac{\frac{\partial X}{\partial u_1} \times \frac{\partial X}{\partial u_2}}{J} \right) J du_1 \wedge du_2 = \mathbf{n} dS_0, \text{ where } J := \left| \frac{\partial X}{\partial u_1} \times \frac{\partial X}{\partial u_2} \right|.$$

[6]

$$\varepsilon_{ijk} = \begin{cases} 1 & \text{if } \{i, j, k\} \text{ has the same permutation as } \{1, 2, 3\} \\ -1 & \text{if } \{i, j, k\} \text{ has the opposite permutation as } \{1, 2, 3\} \\ 0 & \text{if there is a repeated index.} \end{cases}$$

Remark. In the language of differential geometry, the term

$$\nu dS = \star dx^i, \quad \mathbf{n} dS_0 = \star dX^\alpha.$$

The pullback of νdS is

$$\varphi_t^*(\nu^i \cdot \star dx^i) = J \star dX^\alpha$$

See (4.1), Appendix D.

Conservation laws in Lagrangian coordinates Recalling the integral form of the conservation laws (2.7):

$$\int_{\Omega(t)} \partial_t \mathcal{U} \, d\mathbf{x} + \int_{\partial\Omega(t)} \mathcal{F} \cdot \nu \, dS_t = \int_{\Omega(t)} \mathcal{R} \, d\mathbf{x}.$$

Here, we choose Ω in (2.7) to be $\Omega(t) := \varphi_t(\Omega_0)$ for some fixed $\Omega_0 \subset \hat{M}$. Using (2.9), we obtain

$$\frac{d}{dt} \int_{\Omega(t)} \mathcal{U} \, d\mathbf{x} = \int_{\Omega(t)} \partial_t \mathcal{U} \, d\mathbf{x} + \int_{\partial\Omega_t} \mathcal{U} \mathbf{v} \cdot \nu \, dS_t.$$

This leads to the conservation laws becoming

$$\frac{d}{dt} \int_{\Omega(t)} \mathcal{U} \, d\mathbf{x} + \int_{\partial\Omega(t)} (\mathcal{F} - \mathcal{U}\mathbf{v}) \cdot \nu \, dS_t = \int_{\Omega(t)} \mathcal{R} \, d\mathbf{x}.$$

Next, pulling back the integral in the observer's domain to the material domain by the change of variable $\mathbf{x} \mapsto X$, we get

$$\frac{d}{dt} \int_{\Omega(0)} \mathcal{U} J \, dX + \int_{\partial\Omega(0)} (\mathcal{F} - \mathcal{U}\mathbf{V}) \cdot J F^{-T} \cdot \mathbf{n} \, dS_0 = \int_{\Omega(0)} \mathcal{R} J \, dX. \tag{2.11}$$

Here,

$$\frac{d}{dt} := \left.\frac{\partial}{\partial t}\right|_X,$$

and we have used

$$\nu dS_t = J F^{-T} \cdot \mathbf{n} \, dS_0.$$

Thus, the system of conservation laws in the Lagrangian coordinate becomes

$$\boxed{\frac{d}{dt} \mathcal{W} + \nabla_X \cdot \mathcal{G} = \mathcal{R} J,} \tag{2.12}$$

where

$$\mathcal{W} = \mathcal{U} J, \quad \mathcal{G} := (\mathcal{F} - \mathcal{U}\mathbf{V}) \cdot J F^{-T}. \tag{2.13}$$

Since $\rho J = \rho_0$ (see (2.19) in the next section), we get

$$\mathcal{U}J = \begin{bmatrix} \rho_0 \\ \rho_0 \mathbf{v} \\ \rho_0 E \end{bmatrix}, \quad \mathcal{F} - \mathcal{U}\mathbf{v} = \begin{bmatrix} 0 \\ -\sigma \\ -\mathbf{v}\cdot\sigma + \mathbf{q} \end{bmatrix}, \quad \mathcal{G} = \begin{bmatrix} 0 \\ -P \\ -\mathbf{V}\cdot P + \mathbf{Q} \end{bmatrix}, \quad \mathcal{R}J = \begin{bmatrix} 0 \\ \mathbf{f}J \\ \mathbf{V}\cdot \mathbf{f}J \end{bmatrix}.$$

The stress term is transformed to

$$\sigma \cdot \nu \, dS_t = \sigma \cdot JF^{-T} \cdot \mathbf{n} \, dS_0 := P \cdot \mathbf{n} \, dS_0,$$

where the tensor

$$\boxed{P := J\sigma F^{-T}} \tag{2.14}$$

is called the *first Piola stress*. In component form, it reads [7]

$$P_i^\alpha = J\sigma_i^j (F^{-T})_\alpha^j = J\sigma_i^j (F^{-1})_j^\alpha = J\sigma_i^j \frac{\partial X^\alpha}{\partial x^j}.$$

$$P_i^\alpha = J\sigma_i^j \frac{\partial X^\alpha}{\partial x^j}.$$

The work done by the stress is

$$\mathbf{v} \cdot \sigma \cdot \nu \, dS_t = \mathbf{V} \cdot P \cdot \mathbf{n} \, dS_0.$$

And the heat flux $\mathbf{Q}$ in Lagrangian coordinates is

$$\mathbf{q} \cdot \nu \, dS_t = (J\mathbf{q}F^{-T}) \cdot \mathbf{n} \, dS_0 = \mathbf{Q} \cdot \mathbf{n} \, dS_0.$$

Thus,

$$\boxed{\mathbf{Q} = J\mathbf{q}F^{-T},} \tag{2.15}$$

or

$$Q_\alpha = Jq_j (F^{-T})_\alpha^j = Jq_j \frac{\partial X^\alpha}{\partial x^j}.$$

[7] In the terminology of differential geometry (see Appendix), we have

$$P = P_i^\alpha (\star dX^\alpha), \quad \sigma = \sigma_i^j (\star dx^j).$$

$$\varphi_t^*(\star dx^j) = J \frac{\partial X^\alpha}{\partial x^j} (\star dX^\alpha).$$

Thus,

$$P = \varphi_t^*(\sigma).$$

Remarks.

- The continuity equation is trivial (i.e., $\rho(t,X) = \rho_0(X)$).
- The momentum equation and the energy equation do not closed. The corresponding Piola stress P and heat flux Q depend on the deformation gradient F, see (2.14), (2.15). We need an evolution equation for F. It can be derived from
$$\frac{d}{dt}F^i_\alpha(t,X) = \frac{\partial}{\partial t}\frac{\partial x^i}{\partial X^\alpha} = \frac{\partial}{\partial X^\alpha}\frac{\partial x^i}{\partial t} = \frac{\partial}{\partial X^\alpha}v^i(t,X).$$
In tensor form:
$$\boxed{\frac{dF(t,X)}{dt} = \frac{\partial \mathbf{V}(t,X)}{\partial X}.} \tag{2.16}$$
This ODE together with (2.12) closes the system with unknowns $(\mathbf{V}(t,X), F(t,X), S(t,X))$. Note that if there is no heat conduction term $\mathbf{q}$, the entropy satisfies[8]
$$\frac{dS(t,X)}{dt} = 0.$$
We don't need the energy equation. The unknowns are $(\mathbf{V}(t,X), F(t,X))$. The equations are the momentum equation plus the ODE for F. In addition, the constitutive equation is
$$p = p(S,V) = p(S_0, V_0 J) = p(S_0, V_0 \det F).$$
We will have more detailed discussion in subsection 4.1.1.
- The Piola stress $\mathbf{P} = -pJF^{-T}$ is much harder to handle than the Cauchy stress $\sigma = -pI$, both analytically and numerically. In numerical simulations, we usually find the stress in Eulerian coordinates.

2.3 Material Derivatives

2.3.1 Rate-of-changes of geometric variables

Rate-of-change of a scalar field For any scalar field $f(t,\mathbf{x})$, we can track its evolution along a flow path, denoted as $f(t,\mathbf{x}(t,X))$ with X fixed. The derivative of this quantity is referred to **material derivative**
$$\left.\frac{d}{dt}\right|_X f(t,\mathbf{x}(t,X)) = \frac{\partial f}{\partial t} + \dot{\mathbf{x}}(t,X)\frac{\partial f}{\partial \mathbf{x}} = \left(\frac{\partial}{\partial t} + \mathbf{v}\cdot\nabla\right) f(t,\mathbf{x}(t,X))$$
We sometimes abbreviate $\frac{d}{dt}\big|_X$ as $\frac{d}{dt}$ or simply use the dot notation.

[8] See the next section for the entropy equation.

Rate-of-change of the deformation gradient The variation of the flow map $\mathbf{x}(t,X)$ with respect to X is called the *deformation gradient*

$$F(t,X) := \frac{\partial \mathbf{x}}{\partial X}(t,X), \quad \text{or} \quad F^i_\alpha := \frac{\partial x^i}{\partial X^\alpha}.$$

By differentiating

$$\dot{\mathbf{x}}(t,X) = \mathbf{v}(t,\mathbf{x}(t,X))$$

w.r.t. X, we get the evolution equation for F:

$$\frac{d}{dt}\frac{\partial x^i}{\partial X^\alpha} = \frac{\partial \dot{x}^i}{\partial X^\alpha} = \frac{\partial v^i}{\partial X^\alpha} = \frac{\partial v^i}{\partial x^k}\frac{\partial x^k}{\partial X^\alpha}$$

We write it in tensor form:

$$\boxed{\dot{F} = (\nabla \mathbf{v})F}, \quad \text{or} \quad \dot{F}^i_\alpha = \frac{\partial v^i}{\partial x^k}F^k_\alpha. \tag{2.17}$$

where $\dot{F} := \frac{dF}{dt}$. $\nabla \mathbf{v}$ is called deformation rate.

Rate-of-change of the Jacobian Let $J = \det F$ be the Jacobian of the flow map, which measures rate-of-change of volume along the flow path. That is,

$$d\mathbf{x}(t,X) = J(t,X)dX.$$

Then

$$\boxed{\dot{J} = tr(\nabla \mathbf{v})J = (\nabla \cdot \mathbf{v})J.}$$

This follows from the Jacobi's formula below.

Lemma 2.1 (Jacobi's formula)**.** *(i) Let A be an $n \times n$ matrix, and $J := detA$. It holds that*

$$\frac{\partial J}{\partial a_{ij}} = J(A^{-T})_{ij}. \tag{2.18}$$

(ii) Let $A(\varepsilon)$ be a smooth $n \times n$ matrix-valued function. Then

$$\frac{dJ}{d\varepsilon} = tr(\dot{A}A^{-1})J$$

Proof. 1. First, we recall the expansion formula (Laplace formula) of $\det A$:

$$\sum_k a_{ik}A_{jk} = (\det A)\delta_{ij}, \quad \text{or} \quad A(\mathrm{cof}A)^T = (\det A)I = JI,$$

where $\mathrm{cof}A := (A_{ij})$, and A_{ij} is the signed cofactor of A at (i,j), that is, $A_{ij} = (-1)^{i+j}\times$ (determinant of the matrix which eliminates row i and column j from A). We rewrite the above formula by

$$A_{ij} = J(A^{-T})_{ij}.$$

2. We claim that $\partial \det(A)/\partial a_{ij} = A_{ij}$, To see that, we write $\det A$ as
$$\det(A) = \sum_k a_{ik} A_{ik},$$
and note that A_{ik} does not involve a_{ij} for all k. Thus,
$$\frac{\partial \det A}{\partial a_{ij}} = A_{ij}.$$

3. Next,
$$\begin{aligned}\dot{J} = \frac{\partial J}{\partial a_{ij}} \frac{da_{ij}}{d\varepsilon} &= \sum_{i,j} \dot{a}_{ij} A_{ij} \\ &= \sum_{i,j} \dot{a}_{ij} J (A^{-T})_{ij} = J\, tr(\dot{A} A^{-1}).\end{aligned}$$
In the last step, we use $\sum_{i,j} a_{ij} b_{ij} = tr(A^T B) = tr(AB^T)$.

□

2.3.2 Rate-of-changes of thermodynamic variables

Rate-of-change of the density A parcel of fluid centered at X is $\rho_0(X)dX$ initially. At time t, this parcel of fluid is
$$\rho(t, \mathbf{x}(t,X))d\mathbf{x} = \rho(t, \mathbf{x}(t,X))J(t,X)dX,$$
which remains $\rho_0(X)\,dX$ for all time by the conservation of mass. Thus,
$$\boxed{\rho(t, \mathbf{x}(t,X))J(t,X) = \rho_0(X) \quad \text{or equivalently} \quad \frac{d}{dt}(\rho J) = 0.} \tag{2.19}$$
Indeed, this is equivalent to
$$\dot{\rho} J + \rho \dot{J} = \left(\frac{\partial \rho}{\partial t} + \nabla \rho \cdot \mathbf{v} + \rho \nabla \cdot \mathbf{v} \right) J = 0,$$
which is the same continuity equation in the Eulerian framework. Thus, the conservation of mass in Lagrangian form is (2.19). The corresponding rate-of-change of density is
$$\frac{d}{dt}\rho + \rho \nabla \cdot \mathbf{v} = 0. \tag{2.20}$$
This means that
$$\boxed{\nabla \cdot \mathbf{v} = -\frac{\dot{\rho}}{\rho} = \frac{\dot{V}}{V} = \frac{\dot{J}}{J}} \tag{2.21}$$
is the relative rate of change of specific volume. It is called the *volumetric dilatation rate*.

Homework Show
$$-\frac{\dot{\rho}}{\rho} = \frac{\dot{V}}{V} = \frac{\dot{J}}{J}.$$

Rate-of-change of the velocity The momentum equation in Eulerian coordinate is
$$\partial_t(\rho\mathbf{v}) + \nabla\cdot(\rho\mathbf{v}\mathbf{v}) + \nabla p = 0.$$
We expand it to get
$$\rho\frac{\partial\mathbf{v}}{\partial t} + \frac{\partial\rho}{\partial t}\mathbf{v} + \rho\mathbf{v}\cdot\nabla\mathbf{v} + \rho(\nabla\cdot\mathbf{v})\mathbf{v} + \nabla p = 0.$$
Using the continuity equation, we cancel the second and fourth terms to get
$$\frac{\partial\mathbf{v}}{\partial t} + \mathbf{v}\cdot\nabla\mathbf{v} = -\frac{\nabla p}{\rho}. \tag{2.22}$$
$$\boxed{\frac{d\mathbf{v}}{dt} = -\frac{\nabla p}{\rho}.} \tag{2.23}$$
Note that this expression is a mix of Lagrangian representation ($d\mathbf{v}/dt$) and Eulerian representation ($\nabla_{\mathbf{x}}p$).

Rate-of-change of the kinetic energy We multiply (2.23) by $\rho\mathbf{v}$ to get
$$\frac{d}{dt}\left(\frac{1}{2}\rho|\mathbf{v}|^2\right) = -\mathbf{v}\cdot\nabla p.$$
It means that the rate-of-change of the kinetic energy in a parcel is due to the work done by the pressure from outside.

Rate-of-change of the internal energy The energy equation is
$$\rho\left(\partial_t E + \mathbf{v}\cdot\nabla E\right) + \nabla\cdot(p\mathbf{v}) = 0,$$
or
$$\rho\frac{d}{dt}\left(\frac{1}{2}|\mathbf{v}|^2 + U\right) + \nabla\cdot(p\mathbf{v}) = 0.$$
We can subtract the kinetic energy equation from the energy equation to obtain the motion of internal energy:
$$\frac{dU}{dt} + \frac{p}{\rho}\nabla\cdot\mathbf{v} = 0. \tag{2.24}$$

From $\nabla \cdot \mathbf{v} = \frac{1}{V}\frac{dV}{dt}$, we get

$$\frac{dU}{dt} + p\frac{dV}{dt} = 0 \quad \because \rho V = 1.$$

This means that the change of internal energy is due to the volume-change of the fluid.

Rate-of-change of the entropy The above dynamic equation for U together with Gibbs relation

$$dU = T\,dS - p\,dV$$

lead to

$$\boxed{\frac{dS}{dt} = 0.} \tag{2.25}$$

This means that S is constant along particle path. That is, *the flow is adiabatic*, no heat transfer between different fluid parcels.

Rate-of-change of the temperature From caloric equation of state $U(T)$ and the dynamic equation for internal energy, we obtain

$$U'(T)\frac{dT}{dt} = -p\frac{dV}{dt}.$$

This gives

$$\frac{dT}{dt} = -\frac{p}{U'(T)}\frac{dV}{dt}. \tag{2.26}$$

Remark

- In viscous fluids, the entropy increases due to an interaction of fluid parcels with different velocities. The entropy increases in fluid parcel. In particular, the entropy increases as gases pass through a shock front. We shall discuss this in later chapter.

Homework:

1. Given a carolic relation $U = U(T)$, derive a rate equation for T based on $\dot{S} = 0$.

2.4 Lie Derivatives of Scalar Fields and Vector Fields

2.4.1 Basic Notions of Differential Manifolds

Differential Manifolds We shall consider a 3-dimensional differential manifold M.

Differential Forms: The differential forms in a 3-D manifold M are:

- 0-form: it is merely a scalar function $f(\mathbf{x})$ on M. In particular, a coordinate function x^i is a function on M.
- 1-form: it looks like $\eta = \eta_i(\mathbf{x})dx^i$. It is merely the line integral $\int_C \eta_i dx^i$ without the integral symbol $\int$.
- 2-form: it looks like
$$\omega^1 dx^2 \wedge dx^3 + \omega^2 dx^3 \wedge dx^1 + \omega^3 dx^1 \wedge dx^2.$$
It appears in the following surface integral without the integral sign:
$$\int_\Sigma \omega^1 dx^2 \wedge dx^3 + \omega^2 dx^3 \wedge dx^1 + \omega^3 dx^1 \wedge dx^2 = \int_\Sigma \omega \cdot \nu \, dS.$$
where $\omega = (\omega^1, \omega^2, \omega^3)$ is a vector, ν is the outer normal of Σ.
- 3-form: it looks like
$$\zeta = \rho(\mathbf{x}) dx^1 \wedge dx^2 \wedge dx^3.$$
The 3-form $\mu = dx^1 \wedge dx^2 \wedge dx^3$ is called the volume form.
- The set of k-forms on M is denoted by $\Omega^k(M)$. For a 3-D manifold M, we define $\Omega^4(M) = \{0\}$.

The following lemma may give you some intuitions of differential forms.

Lemma 2.2. *Given a surface S in $\mathbb{R}^3$, the normal surface element νdS can be expressed as*
$$\nu dS = (dx^2 \wedge dx^3, dx^3 \wedge dx^1, dx^1 \wedge dx^2).$$

Remark. From this lemma, we see that $dx^1 \wedge dx^2$, as applied to S, is the projection of the vector area element νdS onto the x^1-x^2 plane.

Proof. Let us locally parametrize the surface S by $u = (u^1, u^2)$. That is, the surface S is locally given by $\{\mathbf{x}(u) | u \in \mathscr{U}\}$. An area element on $\mathscr{U}$ is given by $du^1 \wedge du^2$. The two infinitesimal tangents on the surface generated by du_1 and du_2 are
$$\frac{\partial \mathbf{x}}{\partial u^1} du^1, \quad \frac{\partial \mathbf{x}}{\partial u^2} du^2.$$
The normal surface element is defined by
$$\left(\frac{\partial \mathbf{x}}{\partial u^1} du^1\right) \times \left(\frac{\partial \mathbf{x}}{\partial u^2} du^2\right) = \frac{\frac{\partial \mathbf{x}}{\partial u^1} \times \frac{\partial \mathbf{x}}{\partial u^2}}{\left\| \frac{\partial \mathbf{x}}{\partial u^1} \times \frac{\partial \mathbf{x}}{\partial u^2} \right\|} \left\{ \left\| \frac{\partial \mathbf{x}}{\partial u^1} \times \frac{\partial \mathbf{x}}{\partial u^2} \right\| du^1 \wedge du^2 \right\} = \nu dS.$$

On the other hand, from

$$dx^i(u^1,u^2) = \frac{\partial x^i}{\partial u^k} du^k$$

we get

$$\begin{aligned}
\left(\frac{\partial \mathbf{x}}{\partial u^1} du^1\right) \times \left(\frac{\partial \mathbf{x}}{\partial u^2} du^2\right) &= \varepsilon_{ijk} \left(\frac{\partial x^i}{\partial u^1} du^1\right) \left(\frac{\partial x^j}{\partial u^2} du^2\right) e^k \\
&= \sum_{\varepsilon_{ijk}=1} \frac{\partial(x^i,x^j)}{\partial(u^1,u^2)} du^1 \wedge du^2 e^k \\
&= \sum_{\varepsilon_{ijk}=1} dx^i \wedge dx^j e^k.
\end{aligned}$$

Here

$$\frac{\partial(x^i,x^j)}{\partial(u^1,u^2)} := \frac{\partial x^i}{\partial u^1}\frac{\partial x^j}{\partial u^2} - \frac{\partial x^i}{\partial u^2}\frac{\partial x^j}{\partial u^1}.$$

and we have used

$$\begin{aligned}
dx^i \wedge dx^j &= \sum_{k,\ell} \frac{\partial x^i}{\partial u^k}\frac{\partial x^j}{\partial x^\ell} du^k \wedge du^\ell \\
&= \frac{\partial(x^i,x^j)}{\partial(u^1,u^2)} du^1 \wedge du^2
\end{aligned}$$

because $du^2 \wedge du^1 = -du^1 \wedge du^2$ and $du^k \wedge du^k = 0$ for $k = 1,2$. □

Exterior Algebra and Wedge Product

Exterior Derivative:

- The exterior derivative d is defined as $d : \Omega^k(M) \to \Omega^{k+1}(M), k = 0,...,3.$ satisfying
  - (a) d is linear;
  - (b) For $k = 0$, define $df := f_{x^i} dx^i$.
  - (c) For $\omega = w_I(x)dx^I$, define $d\left(w_I(x)dx^I\right) := dw_I(x) \wedge dx^I$.
- Examples:
  - For 0-form: $df = f_{x^1}dx^1 + f_{x^2}dx^2 + f_{x^3}dx^3$.

– For 1-form:

$$
\begin{aligned}
d(A_1dx^1+A_2dx^2+A_3dx^3) &= (A_{1,x^2}dx^2+A_{1,x^3}dx^3)\wedge dx^1 \\
&\quad + (A_{2,x^1}dx^1+A_{2,x^3}dx^3)\wedge dx^2 + (A_{3,x^1}dx^1+A_{3,x^2}dx^2)\wedge dx^3 \\
&= (A_{3,x^2}-A_{2,x^3})dx^2\wedge dx^3 + (A_{1,x^3}-A_{3,x^1})dx^3\wedge dx^1 + (A_{2,x^1}-A_{1,x^2})dx^1\wedge dx^2.
\end{aligned}
$$

– For 2-form:

$$
d(B_1dx^2\wedge dx^3+B_2dx^3\wedge dx^1+B_3dx^1\wedge dx^2) = (B_{1,x^1}+B_{2,x^2}+B_{3,x^3})dx^1\wedge dx^2\wedge dx^3.
$$

– For 3-form: $d(\rho(x)dx^1\wedge dx^2\wedge dx^3) = 0$.

Flow Maps in Fluid Flows

- **Material space and world space:** Let $\hat{M}$ be the initial configuration space (also called the reference space or the material space) and M_t be the configuration space at time t (also called the world space). The volume form $\mu = dx^1\wedge dx^2\wedge dx^3$ in the Eulerian space $\mathbb{R}^3$, where all M_t, $t\geq 0$ are situated. The volume form μ_t of M_t is equal to μ for all t.

- **Flow Map:** The flow map $\varphi_t = \mathbf{x}(t,\cdot)$ is a mapping from $\hat{M}$ to M_t.

- **Pullback:** Functions or differential forms in M_t can be transformed back to $\hat{M}$ through the flow map. This is the pull-back operator. Here are some examples:

  – The 0-form $f(t,\mathbf{x})$ is pulled back to $\varphi_t^*(f)(t,X) := f(t,\mathbf{x}(t,X))$.

  – The 1-form $\eta = \eta_i\, dx^i$ is pulled back to

$$
\varphi_t^*(\eta)(t,X) := \eta_i(t,\mathbf{x}(t,X))\frac{\partial x^i(t,X)}{\partial X^\alpha}dX^\alpha.
$$

  – The volume form μ is pulled back to $\varphi_t^*\mu = J\hat{\mu}$, where $J = det(d\varphi_t)$.

Remarks

- **Mass form** It is assumed that there is a mass form m in the material space $\hat{M}$, which is a 3-form if $\hat{M}$ occupies a 3-dimensional manifold. In geometric formulation, we can avoid the structure of volume form in the reference domain. We only need to assign a mass form in the initial domain $\hat{M}$.

- **Density and Specific Volume** However, if we assign a volume form on $\hat{M}$, i.e. $\hat{\mu}$, or dX, then we can define initial density ρ_0 and the density $\rho(t,\mathbf{x})$ through the following argument. First, the relation between μ_t and $\hat{\mu}$ is

$$\varphi_t^*(\mu) = J(t,X)\hat{\mu}, \quad \text{or} \quad d\mathbf{x} = J(t,X)dX.$$

We define initial density to be

$$\rho_0(X) := \frac{m(X)}{dX}.$$

The density at $(t,\mathbf{x})$ is defined by

$$\rho(t,\mathbf{x}) := \frac{m(X)}{\varphi_t^*(d\mathbf{x})},$$

where $\varphi_t^{-1}(\mathbf{x}) = X$. Both ρ and ρ_0 are 0-forms. They are related through

$$\rho = \frac{m}{\varphi_t^*(d\mathbf{x})} = \frac{\rho_0 dX}{JdX} = \frac{\rho_0}{J}.$$

That is,

$$\rho_0 = J\rho. \tag{2.27}$$

- The specific volume is defined to be

$$V := \frac{1}{\rho} = \frac{\varphi_t^*(\mu)}{m}.$$

V is a 0-form, representing the volume occupied by fluid in a parcel with unit mass.

2.4.2 Fluid Dynamic Equations in terms of Lie derivatives

The advantages of the expressions below are

- We only need differential structure of $\hat{M}$ and M_t, a mass form in $\hat{M}$ and a volume form in M_t.
- The expression uses exterior derivative (a differential structure), and an inner product structure in M_t (to define the kinetic energy, or the momentum).
- It is a coordinate free expression.

Fluid Dynamic Equations In Lagrangian Coordinates

- Let d_t denote for
$$d_t := \left.\frac{\partial}{\partial t}\right|_X .$$
the time derivative with fixed X. We also use dot for time derivative in Lagrangian coordinates.

- Mass conservation: the mass of a fluid parcel is conserved.
$$\boxed{d_t\left(\rho\mu_t\right) = 0.}$$

- The flow is adiabatic .
$$\boxed{d_t S = 0.}$$

- Equation of motion: We have seen that for inviscid flow, the equation of motion is
$$\dot{\mathbf{v}} = -\frac{1}{\rho}\nabla p.$$
Take inner product with $d\mathbf{x}$, we get
$$\dot{\mathbf{v}}\cdot d\mathbf{x} = -\frac{1}{\rho}\nabla_{\mathbf{x}} p\cdot d\mathbf{x} = -\frac{1}{\rho}dp.$$
Let $\eta := v_i dx^i$ be the momentum 1-form. We have
$$\dot{v}_i dx^i = d_t(v_i dx^i) - v_i dv_i = -\frac{1}{\rho}dp,$$
$$\boxed{d_t\eta = \varphi_t^*\left(\frac{1}{2}d|\mathbf{v}|^2 - \frac{1}{\rho}dp\right).} \tag{2.28}$$

Fluid Dynamic Equation in Eulerian coordinates

- The Lie derivative $\partial_t + \mathscr{L}_{\mathbf{v}}$ in the Eulerian coordinate is defined to be
$$d_t = \varphi_t^*\left(\partial_t + \mathscr{L}_{\mathbf{v}}\right).$$

- We can rewrite the above equations in terms of the Lie derivatives in the Eulerian coordinate system:
$$\left\{\begin{array}{l} (\partial_t + \mathscr{L}_{\mathbf{v}})(\rho\mu_t) = 0, \\ (\partial_t + \mathscr{L}_{\mathbf{v}})S = 0, \\ (\partial_t\eta + \mathscr{L}_{\mathbf{v}}\eta) = \frac{1}{2}d|\mathbf{v}|^2 - \frac{1}{\rho}dp. \end{array}\right. \tag{2.29}$$

For details of Lie Derivatives, see the Appendix D.

Viscous flows

- Viscous flows: the deviatoric stress τ is a T^*M-valued $(n-1)$-form. Similar the way we treat for the pressure, we define

$$\tau = \tau^i_j (\star dx^i) \otimes dx^j$$

The equation of motion for viscous fluid flow is

$$\boxed{d_t \eta = \varphi_t^* \left(\frac{1}{2} d|\mathbf{v}|^2 - \frac{1}{\rho} dp + \frac{1}{\rho} \star d\tau \right).}$$

- Vorticity equation: The vorticity $\omega := d\eta$ is a two-form. By taking d operation on the momentum equation, we obtain

$$\boxed{d_t \omega = \varphi_t^* \left(-dV \wedge dp + d\left(V \star d\tau\right)\right).} \tag{2.30}$$

- Expression in terms of Lie derivative. The Lie derivative is defined to be

$$d_t = \varphi_t^* \left(\partial_t + \mathscr{L}_v \right).$$

With this notation, we have

  - Euler equation:
$$\partial_t \eta + \mathscr{L}_{\mathbf{v}} \eta = \frac{1}{2} d|\mathbf{v}|^2 - \frac{1}{\rho} dp.$$

  - Navier-Stokes equation
$$\partial_t \eta + \mathscr{L}_{\mathbf{v}} \eta = \frac{1}{2} d|\mathbf{v}|^2 - \frac{1}{\rho} dp + \frac{1}{\rho} \star d\tau.$$

  - Viscous vorticity equation
$$\partial_t \omega + \mathscr{L}_{\mathbf{v}} \omega = -dV \wedge dp + d\left(V \star d\tau\right).$$

For details, see appendix.

Chapter 3

Flow Invariants

In the preceding chapter, we established that entropy S remains invariant along a fluid parcel's trajectory. In this chapter, we explore additional invariants, focusing on energy-related invariants and vorticity. The theories corresponding to these invariants are the Bernoulli principle and circulation theory.

3.1 Barotropic Flows and Bernoulli Principle

3.1.1 Degenerate thermo relation

Recall that we have two independent thermal variables, say p and V, in fluid dynamics. However, certain fluid flows satisfy $\nabla V \times \nabla p = 0$, indicating that the level sets of V coincide with those of pressure p. This implies a functional dependence between V and p, where there exists only one independent thermodynamic variable. Such flows are termed to have a "degenerate thermo relation."

Examples of flows exhibiting a degenerate thermo relation include:

- **Barotropic flows** Barotropic fluids are fluids where pressure is solely a function of density and vice versa. This frequently occurs in atmospheric flows, where density is a function of pressure. It is important to note that this condition doesn't imply constancy for temperature T or entropy S. A fluid which is not barotropic is *baroclinic*.

- **Isentropic flows** A flow is termed isentropic if the entire flow possesses a single constant entropy S. This approximation holds when the flows exhibit no shocks or very weak shocks. In such cases, we can omit the energy equation, as there is only one thermodynamic independent variable, typically density ρ, determined by the continuity equation. For γ-law gases, the pressure is given by $p = A\rho^{\gamma}$, where A is a constant.

- **Isothermal flows** In flows where $\gamma = 1$ for γ-law gases, the flow is referred to as an isothermal flow. In these scenarios, temperature T remains constant throughout the entire flow due to the relation $p = A\rho$ and the ideal gas law $p\rho^{-1} = RT$. This type of flow characterizes highly compressible gases, where compressing such gases results in the radiative dissipation of energy.
- **Incompressible flows** Incompressible flows satisfy $\frac{D\rho}{Dt} = 0$, which is equivalent to the condition $\nabla \cdot \mathbf{v} = 0$. For these flows, the pressure p is treated as a Lagrangian multiplier (see the variational approach for flow dynamics). This is also a case of thermo degeneracy.

3.1.2 Bernoulli Principle

The Bernoulli principle pertains to the invariance of an energy-related quantity in steady barotropic fluid flows subjected to a conservative body force.

The conservative (per unit mass) body force $\mathbf{f}$ is characterized by the existence of a scalar potential function Φ such that:

$$\mathbf{f}(\mathbf{x}) = -\rho(\mathbf{x})\nabla\Phi(\mathbf{x}).$$

A classical example of such a force is the gravitational force.

Theorem 3.2 (Bernoulli Principle). *For steady barotropic flows under conservative body force $\mathbf{f} = -\rho\nabla\Phi$, the quantity*

$$H := \frac{1}{2}|\mathbf{v}|^2 + h(\rho) + \Phi = constant \tag{3.1}$$

remains constant along every streamline (i.e., the integral curves of the velocity $\mathbf{v}$). Here, $h(\rho) := \int \frac{dp(\rho)}{\rho}$ is the enthalpy.

Proof. With the conservative body force, the momentum equation takes the form:

$$\partial_t \mathbf{v} + \mathbf{v} \cdot \nabla \mathbf{v} + V\nabla p = -\nabla\Phi,$$

where $V = 1/\rho$ is the specific volume. Utilizing the identity

$$\mathbf{v} \cdot \nabla \mathbf{v} = \nabla\left(\frac{1}{2}|\mathbf{v}|^2\right) + \omega \times \mathbf{v},$$

where $\omega := \nabla \times \mathbf{v}$, we obtain

$$\partial_t \mathbf{v} + \omega \times \mathbf{v} + \nabla\left(\frac{1}{2}|\mathbf{v}|^2\right) + V\nabla p = -\nabla\Phi. \tag{3.2}$$

For barotropic flows, $V\nabla p = \nabla h$, where $h = \int \frac{dp}{\rho}$. The Euler equation simplifies to:

$$\boxed{\partial_t \mathbf{v} + \omega \times \mathbf{v} + \nabla H = 0,} \tag{3.3}$$

where

$$H = \frac{1}{2}|\mathbf{v}|^2 + h(\rho) + \Phi(\mathbf{x}).$$

In the case of steady flows, the equation becomes:

$$\omega \times \mathbf{v} + \nabla H = 0. \tag{3.4}$$

Taking the inner product of this equation with $\mathbf{v}$, we obtain:

$$\mathbf{v} \cdot \nabla H = 0.$$

This means that the directional derivative of H in the direction $\mathbf{v}$ is zero, indicating that this quantity remains constant along the integral curve of $\mathbf{v}$, which is the streamline. □

Remarks

1. The Bernoulli theorem is an algebraic relation between kinematic variable $\mathbf{v}$ and thermodynamic variables $h(\rho)$, and the external conservative force.

2. That the Bernoulli principle derived from the momentum equation, is similar to the conservation of total energy derived from momentum equation in classical mechanics. [1]

3. Formula (3.3) indicates that the acceleration is attributed to:

   (i) a rotation ($\omega \times \mathbf{v}$), where $\dot{\mathbf{v}} = -\omega \times \mathbf{v}$ represents a rotation of $\mathbf{v}$. The term $\omega \times \mathbf{v}$ is called the *vorticity force.*

   (ii) a conservative force $\nabla(|\mathbf{v}|^2/2 + h + \Phi)$.

4. For barotropic flows, the pressure p is only a function of density. We express U as a function of ρ as

$$U = -\int^V p\left(\frac{1}{V}\right)\, dV = \int^\rho \frac{p(\rho)}{\rho^2}\, d\rho.$$

   The enthalpy

$$h(\rho) := U + pV$$

[1] In classical mechanics, the momentum equation is $m\ddot{\mathbf{x}} = -\nabla\Phi(\mathbf{x})$, we multiply it by $\dot{\mathbf{x}}$ to get $\frac{d}{dt}\left(\frac{1}{2}m|\mathbf{v}|^2 + \Phi(\mathbf{x})\right) = 0$. This gives $\frac{d}{dt}\left(\frac{1}{2}m|\mathbf{v}|^2 + \Phi(\mathbf{x})\right) = E$ along a particle trajectory.

satisfies
$$h'(\rho) = U'(\rho) + \frac{d}{d\rho}\left(\frac{p}{\rho}\right) = \frac{p'(\rho)}{\rho}.$$
In particular, when $p(\rho) = A\rho^{\gamma}$, where A is a constant, we have
$$h(\rho) = \frac{\gamma}{\gamma - 1}\frac{p}{\rho}.$$

5. For steady barotropic flows, the equation becomes:
$$\omega \times \mathbf{v} + \nabla H = 0. \tag{3.5}$$
We observe that H remains constant along the integral curve of $\mathbf{v}$. Similarly, applying the same procedure, we derive:
$$\omega \cdot \nabla H = 0.$$
This implies that H also remains constant along the integral of ω, referred to as the vortex filament.

6. In the case of $\omega \equiv 0$, such a flow is termed an irrotational flow. For steady, irrotational, and barotropic flows, we have $\nabla H \equiv 0$. Consequently, we obtain:
$$H = constant$$
in every simply connected subdomain of the flow region.

7. Another special case is: $\rho \equiv constant$. In this case, the term $V\nabla p$ in (3.2) is $\nabla\frac{p}{\rho}$. Thus, h in (3.1) is replaced by p/ρ. The Bernoulli principle for constant density case reads:
$$H = \frac{1}{2}|\mathbf{v}|^2 + \frac{p}{\rho} + \Phi(\mathbf{x}) = constant$$
along a streamline.

Applications of Bernoulli Principle

1. Vortex center has low pressure:
    - Typically, the center of a vortex exhibits higher speed, resulting in low pressure at the center.
2. Effect of Strong Wind:
    - In strong winds, the low pressure makes it more challenging to inhale and breathe.

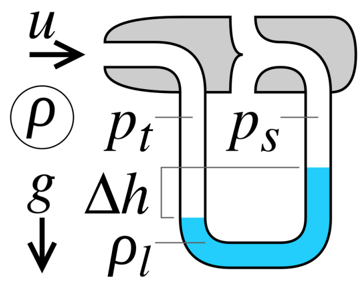

Figure 3.1: Pitot Tube. Credit to Cmglee - Own work, CC BY-SA 4.0, `https://commons.wikimedia.org/w/index.php?curid=74391265http://galileo.phys.virginia.edu/classes/152.mf1i.spring02/Boyle.htm`

3. Pitot Tube, wiki, Video

   - The Pitot tube utilizes Bernoulli's law to measure wind speed, employing the equation:
   $$\frac{1}{2}v^2 + \frac{p_s}{\rho} = \frac{p_t}{\rho}.$$
   Here, p_t is the total pressure or the stagnation pressure, p_s the static pressure. This yields the wind speed equation:
   $$v = \sqrt{\frac{2(p_t - p_s)}{\rho}} = \sqrt{\frac{2\rho_m g h}{\rho}},$$
   where ρ_m is the density of mercury, and ρ is the density of gas.
   - For further applications such as the Venturi effect (for reducing fluid pressure by increasing flow speed), flows through an aperture (Torricelli's Theorem), etc., you can read a classical book: Milne-Thomson, Theoretical Hydrodynamics.

3.2 Vorticity and Circulation Theorem

3.2.1 Circulation Theorem for Barotropic Flows

Vorticity and circulation theory play important roles in fluid dynamics. For thermo degenerate fluid flows, the vorticity equation only involves kinematic variables, the thermodynamic variables do not show up. On the other hand, one can recover the velocity from vorticity. The thermodynamic variables are transported passively.

Circulation and vorticity theory was developed by Cauchy, Hankel, Helmholtz, Kelvin in 19 century. A good historical review article about vorticity and circulation is the article: Uriel Frisch and Barbara Villone, Cauchy's almost forgotten Lagrangian formulation of the Euler equation for 3D incompressible flow (`https://arxiv.org/pdf/1402.4957.pdf`).

Definition 3.2. *Given a closed curve C in the fluid region. We define the circulation of flow field* $\mathbf{v}$ *along C to be*

$$\int_C \mathbf{v}\cdot\mathbf{t}\,ds.$$

The circulation measures how fluid rotates. By the Stokes theorem,

$$\int_C \mathbf{v}\cdot\mathbf{t}\,ds = \int_\Sigma \nabla\times\mathbf{v}\cdot\nu\,dS \tag{3.6}$$

where Σ is any surface with $\partial\Sigma = C$. The quantity $\omega := \nabla\times\mathbf{v}$ is called the *vorticity*. Thus, this circulation is equal to the vorticity flux passing through the surface enclosed by C.

Theorem 3.3 (Circulation Theorem)**.** *In an inviscid fluid flow under a conservative body force with degenerate thermo relation, the circulation is invariant under fluid flow. More precisely, let C_0 be a closed curve and $C(t) := \varphi_t(C_0)$. Then*

$$\frac{d}{dt}\int_{C(t)} \mathbf{v}(t)\cdot\mathbf{t}\,ds_t = 0.$$

Proof. With the thermo degenerate relation, we can find h such that $\nabla h = \nabla p/\rho$. Thus, the Euler equation becomes

$$\dot{\mathbf{v}} = \partial_t\mathbf{v} + \mathbf{v}\cdot\nabla\mathbf{v} = -\frac{1}{\rho}\nabla p - \nabla\Phi = -\nabla\left(h+\Phi\right), \tag{3.7}$$

Let us parametrize the curve C_0 by arc length s. That is $C_0 = \{X(s)\,|\,0\le s\le L\}$ with $X(0) = X(L)$. The curve $C(t)$ in the observer's space is $C(t) = \{\mathbf{x}(t,X(s))|0\le s\le L\}$. Its tangent is

$$\mathbf{t} = \frac{\frac{\partial\mathbf{x}(t,X(s))}{\partial s}}{\|\frac{\partial\mathbf{x}(t,X(s))}{\partial s}\|}$$

and the arc length is

$$ds_t = \left\|\frac{\partial\mathbf{x}(t,X(s))}{\partial s}\right\| ds.$$

Let us write

$$\frac{\partial\mathbf{x}(t,X(s))}{\partial s} = \mathbf{x}'(t,X(s))$$

Let us write the evolution of circulation in Lagrange coordinate:

$$\int_{C(t)} \mathbf{v}(t,\mathbf{x}) \cdot \mathbf{t}\, ds_t = \int_0^L \mathbf{v}(t,\mathbf{x}(t,X(s)) \cdot \mathbf{x}'(t,X(s))\, ds.$$

We differentiate this equation in t with fixed $X(s)$.

$$\begin{aligned}
\frac{d}{dt}\int_{C(t)} \mathbf{v}(t,\mathbf{x}) \cdot \mathbf{t}\, ds &= \frac{d}{dt}\int_0^L \mathbf{v}(t,\mathbf{x}(t,X(s)) \cdot \mathbf{x}'(t,X(s))\, ds \\
&= \int_0^L \dot{\mathbf{v}} \cdot \mathbf{x}'(s) + \mathbf{v} \cdot \dot{\mathbf{x}}'\, ds \\
&= \int_0^L \nabla(-\Phi - h) \cdot \mathbf{x}' + \mathbf{v} \cdot (\nabla \mathbf{v} \cdot \mathbf{x}')\, ds \qquad \because \dot{\mathbf{x}}' = \frac{d}{ds}\mathbf{v} = \nabla \mathbf{v} \cdot \mathbf{x}' \\
&= \int_0^L \nabla\left(-\Phi - h + \frac{1}{2}|\mathbf{v}|^2\right) \cdot \mathbf{x}'\, ds \\
&= \int_0^L \frac{d}{ds}\left(\frac{1}{2}|\mathbf{v}|^2 - h - \Phi\right) ds \\
&= 0. \qquad \because C(0) \text{ is a closed curve.}
\end{aligned}$$

□

Corollary 3.2. *For fluid flows with degenerate thermo relation and under conservative force field, its vorticity 2-form is invariant with the flow. In other words, if Σ is a closed surface and $\Sigma(t) = \varphi_t(\Sigma)$, then*

$$\frac{d}{dt}\int_{\Sigma(t)} \omega \cdot \nu\, dS_t = 0. \tag{3.8}$$

Proof. From the Stokes theorem,

$$\frac{d}{dt}\int_{\Sigma(t)} \nabla \times \mathbf{v} \cdot \nu\, dS_t = \frac{d}{dt}\int_{\partial\Sigma(t)} \mathbf{v} \cdot \mathbf{t}\, ds = 0.$$

□

3.2.2 Vorticity Equation in Eulerian coordinate

In this subsection, we derive a vorticity equation, which can be thought of as a differential form of the circulation theorem.

1. We assume the specific body force is conservative. The Euler equation reads

$$\partial_t \mathbf{v} + \boldsymbol{\omega} \times \mathbf{v} + \nabla\left(\frac{1}{2}|\mathbf{v}|^2\right) + V\nabla p = -\nabla\Phi,$$

   By taking *curl* (i.e., $\nabla\times$) on this equation, we can eliminate those gradient terms and leave only kinematic variables:

$$\boxed{\partial_t \boldsymbol{\omega} + \mathbf{v}\cdot\nabla\boldsymbol{\omega} - (\boldsymbol{\omega}\cdot\nabla)\,\mathbf{v} + \boldsymbol{\omega}\,(\nabla\cdot\mathbf{v}) = \nabla p \times \nabla V.} \tag{3.9}$$

   This is the vorticity equation in the Eulerian coordinates. In the derivation, we have used the identities from vector calculus

$$\nabla\times(\boldsymbol{\omega}\times\mathbf{v}) = (\mathbf{v}\cdot\nabla)\boldsymbol{\omega} - \boldsymbol{\omega}\cdot\nabla\mathbf{v} + \boldsymbol{\omega}(\nabla\cdot\mathbf{v}) - \mathbf{v}(\nabla\cdot\boldsymbol{\omega})$$
$$\nabla\cdot\boldsymbol{\omega} = \nabla\cdot\nabla\times\mathbf{v} = 0$$
$$\nabla\times(V\nabla p) = \nabla V\times\nabla p + V\nabla\times(\nabla p) = \nabla V\times\nabla p.$$

2. Note that from the first law of thermodynamics

$$\nabla U = T\nabla S - p\nabla V.$$

   We take curl on both sides, using $\nabla\times(T\nabla S) = \nabla T\times\nabla S$ to get

$$0 = \nabla T\times\nabla S - \nabla p\times\nabla V.$$

   Thus, the vorticity equation is equivalent to

$$\boxed{\partial_t \boldsymbol{\omega} + \mathbf{v}\cdot\nabla\boldsymbol{\omega} - (\boldsymbol{\omega}\cdot\nabla)\,\mathbf{v} + \boldsymbol{\omega}\,(\nabla\cdot\mathbf{v}) = \nabla T \times \nabla S.} \tag{3.10}$$

3. Each term in the vorticity has a name:

   - $\mathbf{v}\cdot\nabla\boldsymbol{\omega}$: the advection term
   - $(\boldsymbol{\omega}\cdot\nabla)\,\mathbf{v}$ the deformation (stretching or expansion) term
   - $\boldsymbol{\omega}\,(\nabla\cdot\mathbf{v})$ the source term.

4. The circulation conservation is valid on the level set of entropy, where $\nabla S = 0$. In fact, it is valid on the level set of S, or T, or p, or V.

5. For fluid flows with degenerate thermo relation and under conservative force field, the thermo area element degenerate. The vorticity equation becomes

$$\boxed{\partial_t \boldsymbol{\omega} + \mathbf{v}\cdot\nabla\boldsymbol{\omega} - (\boldsymbol{\omega}\cdot\nabla)\,\mathbf{v} + \boldsymbol{\omega}\,(\nabla\cdot\mathbf{v}) = 0.} \tag{3.11}$$

   This gives the circulation theorem.

Homeworks Let $\omega := \nabla \times \mathbf{v}$, show the following identities in vector calculus:

1. $\mathbf{v} \cdot \nabla \mathbf{v} = \nabla \left(\frac{1}{2}|\mathbf{v}|^2\right) + \omega \times \mathbf{v}$.
2. $\nabla \times (\omega \times \mathbf{v}) = \omega(\nabla \cdot \mathbf{v}) - \mathbf{v}(\nabla \cdot \omega) + (\mathbf{v} \cdot \nabla)\omega - \omega \cdot \nabla \mathbf{v}$
3. $\nabla \cdot \nabla \times \mathbf{v} = 0$
4. $\nabla \times (V \nabla p) = \nabla V \times \nabla p + V \nabla \times (\nabla p) = \nabla V \times \nabla p$.

3.2.3 Vorticity equation in Lagrangian coordinate

1. There is a very good interpretation of the above vorticity equation in differential geometry. Let us define the vorticity 2-form as

$$\omega = \omega \cdot \nu dS = \omega_1 dx^2 \wedge dx^3 + \omega_2 dx^3 \wedge dx^1 + \omega_3 dx^1 \wedge dx^2.$$

In (3.8), let us change the integration back to initial time:

$$\frac{d}{dt}\int_{\Sigma(t)} \omega = \frac{d}{dt}\int_{\Sigma(0)} \varphi_t^* \omega = \int_{\Sigma(0)} \frac{d}{dt} \varphi_t^* \omega$$

The term $\varphi_t^* \omega$ is a 2-form at time 0, called the pullback of ω by the flow map φ_t:

$$\begin{aligned} \varphi_t^* \omega(t,X) := {} & \omega^1(t,\mathbf{x}(t,X)) dx^2(t,X) \wedge dx^3(t,X) \\ & + \omega^2(t,\mathbf{x}(t,X)) dx^3(t,X) \wedge dx^1(t,X) \\ & + \omega^3(t,\mathbf{x}(t,X)) dx^1(t,X) \wedge dx^2(t,X). \end{aligned}$$

2. Let d_t be the abbreviation of d/dt, which is the partial derivative in t with fixed X, i.e. the material derivative.

$$\begin{aligned} d_t \varphi_t^* \omega = {} & (d_t \omega^1) dx^2 \wedge dx^3 + (d_t \omega^2) dx^3 \wedge dx^1 + (d_t \omega^3) dx^1 \wedge dx^2 \\ & + \omega^1 d_t(dx^2 \wedge dx^3) + \omega^2 d_t(dx^3 \wedge dx^1) + \omega^3 d_t(dx^1 \wedge dx^2) \\ = {} & \left[(\partial_t + \mathbf{v} \cdot \nabla)\omega^1 + \omega^1 \left(\frac{\partial v^2}{\partial x^2} + \frac{\partial v^3}{\partial x^3}\right) - \omega^2 \frac{\partial v^1}{\partial x^2} - \omega^3 \frac{\partial v^1}{\partial x^3} \right] dx^2 \wedge dx^3 \\ & + \left[(\partial_t + \mathbf{v} \cdot \nabla)\omega^2 + \omega^2 \left(\frac{\partial v^1}{\partial x^1} + \frac{\partial v^3}{\partial x^3}\right) - \omega^3 \frac{\partial v^2}{\partial x^3} - \omega^1 \frac{\partial v^2}{\partial x^1} \right] dx^3 \wedge dx^1 \\ & + \left[(\partial_t + \mathbf{v} \cdot \nabla)\omega^3 + \omega^3 \left(\frac{\partial v^1}{\partial x^1} + \frac{\partial v^2}{\partial x^2}\right) - \omega^3 \frac{\partial v^3}{\partial x^1} - \omega^1 \frac{\partial v^3}{\partial x^2} \right] dx^1 \wedge dx^2 \end{aligned}$$

For each component, we have

$$d_t\omega^i = \partial_t\omega^i + v^k\frac{\partial\omega^i}{\partial x^k} + \omega^i\frac{\partial v^k}{\partial x^k} - \frac{\partial v^i}{\partial x^k}\omega^k$$

In vector calculus, we define $\omega = (\omega^1, \omega^2, \omega^3)^T$. In vector form, it is

$$\boxed{d_t\omega = \partial_t\omega + \mathbf{v}\cdot\nabla\omega + \omega\nabla\cdot\mathbf{v} - (\nabla\mathbf{v})\omega,} \tag{3.12}$$

Thus, we get

$$\boxed{d_t\omega = \varphi_t^*\left(dp\wedge dV\right).} \tag{3.13}$$

3. Expression in terms of Lie derivative. The Lie derivative is defined to be

$$d_t = \varphi_t^*\left(\partial_t + \mathscr{L}_v\right).$$

With this notation, we have

$$\boxed{\partial_t\omega + \mathscr{L}_{\mathbf{v}}\omega = dp\wedge dV = dT\wedge dS.} \tag{3.14}$$

The last equality is obtained from $0 = d^2U = dT\wedge dS - dp\wedge dV$.

3.2.4 Helmholtz's Vorticity Equation: Deformation of ω/ρ

In the vorticity equation:

$$\partial_t\omega + \mathbf{v}\cdot\nabla\omega - (\omega\cdot\nabla)\,\mathbf{v} + \omega\,(\nabla\cdot\mathbf{v}) = \nabla p\times\nabla V. \tag{3.15}$$

Helmholtz derived another form of vorticity equation without the source term $\omega\,(\nabla\cdot\mathbf{v})$. Recall the continuity equation:

$$\partial_t V + \mathbf{v}\cdot\nabla V = V(\nabla\cdot\mathbf{v}). \tag{3.16}$$

By V(3.15) $+\omega$ (3.16), we can cancel the source term to get

$$\boxed{\partial_t\,(V\omega) + \mathbf{v}\cdot(V\omega) - (V\omega\cdot\nabla)\,\mathbf{v} = V\nabla p\times\nabla V.} \tag{3.17}$$

In terms of the density $\rho := 1/V$, it reads

$$\frac{d}{dt}\left(\frac{\omega}{\rho}\right) - \left(\frac{\omega}{\rho}\cdot\nabla\right)\mathbf{v} = \frac{1}{\rho^3}\nabla\rho\times\nabla p. \tag{3.18}$$

Remarks.

- The term $\left(\frac{\omega}{\rho}\cdot\nabla\right)\mathbf{v}$ (i.e., $\frac{\omega^k}{\rho}\frac{\partial}{\partial x^k}v^i$) can be expressed as $(\nabla\mathbf{v})(\omega/\rho)$ (i.e., $\frac{\partial v^i}{\partial x^k}\omega^k/\rho$). It is a deformation term. We may diagonalize $\nabla\mathbf{v}$ and observe how ω/ρ changes along the eigenvectors of $\nabla\mathbf{v}$. In the expansion direction (the corresponding eigenvalue of $\nabla\mathbf{v}$ is positive), the corresponding component of ω/ρ increases exponentially, whereas in the shrinking direction, the component of ω/ρ decreases exponentially.

- The term on the right-hand side $\frac{1}{\rho^3}\nabla\rho\times\nabla p$ is called the buoyancy source.

- The compressible vortex ω/ρ is transported like a vector.

In the case of thermo degeneracy where $\nabla V\times\nabla p = 0$, we have the following theorem.

Theorem 3.4. *For fluid flows with degenerate thermo relation and under conservative force field, we have*

$$\frac{d}{dt}\left(\frac{\omega}{\rho}\right) = \left(\frac{\omega}{\rho}\cdot\nabla\right)\mathbf{v} \tag{3.19}$$

and

$$\boxed{\frac{\omega}{\rho}(t) = \frac{\partial\mathbf{x}(t,X)}{\partial X}\frac{\omega}{\rho}(0).} \tag{3.20}$$

It means that $\frac{\omega}{\rho}$ is transported like a tangent vector along a particle path.

Proof. 1. Formulae (3.19) is obtained from (3.18) because of the degenerate thermo relation.

2. Equation (3.19) in matrix form is

$$\frac{d}{dt}\left(\frac{\omega}{\rho}\right) = (\nabla\mathbf{v})\left(\frac{\omega}{\rho}\right).$$

This is identical to the perturbation equation of the flow map equation:

$$\dot{\mathbf{x}} = \mathbf{v}(t,\mathbf{x}),$$

which is

$$\frac{d}{dt}\delta\mathbf{x} = \frac{\partial\mathbf{v}}{\partial\mathbf{x}}\delta\mathbf{x}.$$

Its solution is

$$\delta\mathbf{x}(t) = \frac{\partial\mathbf{x}}{\partial X}\mathbf{x}(0).$$

This is because it satisfies the perturbation equation:

$$\frac{d}{dt}\delta\mathbf{x}(t) = \frac{d}{dt}\frac{\partial\mathbf{x}}{\partial X}\mathbf{x}(0) = \frac{\partial\mathbf{v}}{\partial X}\mathbf{x}(0) = \frac{\partial\mathbf{v}}{\partial\mathbf{x}}\frac{\partial\mathbf{x}}{\partial X}\mathbf{x}(0) = (\nabla\mathbf{v})\,\mathbf{x}(t),$$

and the solution is unique.

3. Thus, we may think $\frac{\omega}{\rho}(0)$ as a tangent vector at $(t=0,X)$, $\frac{\omega}{\rho}(t)$ as a tangent vector at $(t,\mathbf{x}(t,X))$. The tangent vector $\frac{\omega}{\rho}(t)$ is transported along the flow trajectory.

□

Corollary 3.3. *For fluid flows with degenerate thermo relation and under conservative force field, if $\omega \equiv 0$ initially, then it stays $\omega(t) \equiv 0$ for all later time. In other words, for thermo degenerate fluids, if the flow is irrotational initially, it stays irrotational in all later time.*

Remarks In terms of the Language of differential geometry,

- an equivalent formulation of the above theorem is

$$\boxed{\omega^i(t) = \frac{1}{J} F^i_\alpha \omega_0^\alpha.}$$

- The push forward of the vorticity two form is

$$\star_t \omega(t) = F \star_0 \omega_0.$$

  The ratio of the two stars ($\star_t$ and $\star_0$) gives the J term.

- One can express ω/ρ as $\frac{\omega_i}{\rho}\frac{\partial}{\partial x^i}$.

Vortex filament

- Let us define the vortex filament to be the integral curve of the vorticity field ω. Let $X(\alpha)$ be a vortex filament at $t=0$. That is,

$$\frac{dX}{d\alpha} = \frac{\omega(X,0)}{\rho(X,0)}.$$

  Let us investigate this line following the flow $\mathbf{x}(t,X(\alpha))$. Its tangent is

$$\begin{aligned}
\frac{d}{d\alpha}\mathbf{x}(t,X(\alpha)) &= \frac{\partial \mathbf{x}}{\partial X}\frac{dX}{d\alpha} \\
&= \frac{\partial \mathbf{x}}{\partial X}\frac{\omega}{\rho}(0) \\
&= \frac{\omega}{\rho}(t).
\end{aligned}$$

  This shows that the vortex filament stays as a vortex filament. Thus, a vortex filament flows with the fluid flow.

- The vortex filaments through each point of a closed surface Σ constitute a vortex tube Ω. Thus, a vortex filament is an infinitesimal vortex tube. The circulation theorem implies that the vortex tube (filament) stays as a vortex tube (filament) as it flows with the fluid.

3.2.5 Potential Vorticity

- Ertel (1942) derived another form of vorticity equation, which removed the buoyancy term and the stretching term. It is useful in rotating fluid dynamics. The idea is to introduce a free advected thermo parameter, called ψ. It has two properties:
  - $\nabla\psi \cdot (\nabla V \times \nabla p) = 0$
  - ψ is freely advected by the flow:
$$\partial_t \psi + \mathbf{v} \cdot \nabla \psi = 0.$$
- Examples of such function Ψ are
  - Entropy S
  - Potential temperature θ
$$\theta := T\left(\frac{p_0}{p}\right)^{R/c_p} = T\left(\frac{p_0}{p}\right)^{\gamma-1)/\gamma}$$
where p_0 is a standard reference pressure, usually $1,000\,hPa$ $(1,000mb)$. (The standard atmosphere (symbol: atm) is a unit of pressure defined as $1,013.25\,hPa$.)
- If we take the dot product of the vorticity equation (3.17) with $\nabla\psi$, then the right-hand side disappears because there are only two independent thermo parameters.
- **Potential Vorticity** Define
$$q := \frac{\omega \cdot \nabla\psi}{\rho} = \frac{\nabla \cdot (\psi\omega)}{\rho} \qquad (\because \nabla \cdot \omega = 0). \tag{3.21}$$
It is called the *potential vorticity* associated with the advected quantity ψ.
- **Ertel's Theorem:** *The potential vorticity is freely advected:*
$$\boxed{\frac{Dq}{Dt} = 0.} \tag{3.22}$$
That is, q is invariant along the parcel trajectory.

Proof. 1. Let us rewrite the Helmholtz vorticity equation (3.17) as

$$\frac{D}{Dt}\xi - \xi \cdot \nabla \mathbf{v} = V\nabla V \times \nabla p. \tag{3.23}$$

where $\xi := V\omega = \omega/\rho$.

2. We take ∇ to the free advection equation of ψ:

$$\begin{aligned} 0 &= \nabla\left(\partial_t \psi + \mathbf{v}\cdot\nabla\psi\right) \\ &= \partial_t(\nabla\psi) + (\nabla\mathbf{v})\cdot(\nabla\psi) + \mathbf{v}\cdot\nabla(\nabla\psi) \\ &= \frac{D}{Dt}(\nabla\psi) + (\nabla\mathbf{v})\cdot(\nabla\psi) \end{aligned} \tag{3.24}$$

3. We take

$$\nabla\psi \cdot (3.23) + \xi \cdot (3.24),$$

Using $\nabla\psi \cdot (\nabla V \times \nabla p) = 0$, we get

$$\nabla\psi \cdot \frac{D}{Dt}\xi + \xi \frac{D}{Dt}(\nabla\psi) = 0.$$

□

- **Remarks.**
  1. The potential vorticity is a 0-form.
  2. The Ertel Theorem can also be derived from the relabeling symmetry (see Salmon, 1988).

References

1. P.G. Saffman, Vortex Dynamics (1992)
2. Lamb, Hydrodynamics (1932).

3.3 Vortex Momentum

3.3.1 Vortex Momentum

Ref. Saffman, Vortex Dynamics, Chapter 3.

3.3.2 Some Flow Conservative Quantities

The following statement is copied from Majda and Bertozzi, Vorticity and Incompressible Flow (pp. 24) For incompressible inviscid flows which are vanishing at infinity, the following quantities are conserved in time:

- total velocity: $\int \mathbf{v}\, d\mathbf{x}$
- total vorticity: $\int \omega\, d\mathbf{x}$
- total kinetic energy:
$$\frac{1}{2}\int |\mathbf{v}|^2\, d\mathbf{x} = \int \mathbf{v}\cdot(\mathbf{x}\times\omega)\, d\mathbf{x}.$$
- Helicity:
$$\int \mathbf{v}\cdot\omega\, d\mathbf{x}$$
- Impulse:
$$\frac{1}{2}\int \mathbf{x}\times\omega\, d\mathbf{x}.$$
- Moment of fluid impulse:
$$\frac{1}{3}\int \mathbf{x}\times(\mathbf{x}\times\omega)\, d\mathbf{x}.$$

We are interested in global mechanical properties expressed in terms of $\mathbf{v}$ and ω. For instance, we can project the impulse to a direction $\mathbf{a}$ to get the impulse in the $\mathbf{a}$ direction:

$$\begin{aligned}
\int \langle \mathbf{x}\times\omega(\mathbf{x}), \mathbf{a}\rangle\, d\mathbf{x} &= \int \langle \omega(\mathbf{x})\times\mathbf{a}, \mathbf{x}\rangle\, d\mathbf{x} \\
&= \int \left(\nabla_{\mathbf{a}}\langle \mathbf{x},\mathbf{v}\rangle - \langle \mathbf{v}, \nabla_{\mathbf{x}}\mathbf{a} - \nabla_{\mathbf{a}}\mathbf{x}\rangle - \nabla_{\mathbf{x}}\langle \mathbf{a},\mathbf{v}\rangle\right) d\mathbf{x} \\
&= \int \left(\langle \mathbf{v},\mathbf{a}\rangle + (\nabla\cdot\mathbf{x})\langle \mathbf{a},\mathbf{v}\rangle\right) d\mathbf{x} \\
&= 4\int \langle \mathbf{v},\mathbf{a}\rangle\, d\mathbf{x}.
\end{aligned}$$

Chapter 4

Variational Principles for Fluid Flows

The approach of variational principles in analytic mechanics has a long history. You can see wiki page on the "the History of Variational Principles in Physics". Below is a brief list of historical developments:

- (1705) Gottfried Leibniz, least action principle
- (1744) Euler and Pierre Louis Maupertuis, Least action principle
- (1757) Euler: Euler equation (continuity equation and momentum equation)
- (1788) Lagrange formulated Lagrange mechanics and derived Euler equation based on the variational principle in Lagrangian coordinates.
- (1809) Poisson introduced the Poisson bracket.
- (1833) Hamilton formulated Hamiltonian mechanics based on Lagrange mechanics

We shall derive the equations of fluid dynamics via the variational approach. There are two approaches, one uses Lagrangian coordinates, the other uses Eulerian coordinates.

4.1 Lagrange's Variational Approach

In 1788, Lagrange derived the Euler equation based on the variational principle in Lagrangian coordinates. Mimicking the variational approach in classical mechanics, we shall take the variation of the action with respect to parcel paths $\mathbf{x}(t, X)$, or equivalently, the flow maps.

- **Action** Given a flow map $\mathbf{x}(\cdot,\cdot)$, we define its *action* in the Lagrangian coordinates to be

$$\mathcal{S}[\mathbf{x}] = \mathscr{T}[\mathbf{x}] - \mathscr{U}[\mathbf{x}] := \int_{t_0}^{t_1}\int_{\Omega_0}\left(\frac{1}{2}\rho_0(X)|\dot{\mathbf{x}}(t,X)|^2 - W\left(\frac{\partial \mathbf{x}}{\partial X}\right)\right) dX\,dt.$$

  Here, the first term is the kinetic energy, while the second term $W(F)$ is the potential energy, which is the energy stored in a fluid parcel through the deformation gradient $F = \frac{\partial \mathbf{x}}{\partial X}$.

- In the case of fluid mechanics, $W(F(t,X)) = \rho_0(X)U(S_0(X),V)$ for a fluid parcel. The specific volume V is

$$V := \frac{1}{\rho} = \frac{J}{\rho_0} = \frac{\det(F)}{\rho_0}$$

- Note that the specific entropy S is assumed as a constant along a parcel path. Therefore, $W = \rho_0(X)U(S,V)$ is a function of $det(F)$ along a parcel path.

We will derive the equation of motion in Lagrangian coordinates without the body force. First, we work for compressible fluid flows. Next, we work out incompressible fluid flows.

4.1.1 Variation of Action w.r.t. Flow Maps for Compressible Flows

Equation of motion for the flow maps $\mathbf{x}(t,X)$

1. **Variation of flow maps** We will study the variation of the action with respect to the flow map $\mathbf{x}(\cdot,\cdot)$. Let us perturb the flow map by $\mathbf{x}^\varepsilon(t,X)$ with $\mathbf{x}^0(t,X) = \mathbf{x}(t,X)$, the original unperturbed flow map. We denote

$$\delta\mathbf{x}(t,X) := \frac{\partial}{\partial\varepsilon}|_{\varepsilon=0}\mathbf{x}^\varepsilon(t,X), \tag{4.1}$$

   as the variation of the flow map $\mathbf{x}(\cdot,\cdot)$. We represent the variation of $\mathbf{x}$ by $\delta\mathbf{x}$. Since, $\mathbf{x}^\varepsilon(t,\cdot)$ are flow maps, its variation $\delta\mathbf{x}$ is an infinitesimal variation of position, can be called a virtual displacement.

2. **Variation of a functional** The variation of a functional $I[\mathbf{x}]$ in the direction of $\delta\mathbf{x}$ means that

$$\delta I[\mathbf{x}] := \frac{d}{d\varepsilon}|_{\varepsilon=0}I[\mathbf{x}^\varepsilon].$$

   The derivative $\frac{\delta I}{\delta \mathbf{x}}$ is defined to be

$$\delta I[\mathbf{x}] = \frac{\delta I}{\delta\mathbf{x}}\cdot\delta\mathbf{x}.$$

3. **Variation of action with respective to flow maps** We shall study the variation of action w.r.t. flow maps. We choose those variations $\delta\mathbf{x}$ satisfying $\delta\mathbf{x}(t,X)=0$ for $t=t_0$ and $t=t_1$ so that we can take integration by part for t in the action integral, no boundary terms appear.

$$
\begin{aligned}
\delta\mathcal{S}[\mathbf{x}] &= \int_{t_0}^{t_1}\int_{\Omega_0}\big(\rho_0(X)\dot{\mathbf{x}}(t,X)\cdot\delta\dot{\mathbf{x}}-W'(F)\delta F\big)\,dX\,dt\\
&= \int_{t_0}^{t_1}\int_{\Omega_0}\left(-\frac{d}{dt}\left(\rho_0(X)\dot{\mathbf{x}}(t,X)\right)\cdot\delta\mathbf{x}-W'(F)\frac{\delta\partial\mathbf{x}}{\partial X}\right)dX\,dt\\
&= \int_{t_0}^{t_1}\int_{\Omega_0}\left(-\rho_0(X)\ddot{\mathbf{x}}(t,X)\cdot\delta\mathbf{x}-W'(F)\frac{\partial\delta\mathbf{x}}{\partial X}\right)dX\,dt\\
&= \int_{t_0}^{t_1}\int_{\Omega_0}\left(-\rho_0(X)\ddot{\mathbf{x}}(t,X)\cdot\delta\mathbf{x}-\frac{\partial}{\partial X}\cdot\big(W'(F)\delta\mathbf{x}\big)+\left(\frac{\partial}{\partial X}\cdot W'(F)\right)\cdot\delta\mathbf{x}\right)dX\,dt\\
&= \int_{t_0}^{t_1}\int_{\Omega_0}\left(-\rho_0(X)\ddot{\mathbf{x}}(t,X)+\frac{\partial}{\partial X}\cdot W'(F)\right)\cdot\delta\mathbf{x}\,dX\,dt.
\end{aligned}
$$

Here, we have chosen those variations satisfying

$$\int_{\Omega_0}\frac{\partial}{\partial X}\cdot\big(W'(F)\delta\mathbf{x}\big)\,dX=\int_{\partial\Omega_0}W'(F)\delta\mathbf{x}\cdot\mathbf{n}\,dS_0=0. \tag{4.2}$$

4. **Equation of motion for the flow map** The least action principle states that

$$\frac{\delta\mathcal{S}}{\delta\mathbf{x}}[\mathbf{x}]=0 \tag{4.3}$$

along a physical flow map $\mathbf{x}$. That is

$$\boxed{\frac{\delta\mathcal{S}}{\delta\mathbf{x}}=-\rho_0(X)\ddot{\mathbf{x}}(t,X)+\nabla_X\cdot P\left(\frac{\partial\mathbf{x}}{\partial X}\right)=0.} \tag{4.4}$$

Here, $P=W'(F)$ is called the first Piola stress tensor. The component form of the above equation is

$$P_i^\alpha=\frac{\partial W}{\partial F_\alpha^i},\quad F_\alpha^i:=\frac{\partial x^i}{\partial X_\alpha},\quad (\nabla_X\cdot P)^i=\frac{\partial}{\partial X^\alpha}P_i^\alpha.$$

This is the equation of motion in Lagrangian coordinates for the flow map $\mathbf{x}(t,X)$. It is a second-order partial differential equations.

Equation (4.3) is called the Euler-Lagrange equation corresponding to the action $\mathcal{S}$.

Equation of motion for $(\mathbf{v}, F)$

1. **Equation of motion for $(\mathbf{v}, F)$** Let us express this equation of motion in terms of $\mathbf{v}$ and thermo variables in Lagrangian coordinate. First, the Euler-Lagrange equation (4.4) can be rewritten as
$$\rho_0 \dot{\mathbf{v}} = \nabla_X \cdot P.$$
Next, we express the first Piola stress in terms of thermo variables. Recall that
$$W(F) = \rho_0(X) U(S_0(X), V),$$
because the entropy S is constant along particle path. The first Piola stress $P = W'(F)$ becomes
$$\begin{aligned} P = W'(F) &= \frac{\partial(\rho_0(X)U(S_0(X),V))}{\partial F} = \rho_0 \frac{\partial U}{\partial V}\frac{\partial V}{\partial F} \\ &= -\rho_0 p \frac{\partial V}{\partial F} = -p\frac{\partial(\rho_0 V)}{\partial F} = p\frac{\partial J}{\partial F} = -pJF^{-T}. \end{aligned}$$
Here, we have used $V = 1/\rho$, $\rho J = \rho_0$ and $\partial \det(F)/\partial F = JF^{-T}$, which is (2.18). Thus, the equation of motion is
$$\begin{cases} \rho_0 \dot{\mathbf{v}} = \nabla_X \cdot P(F) \\ \dot{F} = \frac{\partial \mathbf{v}(t,X)}{\partial X} \end{cases} \tag{4.5}$$
where
$$P = -pJF^{-T}. \tag{4.6}$$
The thermodynamic variable p is a function of (S,V). With fixed X, we have $S(t,X) = S_0(X)$. The variable $V = 1/\rho = J/\rho_0 = \det(F)/\rho_0(X)$. Thus,
$$p(S,V) = p\left(S_0(X), \frac{\det(F)}{\rho_0(X)}\right)$$
is only a function of F and X. The system (4.5), (4.6) is closed with unknowns $\mathbf{v}(t,X)$ and $F(t,X)$.

2. **Compatibility condition** The above derivation shows that if $\mathbf{x}(t,X)$ satisfies PDE (4.4), then its derivatives $(\mathbf{v}(t,X), F(t,X))$ satisfies PDE (4.5). In addition, from
$$\frac{\partial^2 \mathbf{x}}{\partial X^\beta \partial X^\alpha} = \frac{\partial^2 \mathbf{x}}{\partial X^\alpha \partial X^\beta}$$
and
$$\frac{\partial^2 \mathbf{x}}{\partial t \partial X^\alpha} = \frac{\partial^2 \mathbf{x}}{\partial X^\alpha \partial t},$$

we see that necessarily F satisfies the following *compatibilty conditions* (or *integrability condition*):

$$\frac{\partial F^i_\alpha}{\partial X^\beta} = \frac{\partial F^i_\beta}{\partial X^\alpha} \tag{4.7}$$

and

$$\dot{F}^i_\alpha = \frac{\partial v^i}{\partial X^\alpha}. \tag{4.8}$$

The second one is already appeared in our equation (4.5). So (4.7) is an addition condition.

Conversely, if a pair of functions $(\mathbf{v}(t,X), F(t,X))$ satisfies PDE (4.5), does there exist a function $\mathbf{x}(t,X)$ satisfying $\dot{\mathbf{x}}(t,X) = \mathbf{v}(t,X)$, $\frac{\partial \mathbf{x}}{\partial X} = F(t,X)$ and equation (4.4)? Certainly there is no guarantee that F satisfies (4.7). However, if F satisfies (4.7) at $t = 0$, we claim that F satisfies (4.7) for all later time. This is because

$$\frac{d}{dt}\left(\frac{\partial F^i_\alpha}{\partial X^\beta} - \frac{\partial F^i_\beta}{\partial X^\alpha}\right) = \frac{\partial^2 v^i}{\partial\beta\partial\alpha} - \frac{\partial^2 v^i}{\partial\alpha\partial\beta} = 0.$$

If $\mathbf{v}$ and F satisfy the compatibility conditions (4.7), (4.8), then we can find its integral $\mathbf{x}(t,X)$ with $\dot{\mathbf{x}}(t,X) = \mathbf{v}(t,X)$ and $\frac{\partial \mathbf{x}}{\partial X} = F(t,X)$.

Equation of motion in Eulerian coordinates The equation of motion in Eulerian coordinates is simpler. From (2.14) and (4.6), the Cauchy stress for fluids is

$$\sigma = J^{-1}W'(F)F^T = -J^{-1}pJF^{-T}F^T = -pI.$$

Using the Euler-Lagrange transformation formula, we obtain

$$\rho\left(\partial_t \mathbf{v} + \mathbf{v}\cdot\nabla_{\mathbf{x}}\mathbf{v}\right) = -\nabla p.$$

Recall that the thermo variables ρ and S in Lagrangian frame satisfy

$$\rho(t,\mathbf{x}(t,X))J(t,X) = \rho_0(X), \quad S(t,\mathbf{x}(t,X)) = S_0(X). \tag{4.9}$$

They are not needed in the equation of motion in Lagrangian formulation because we can treat pressure p as a function of X and F based on the conservation of mass and adiabaticity assumption. However, ρ and S are needed in the equation of motion in Eulerian formulation. Thus, we need dynamical equations for ρ and S, which are

$$\partial_t\rho + \nabla_{\mathbf{x}}(\rho\mathbf{v}) = 0,$$

$$\partial_t S + \mathbf{v}\cdot\nabla_{\mathbf{x}}S = 0.$$

They are obtained by differentiating (4.9) in t.

Boundary conditions In the above derivation of the Euler-Lagrange equation (4.4), we require the boundary condition (4.2) for $\delta\mathbf{x}$. Express this in component form reads

$$P_i^\alpha n_\alpha \delta x^i dS_0 = 0 \tag{4.10}$$

on the boundary $\partial\Omega_0$. Note that P is a function of F, which is $\frac{\partial \mathbf{x}}{\partial X}$. For the fluid mechanics, $P = -pJF^{-T}$. This gives

$$0 = p\delta\mathbf{x}\cdot JF^{-T}\mathbf{n}dS_0 = p\delta\mathbf{x}\cdot \nu dS_t.$$

Thus, a natural boundary condition is

$$\delta\mathbf{x}(t,X)\cdot\nu(\mathbf{x}(t,X)) = 0 \text{ for } X\in\partial\Omega_0.$$

The condition

$$\mathbf{v}\cdot\nu = 0 \text{ on } \partial\Omega_t$$

implies $\delta\mathbf{x}\cdot\nu = 0$ on $\partial\Omega_t$. [1] This is called the natural boundary condition. This is also an advantage of the variational approach, easier to find a natural boundary condition.

4.1.2 Variation of Action w.r.t. Flow Maps for Incompressible Flows

Incompressibility

- When the density of each fluid parcel is unchanged during its motion, such fluid is called incompressible. That is
$$\boxed{\partial_t\rho + \mathbf{v}\cdot\nabla\rho = 0.} \tag{4.11}$$
- Incompressibility is equivalent to
$$\boxed{\nabla\cdot\mathbf{v} = 0.} \tag{4.12}$$
This follows from the definition of incompressibility and the continuity equation
$$\partial_t\rho + \mathbf{v}\cdot\nabla\rho + \rho\nabla\cdot\mathbf{v} = 0$$
- Incompressibility is also equivalent to
$$\boxed{J(t,X) := \det F = 1.} \tag{4.13}$$
where $F = \frac{\partial x^i}{\partial X^j}$ is the deformation gradient. This follows from
$$\left(\frac{d}{dt}(\rho J) = 0,\ \frac{d}{dt}\rho = 0\right) \quad\Rightarrow\quad \frac{d}{dt}J = 0.$$
Since $J(0,X) = 1$, we get $J(t,X) = 1$ for all t.

[1] When $\mathbf{v}\cdot\nu$, the flow is required to slip on the boundary. This means that $\delta\mathbf{x}(t,X)\parallel\partial\Omega$.

Variation of action with incompressibility constraint

1. The incompressibility is equivalent to the constraint

$$\det F(t,X) = 1.$$

Thus, in the above variation of action, we should add a constraint term with a Lagrange multiplier:

$$\delta \mathcal{S}[\mathbf{x}] + \delta \int_{t_0}^{t_1} \int p(t,X)(\det F - 1)\, dX\, dt = 0.$$

Here, p is the Lagrange multiplier.

2. The variation of $\mathcal{S}[\mathbf{x}]$ gives

$$\delta \mathcal{S} = \int_{t_0}^{t_1} \int [-\rho_0(X)\ddot{\mathbf{x}} + \nabla_X P] \cdot \delta \mathbf{x}\, dX\, dt.$$

The Piola stress

$$P = W'(F) = \frac{\partial W}{\partial V}\frac{\partial V}{\partial F} = \frac{\partial W}{\partial V}\frac{1}{\rho_0(X)}\frac{\partial J}{\partial F} = 0, \quad \because J \equiv 1.$$

3. The variation

$$\delta(\det F) = tr(F^{-T} \cdot (\delta F)) \det F = tr(F^{-T} \cdot (\delta F)).$$

where

$$tr(F^{-T} \cdot (\delta F)) = \sum_{i,\alpha} (F^{-T})_i^\alpha (\delta F)_\alpha^i = \sum_{i,\alpha} (F^{-T})_i^\alpha \frac{\partial \delta x^i}{\partial X^\alpha}$$

We take integration by part in the variation form below to get

$$\begin{aligned}
&\delta \int_{t_0}^{t_1} \int p(t,X)(\det F - 1)\, dX\, dt = \int_{t_0}^{t_1} \int p(t,X)\, \delta \det F\, dX\, dt \\
&= \int_{t_0}^{t_1} \int p \sum_{i,\alpha} (F^{-T})_i^\alpha \frac{\partial \delta x^i}{\partial X^\alpha}\, dX\, dt = -\int_{t_0}^{t_1} \int \sum_{i,\alpha} \left[\frac{\partial}{\partial X^\alpha}(pF^{-T})_i^\alpha\right] \delta x^i\, dX\, dt \\
&= -\int_{t_0}^{t_1} \int [\nabla_X \cdot \left(pF^{-T}\right)] \cdot \delta \mathbf{x}\, dX\, dt
\end{aligned}$$

4. **Euler-Lagrange equation in Lagrangian coordinate for the constrained flow** Combining the above two calculations, we obtain the following constraint-flow equation
$$\rho_0 \ddot{\mathbf{x}} = -\nabla_X \cdot (pF^{-T}), \quad \det F = 1, \quad F := \frac{\partial \mathbf{x}}{\partial X}$$
for the unknown $\mathbf{x}(t,X)$ and $p(t,X)$. Here, the boundary terms appeared in the integration-by-part is
$$\int_{t_0}^{t_1} \int_{\partial \hat{M}} \delta \mathbf{x} \cdot \left(pF^{-T}\right) \cdot \mathbf{n} \, dS_0 \, dt.$$
We choose those $\delta \mathbf{x}$ to make this term to be zero.

   We can express this second-order equation as a system of first-order equations:
$$\begin{cases} \rho_0 \dot{\mathbf{v}} = -\nabla_X \cdot (pF^{-T}) \\ \dot{F} = \frac{\partial \mathbf{v}(t,X)}{\partial X} \\ \det F(t,X) = 1. \end{cases}$$
The unknowns are $(F, \mathbf{v}, p)$.

Eulerian formulation Through the transformation formula, we get that the equation of motion in Eulerian coordinate is
$$\partial_t (\rho \mathbf{v}) + \nabla \cdot (\rho \mathbf{v}\mathbf{v}) + \nabla p = 0.$$
We still need the continuity equation for ρ. The incompressibility constraint is expressed as
$$\nabla \cdot \mathbf{v} = 0.$$
We summarize them as
$$\begin{cases} \partial_t \rho + \nabla \cdot (\rho \mathbf{v}) = 0 \\ \partial_t (\rho \mathbf{v}) + \nabla \cdot (\rho \mathbf{v}\mathbf{v}) + \nabla p = 0. \\ \nabla \cdot \mathbf{v} = 0 \end{cases}$$
The unknowns are $(\rho, \mathbf{v}, p)$.

Equation of motion Consider incompressible simple fluids (i.e. no stress appears, fluid particles have only free motion). The governing equations are

- Continuity equation
$$\rho_t + \nabla \cdot (\rho \mathbf{v}) = 0.$$

- Incompressibility

$$\nabla \cdot \mathbf{v} = 0.$$

- Equation of motion

$$\boxed{\rho \frac{d\mathbf{v}}{dt} + \nabla p = \mathbf{f}.} \tag{4.14}$$

Here, we have $(\rho, p, \mathbf{v})$ as our unknowns.

Remark For incompressible flows, the is only one thermo variable. Thus, we cannot include the energy equation. The role of pressure p is a Lagrange multiplier from the constraint $\det F = 1$ or $\nabla \cdot \mathbf{v} = 0$.

Boundary Conditions We impose the boundary condition

$$\mathbf{v} \cdot \nu = 0, \quad \mathbf{x} \in \partial D. \tag{4.15}$$

It means that the fluid can not flow through the boundary ∂D.

Simple Flows When $\rho \equiv 1$, we have

$$\frac{d\mathbf{v}}{dt} + \nabla p = 0, \quad \nabla \cdot \mathbf{v} = 0.$$

This is called the simple flow. The unknown are $(\mathbf{v}, p)$.

Barotropic Flows Barotropic flow: the pressure is a function of ρ. In this case, we can find a potential (the enthalpy) h such that $h'(\rho) = p'(\rho)/\rho$. Then the barotropic flow equation becomes

$$\frac{d\mathbf{v}}{dt} + \nabla h = 0,$$

The equation for ρ is still the continuity equation

$$\frac{d\rho}{dt} + \rho \nabla \cdot \mathbf{v} = 0.$$

4.2 Eulerian Variational Approach

There are several ways to derive the Euler equation via variational principle in Eulerian coordinate. These include

- Euler-Poincarè-Hamel's approach,
- Herivel-Lin's approach approach.

The references are

1. R.L. Seliger and G.B. Whitham, F.R.S., Variational Principles in Continuum Mechanics, Proc. Roy. Soc. A 305, 1-25 (1968).
2. Rick Salmon, Hamiltonian Fluid Mechanics, Ann. Rev. Fluid Mech. 20, 225-256 (1988).
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4. N. Padhye and P.J. Morrison, Relabeling Symmetries in Hydrodynamics and Magnetohydrodynamics, Plasma Physics Report (1996).
5. J. Serrin, Mathematical Principles of Classical Fluid Mechanics (1959).
6. Beris and Edwards, Thermodynamics of Flowing Systems (1994).

4.2.1 Euler-Poincarè-Hamel's Approach (Dynamically accessible variation)

1. **Dynamically accessible flow maps** Let $\mathbf{x}(t,X)$ be a flow map. Consider a variation of $\mathbf{x}(t,X)$: it is a one-parameter family of flow maps $\mathbf{x}^s(t,X)$ with $\mathbf{x}^0(t,X) = \mathbf{x}(t,X)$. It is called dynamically accessible if it satisfies the constraints that $\mathbf{x}(t,X)$ satisfies. That is, the density and entropy constraints:

$$\rho(t,\mathbf{x}^s(t,X))J^s(t,X) = \rho_0(X), \quad J^s(t,X) := \det\left(\frac{\partial \mathbf{x}^s}{\partial X}\right) \tag{4.16}$$

$$S(t,\mathbf{x}^s(t,X)) = S_0(X). \tag{4.17}$$

2. **Dynamically accessible flow variations w:** We recall that the variation of the flow map is defined as

$$\delta\mathbf{x}(t,X) := (\partial_s|_{s=0})_X \mathbf{x}^s(t,X).$$

We now define the *flow variation* or the *virtual velocity in Eulerian coordinate* to be

$$\mathbf{w}(t,\mathbf{x}) := \delta\mathbf{x}(t,\varphi_t^{-1}(\mathbf{x})),$$

where $\varphi_t(X) = \mathbf{x}(t,X)$ is the flow map. The role of $\mathbf{w}$ is similar to $\mathbf{v}$. Both of them are defined in the Eulerian coordinates, and

$$\mathbf{v}(t,\mathbf{x}(t,X)) = (\partial_t)_X \mathbf{x}(t,X), \quad \mathbf{w}(t,\mathbf{x}(t,X)) = (\partial_s|_{s=0})_X \mathbf{x}^s(t,X)$$

Note that (t,s) are independent in $\mathbf{x}^s(t,X)$. This implies

$$(\partial_s)_X (\partial_t)_X \mathbf{x}^s(t,X) = (\partial_t)_X (\partial_s)_X \mathbf{x}^s(t,X).$$

We also note that

$$(\partial_s)_X = (\partial_s)_{\mathbf{x}} + \mathbf{w}\cdot\nabla_{\mathbf{x}}, \quad (\partial_t)_X = (\partial_t)_{\mathbf{x}} + \mathbf{v}\cdot\nabla_{\mathbf{x}}. \tag{4.18}$$

This gives

$$(\partial_s)_{\mathbf{x}} \mathbf{v} + \mathbf{w}\cdot\nabla\mathbf{v} = \partial_t \mathbf{w} + \mathbf{v}\cdot\nabla\mathbf{w}. \tag{4.19}$$

3. **Dynamically Accessible Variations** The dynamically accessible flow variation $\mathbf{w}$ induces other *dynamically accessible variations* on $\mathbf{v}$, ρ and S in Eulerian coordinate as the follows:

$$\begin{aligned}
\delta\mathbf{v}(t,\mathbf{x}) &:= \left(\frac{\partial}{\partial s}\bigg|_{s=0}\right)_{\mathbf{x}} \mathbf{v}(t,\mathbf{x}^s(t,X)),\\
\delta\rho(t,\mathbf{x}) &:= \left(\frac{\partial}{\partial s}\bigg|_{s=0}\right)_{\mathbf{x}} \rho(t,\mathbf{x}^s(t,X)),\\
\delta S(t,\mathbf{x}) &:= \left(\frac{\partial}{\partial s}\bigg|_{s=0}\right)_{\mathbf{x}} S(t,\mathbf{x}^s(t,X)),
\end{aligned}$$

with $\mathbf{x} = \mathbf{x}(t,X)$ fixed, where $\frac{\partial}{\partial s}$ is evaluated at $s=0$. The right-hand sides are evaluated at $X = \varphi_t^{-1}(\mathbf{x})$. We have the following lemma.

Lemma 4.3. *The dynamically accessible variations $\delta\mathbf{v}$, $\delta\rho$ and δS satisfy*

$$\delta\mathbf{v} + \mathbf{w}\cdot\nabla\mathbf{v} = \partial_t\mathbf{w} + \mathbf{v}\cdot\nabla\mathbf{w}, \tag{4.20}$$
$$\delta\rho + \nabla\cdot(\rho\mathbf{w}) = 0, \tag{4.21}$$
$$\delta S + \mathbf{w}\cdot\nabla S = 0. \tag{4.22}$$

Here, the ∇ denotes for $\nabla_{\mathbf{x}}$.

Proof. (a) (4.20) is the equation (4.19).

(b) Next, we compute $(\partial_s|_{s=0})_X J$: Using $\mathbf{x}^s(t,X)$ being flow maps. We have

$$(\partial_s)_X \frac{\partial \mathbf{x}^s}{\partial X} = \frac{\partial}{\partial X}(\partial_s)_X \mathbf{x}^s = \frac{\partial}{\partial X}\mathbf{w}^s(t,\mathbf{x}) = \frac{\partial \mathbf{w}}{\partial \mathbf{x}}\frac{\partial \mathbf{x}^s}{\partial X}$$

Thus,

$$(\partial_s)_X \left(\frac{\partial \mathbf{x}^s}{\partial X}\right) = \nabla_{\mathbf{x}}\mathbf{w}\left(\frac{\partial \mathbf{x}^s}{\partial X}\right).$$

Its determinant $\det\left(\frac{\partial \mathbf{x}^s}{\partial X}\right) = J^s$ satisfies

$$(\partial_s|_{s=0})_X J = \delta J + \mathbf{w}\cdot\nabla J = (\nabla\cdot\mathbf{w})J.$$

(c) Recall that $\mathbf{x}^s(t,X)$ satisfies the density and entropy constraints:

$$\rho(t,\mathbf{x}^s(t,X))J^s(t,X) = \rho_0(X) \tag{4.23}$$
$$S(t,\mathbf{x}^s(t,X)) = S_0(X). \tag{4.24}$$

Differentiating (4.23) in s fixing X, using (4.18), we get

$$\begin{aligned} 0 &= (\partial_s)_X\left(\rho(t,\mathbf{x}^s(t,X))J^s(t,X)\right) = (\partial_s)_X\left(\rho(t,\mathbf{x}^s(t,X))\right)J^s + \rho\,(\partial_s)_X J^s \\ &= (\delta\rho + \mathbf{w}\cdot\nabla\rho)J + \rho(\nabla\cdot\mathbf{w})J = (\delta\rho + \nabla\cdot(\rho\mathbf{w}))J. \end{aligned}$$

This gives (4.21). Similarly, differentiating (4.24) in s with fixed X, we get (4.22).

□

4. **Variation of action w.r.t. the dynamically accessible variations** The action is defined to be

$$\mathcal{S}[\rho,\mathbf{v},S] := \int_{t_0}^{t_1}\int_\Omega \left(\frac{1}{2}\rho|\mathbf{v}|^2 - \rho U(\rho,S)\right) d\mathbf{x}\,dt. \tag{4.25}$$

The variation of a functional $\mathcal{S}$ w.r.t. $\rho, S, \mathbf{v}$ is

$$\begin{aligned} \delta\mathcal{S}[\rho,\mathbf{v},S] &= \int_{t_0}^{t_1}\int_\Omega \left[\delta\rho\frac{1}{2}|\mathbf{v}|^2 + \rho\mathbf{v}\cdot\delta\mathbf{v} - (\delta\rho)U - \rho\left(\frac{\partial U}{\partial\rho}\delta\rho + \frac{\partial U}{\partial S}\delta S\right)\right] d\mathbf{x}\,dt \\ &= \int_{t_0}^{t_1}\int_\Omega \left[\left(\frac{1}{2}|\mathbf{v}|^2 - U - \frac{p}{\rho}\right)\delta\rho - \rho T\delta S + \rho\mathbf{v}\cdot\delta\mathbf{v}\right] d\mathbf{x}\,dt. \end{aligned}$$

Here, $\rho\frac{\partial U}{\partial\rho} = -\frac{p}{\rho}$. The variations $\delta\rho$, δS and $\delta\mathbf{v}$ are induced by $\mathbf{w}$. We now express them in terms of $\mathbf{w}$:

$$\begin{aligned} \delta\mathcal{S} &= \int_{t_0}^{t_1}\int_\Omega \left(\frac{1}{2}|\mathbf{v}|^2 - U - \frac{p}{\rho}\right)(-\nabla\cdot(\rho\mathbf{w})) + \rho T(\nabla S\cdot\mathbf{w}) + \rho\mathbf{v}(\mathbf{w}_t + \mathbf{v}\cdot\nabla\mathbf{w} - \nabla\mathbf{v}\cdot\mathbf{w})\,d\mathbf{x}\,dt \\ &= \int_{t_0}^{t_1}\int_\Omega [-(\rho\mathbf{v})_t - \nabla\cdot(\rho\mathbf{v}\mathbf{v}) - \nabla p]\cdot\mathbf{w} - \rho[\nabla U - \frac{p}{\rho^2}\nabla\rho - T\nabla S]\cdot\mathbf{w}\,d\mathbf{x}\,dt \end{aligned} \tag{4.26}$$

Here, we have performed integration by part and used $\mathbf{w}\cdot\nu = 0$ on the boundary. Using the first law of thermodynamics

$$\nabla U - \frac{p}{\rho^2}\nabla\rho - T\nabla S = 0,$$

we get

$$\int_{t_0}^{t_1}\int_\Omega [-(\rho\mathbf{v})_t - \nabla\cdot(\rho\mathbf{v}\mathbf{v}) - \nabla p]\cdot\mathbf{w}\,d\mathbf{x}\,dt = 0 \text{ for all } \mathbf{w}.$$

This recovers Euler's equation of motion.

4.2.2 Herivel-Lin's Approach (Constrained Variation)

- Herivel-Lin treat the equations for thermodynamic variables ρ and S as two constraints:

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

$$\partial_t S + \mathbf{v}\cdot\nabla S = 0$$

in the variational problem $\delta\mathcal{S}[\mathbf{v},\rho,S]$. These give the unconstrained variational problem:

$$\delta\mathcal{S}[\mathbf{v},\rho,S,\varphi,\eta] = \delta\int_{t_0}^{t_1}dt\int_\Omega d\mathbf{x}\left\{\frac{1}{2}\rho|\mathbf{v}|^2 - \rho U(\rho,S) + \varphi[\rho_t + \nabla\cdot(\rho\mathbf{v})] - \rho\eta[S_t + \mathbf{v}\cdot\nabla S]\right\}. \tag{4.27}$$

Here, φ and $\rho\eta$ are the Lagrange multipliers.[2]

From

$$0 = \frac{\delta\mathcal{S}}{\delta\mathbf{v}} = \rho\mathbf{v} - \rho\nabla\varphi - \rho\eta\nabla S,$$

we get

$$\mathbf{v} = \nabla\varphi + \eta\nabla S. \tag{4.28}$$

This is called a *Clesch representation* of $\mathbf{v}$ in terms of (ρ,S,φ,η). We can plug (4.28) into (4.27) to eliminate $\mathbf{v}$. The unstrained variational problem becomes

$$\delta\mathcal{S}[\rho,S,\varphi,\eta] = \delta\int_{t_0}^{t_1}dt\int_\Omega d\mathbf{x}\left\{\frac{1}{2}\rho|\mathbf{v}|^2 - \rho U(\rho,S) + \varphi[\rho_t + \nabla\cdot(\rho\mathbf{v})] - \rho\eta[S_t + \mathbf{v}\cdot\nabla S]\right\} \tag{4.29}$$

[2]These are called conjugate variables. Note that $\rho\,d\mathbf{x}$ is an n-form. Its conjugate variable φ is a 0-form. On the other hand, S is a 0-form, so its conjugate variable $\rho\eta\,d\mathbf{x}$ is an n-form.

with $\mathbf{v}$ given by (4.28). The variation of $\mathcal{S}$ w.r.t. ρ, S, φ, η give the following equations for these 4 unknowns:

$$
\begin{aligned}
\frac{\delta \mathcal{S}}{\delta \rho} &= \frac{1}{2}|\mathbf{v}|^2 - U - \frac{p}{\rho} - \varphi_t - \mathbf{v}\cdot\nabla\varphi = 0 \\
\frac{\delta \mathcal{S}}{\delta S} &= (\rho\eta)_t + \nabla\cdot(\rho\eta\mathbf{v}) - \rho T = 0 \\
\frac{\delta \mathcal{S}}{\delta \varphi} &= \rho_t + \nabla\cdot(\rho\mathbf{v}) = 0 \\
\frac{\delta \mathcal{S}}{\delta \eta} &= S_t + \mathbf{v}\cdot\nabla S = 0.
\end{aligned}
$$

It involves 4 unknowns (ρ, S, φ, η) and 4 equations. However, the Euler equations should have 5 independent variables. Thus, this representation can only form a subset of solutions of the Euler equations. In fact, if $S = constant$, then $\mathbf{v} = \nabla\varphi$, allowing only potential flows. Furthermore, one can show that the corresponding fluid flows always have zero helicity: [Graham and Henyey, 2000]

$$\int \mathbf{v}\cdot\nabla\times\mathbf{v}\, d\mathbf{x} = 0.$$

- **Lin's relabel symmetry** It was noticed by C.C. Lin that there is another constraint, the relabeling symmetry, which is crucial in the representation of velocity. Let $X(t,\mathbf{x})$ be the inversion of $\mathbf{x}(t,X)$. Then $X(t,\mathbf{x})$ (which is φ_t^{-1}) satisfies[3]

$$\partial_t X + \mathbf{v}\cdot\nabla X = 0.$$

By introducing the Lagrange multiplier $\varphi, \rho\eta$ and $\rho\gamma = \rho(\gamma^1, \gamma^2, \gamma^3)$, Lin considered the following action

$$
\begin{aligned}
\mathcal{S}[\mathbf{v}, \rho, S, X, \varphi, \eta, \gamma] = \int_{t_0}^{t_1} dt \int_\Omega d\mathbf{x} \Big\{ & \frac{1}{2}\rho|\mathbf{v}|^2 - \rho U(\rho, S) \\
& + \varphi[\rho_t + \nabla\cdot(\rho\mathbf{v})] - \rho\eta[S_t + \mathbf{v}\cdot\nabla S] - \rho\gamma\cdot[X_t + \mathbf{v}\cdot\nabla X] \Big\}.
\end{aligned}
$$

Taking the variation of the action w.r.t. the Lagrange multipliers $(\varphi, \rho\eta, \rho\gamma)$ lead to

[3]This is called the Lin constraints.

the constraints. The variations of the action w.r.t. $\mathbf{v}$, ρ, S, X are listed below.

$$
\begin{aligned}
\frac{\delta \mathcal{S}}{\delta \mathbf{v}} &= \rho \mathbf{v} - \rho \nabla \varphi - \rho \eta \nabla S - \rho \gamma \cdot \nabla X = 0 \\
\frac{\delta \mathcal{S}}{\delta \rho} &= \frac{1}{2}|\mathbf{v}|^2 - U - \frac{p}{\rho} - \varphi_t - \mathbf{v} \cdot \nabla \varphi = 0 \\
\frac{\delta \mathcal{S}}{\delta S} &= (\rho \eta)_t + \nabla \cdot (\rho \eta \mathbf{v}) - \rho T = 0 \\
\frac{\delta \mathcal{S}}{\delta X} &= (\rho \gamma)_t + \nabla \cdot (\rho \gamma \mathbf{v}) = 0
\end{aligned}
$$

These give

$$
\begin{cases}
\mathbf{v} & = \nabla \varphi + \eta \nabla S + \gamma \cdot \nabla X, \\
\dot{\varphi} & = \frac{1}{2}|\mathbf{v}|^2 - U - \frac{p}{\rho}, \\
\dot{\eta} & = T, \\
\dot{\gamma} & = 0,
\end{cases}
\tag{4.30}
$$

where the dot means the material derivative. Let us write $\mathbf{v} = \nabla \varphi + \eta \nabla S + \gamma \cdot \nabla X = \sum_k b_k \nabla a_k$. Applying the material derivative to $\mathbf{v}$ to get

$$
\begin{aligned}
\dot{\mathbf{v}} &= \sum_k \left(\dot{b}_k \nabla a_k + b_k (\partial_t + v_j \partial_j) \nabla a_k \right) \\
&= \sum_k \left(\dot{b}_k \nabla a_k + b_k \nabla (\partial_t + v_j \partial_j) a_k - b_k \nabla a_k \cdot \nabla \mathbf{v} \right) \\
&= \sum_k \left(\dot{b}_k \nabla a_k + b_k \nabla (\partial_t + v_j \partial_j) a_k \right) - \mathbf{v} \cdot \nabla \mathbf{v} \\
&= \sum_k \left(\dot{b}_k \nabla a_k + b_k \nabla \dot{a}_k \right) - \frac{1}{2} \nabla |\mathbf{v}|^2 \\
&= \nabla \dot{\varphi} + \dot{\eta} \nabla S + \eta \nabla \dot{S} + \dot{\gamma} \cdot \nabla X + \gamma \nabla \dot{X} - \frac{1}{2} \nabla |\mathbf{v}|^2 \\
&= \nabla \left(-\frac{1}{2}|\mathbf{v}|^2 + \dot{\varphi} \right) + \dot{\eta} \nabla S \\
&= -\nabla \left(U + \frac{p}{\rho} \right) + T \nabla S \\
&= -\frac{\nabla p}{\rho}.
\end{aligned}
$$

Here, we have used

$$
\dot{\varphi} = \frac{1}{2}|\mathbf{v}|^2 - U - \frac{p}{\rho}, \quad \dot{\eta} = T, \quad \dot{S} = 0, \quad \dot{\gamma} = 0, \quad \dot{X} = 0,
$$

and

$$\nabla U = T\nabla S + \frac{p}{\rho^2}\nabla\rho.$$

The formula $\dot{\mathbf{v}} = -\nabla p/\rho$ is the Euler equation. This means that we can recover the Euler equations through the representation:

$$\mathbf{v} = \nabla\varphi + \eta\nabla S + \gamma\cdot\nabla X.$$

- **Can we have smaller number of constraints?** Note that there are 10 unknowns in this unconstrained variational problem:

$$\delta\mathcal{S}[\rho, S, X, \varphi, \eta, \gamma].$$

However, the Euler equations has only 5 unknowns. This suggests we can eliminate some of Lin's constraints. We need 2 labelling constraints at least. By adding just one constraint:

$$a_t + \mathbf{v}\cdot\nabla a = 0, \tag{4.31}$$

where a is a scalar, the Clebsch representation of $\mathbf{v}$ is

$$\mathbf{v} = \nabla\varphi + \eta\nabla S + \zeta\nabla a. \tag{4.32}$$

which involves exactly 5 unknowns $(\varphi, \eta, S, \zeta, a)$.

By eliminating $\mathbf{v}$ from the above unconstrained variational problem, we get

$$\delta\mathcal{S}[\rho, S, a, \varphi, \eta, \zeta] = \delta\int_{t_0}^{t_1} dt \int_\Omega d\mathbf{x}\left\{\frac{1}{2}\rho|\mathbf{v}|^2 - \rho U(\rho, S)\right.$$
$$\left. + \varphi[\rho_t + \nabla\cdot(\rho\mathbf{v})] - \rho\eta[S_t + \mathbf{v}\cdot\nabla S] - \rho\zeta[a_t + \mathbf{v}\cdot\nabla a]\right\}.$$

There are 6 unknowns $(\rho, S, a, \varphi, \eta, \zeta)$. Their equations are

$$\dot{\varphi} = \frac{1}{2}|\mathbf{v}|^2 - U - \frac{p}{\rho}, \quad \dot{\rho} = -\rho\nabla\cdot\mathbf{v}$$
$$\dot{\eta} = T, \quad \dot{S} = 0, \quad \dot{a} = 0, \quad \dot{\zeta} = 0.$$

We have to make sure this Clebsch representation (4.32) can cover arbitrary velocity vector field $\mathbf{v}$ initially. This means that: given a vector field $\mathbf{v}_0$, (as well as S_0), can we find scalar functions φ_0, η_0, ζ_0 and a_0 such that

$$\mathbf{v}_0 = \nabla\varphi_0 + \eta_0\nabla S_0 + \zeta_0\nabla a_0?$$

The answer is YES. This is the Darboux Theorem.

- **Relation of the Clebsch representation of velocity and the vorticity** By taking *curl* of (4.32), we get

$$\omega = \nabla\eta \times \nabla S + \nabla\zeta \times \nabla a + \nabla\xi \times \nabla b. \tag{4.33}$$

  Taking the Lie derivative gives

$$\dot{\omega} = \nabla\dot{\eta} \times \nabla S + \nabla\eta \times \nabla\dot{S} + \nabla\dot{\zeta} \times \nabla a + \nabla\zeta \times \nabla\dot{a} + \nabla\dot{\xi} \times \nabla b + \nabla\xi \times \nabla\dot{b} = \nabla T \times \nabla S.$$

  The formula shows that the relabeling a and b does not affect $\dot{\omega}$ because they advect along the flow.

- **Connection between relabeling symmetry and the conservation of circulations** In the case of constant entropy or constant temperature, we have $\nabla T \times \nabla S = 0$. Thus,

$$\dot{\omega} = 0.$$

  Thus, the vorticity is invariant along the fluid flow.

  The term a comes from the relabeling of the initial mass. The appearance a and its conjugate ζ allow us to construct any initial vorticity field:

$$\omega(t=0) = \nabla\zeta \times \nabla a(t=0).$$

  Thus, the relabeling, which corresponds to a perturbation of flow path, induces an invariant, the vorticity. "*The vorticity laws arise from the particle-relabling symmetry*", quoted from Salmon. [4]

  In general, the vorticity law holds on the constant entropy surfaces. For more concise explanation, see
  Padhye and Morrison, Relabeling Symmetries in Hydrodynamics and Magnetohydrodynamics (1996).

[4] Rick Salmon, Hamiltonian Fluid Mechanics (1998). In fact, Salmon derives the potential vorticity and the vorticity equation (in Lagrangian coordinate) via variation of action with respect to the material variable $\mathbf{a}$ (where $d\mathbf{a} = \rho_0(X)\,dX$) using the relabeling symmetry.

Chapter 5

Hamiltonian Fluid Mechanics

5.1 Hamiltonian Fluid Mechanics in Lagrangian coordinates

5.1.1 Hamiltonian Mechanics in Lagrangian Variables

1. Let us define the configuration space to be the space of all flow maps:

$$\mathcal{Q} := \{\mathbf{x} : \Omega_0 \to \mathbb{R}^3 \text{ is 1-1, onto and Lipschitz continuous}\}.$$

   Define the phase spaces

$$\mathcal{M} := \mathcal{T}\mathcal{Q} = \{(\mathbf{x},\mathbf{v}) : \Omega_0 \to \mathbb{R}^3 \times \mathbb{R}^3\},$$
$$\mathcal{M}^* := \mathcal{T}^*\mathcal{Q} = \{(\mathbf{x},\mathbf{p}) : \Omega_0 \to \mathbb{R}^3 \times \mathbb{R}^3\}.$$

   We call $(\mathbf{x},\mathbf{p})$ the Lagrangian variables. Sometimes we use $(\mathbf{q},\mathbf{p})$, because $\mathbf{x}$ is used as a spatial variable, or the flow map function $\mathbf{x}(t,X)$ in this note.

2. We assume: on the target space $\mathbb{R}^3$, there is a natural volume measure $d\mathbf{x}$, while in the material space Ω_0, there is a mass measure $\rho_0(X)\,dX$. The density associate with an $\mathbf{x} \in \mathcal{Q}$ is defined to be

$$\rho\, d\mathbf{x} = \rho_0 dX,$$

   and the specific volume $V := 1/\rho$. In addition, we assume there exists an entropy function $S_0 : \Omega \to \mathbb{R}$ and an internal energy $U(V,S_0)$.

3. Define Lagrangian density

$$L\left(\mathbf{x}, \frac{\partial \mathbf{x}}{\partial X}, \mathbf{v}\right) := \rho_0(X)\frac{|\mathbf{v}(X)|^2}{2} - \rho_0 U(S_0(X), V(\mathbf{x}(X)))$$

The Lagrangian $\mathscr{L} : \mathcal{M} \to \mathbb{R}$ is defined by

$$\mathscr{L}[\mathbf{x},\mathbf{v}] := \int_{\Omega_0} L(\mathbf{x}, \frac{\partial \mathbf{x}}{\partial X}, \mathbf{v})\, dX.$$

A path is a trajectory on $\mathcal{M}$. That is $(\mathbf{x},\mathbf{v}) : [t_0,t_1] \to \mathcal{M}$. Associate with a path $(\mathbf{x}(\cdot),\mathbf{v}(\cdot))$ we define the action to be

$$\mathcal{S}[\mathbf{x}] := \int_{t_0}^{t_1} \mathscr{L}[\mathbf{x}(t),\dot{\mathbf{x}}(t)]\, dt.$$

4. The Euler-Lagrange equation is governed by $\delta\mathcal{S}/\delta\mathbf{x} = 0$, which is

$$\frac{d}{dt}\frac{\delta\mathscr{L}}{\delta\mathbf{v}} + \frac{\delta\mathscr{L}}{\delta\mathbf{x}} = 0.$$

Here,

$$\begin{aligned}\frac{\delta\mathscr{L}}{\delta\mathbf{v}}[\mathbf{x},\dot{\mathbf{x}}] &= \rho_0\dot{\mathbf{x}}\\ \frac{\delta\mathscr{L}}{\delta\mathbf{x}}[\mathbf{x},\dot{\mathbf{x}}] &= \nabla_X\cdot(pJF^{-T}),\end{aligned}$$

with

$$F := \frac{\partial \mathbf{x}}{\partial X}, \quad J = det(F),$$
$$p := \frac{\partial U}{\partial V}, \quad V = \frac{J}{\rho_0}.$$

Variations $\delta\mathbf{x}, \delta\mathbf{v}$ are 1-forms on $\mathcal{M}$, while $\delta\mathscr{L}/\delta\mathbf{x}$ and $\delta\mathscr{L}/\delta\mathbf{v}$ are tangent vectors on $\mathcal{M}$. Thus,

$$\left(\frac{\delta\mathscr{L}}{\delta\mathbf{v}}, \frac{\delta\mathscr{L}}{\delta\mathbf{x}}\right) \in \mathcal{T}\mathcal{M}.$$

5. The Hamiltonian $\mathscr{H}$ is defined on $\mathcal{T}^*\mathcal{Q}$ by

$$\mathscr{H}[\mathbf{x},\mathbf{p}] := \langle\mathbf{p},\mathbf{v}\rangle - \mathscr{L}[\mathbf{x},\mathbf{v}]$$

with $\mathbf{v}$ obtained from the relation:

$$\mathbf{p} = \delta\mathscr{L}/\delta\mathbf{v}[\mathbf{x},\mathbf{v}]. \tag{5.1}$$

This relation gives $\mathbf{v} = \mathbf{p}/\rho_0$. Thus,

$$\boxed{\mathscr{H}[\mathbf{x},\mathbf{p}] = \int_{\Omega_0} H(\mathbf{x}, \frac{\partial \mathbf{x}}{\partial X}, \mathbf{p})\, dX := \int_{\Omega_0} \frac{|\mathbf{p}|^2}{2\rho_0} + \rho_0 U(\rho_0/J, S_0)\, dX.} \tag{5.2}$$

The variations $(\frac{\delta \mathscr{H}}{\delta \mathbf{x}}, \frac{\delta \mathscr{H}}{\delta \mathbf{p}})$ is considered as a vector field on $\mathcal{T}^*\mathcal{Q}$. The Hamilton's equation of motion is

$$\begin{cases} \dot{\mathbf{x}} = \frac{\delta \mathscr{H}}{\delta \mathbf{p}} \\ \dot{\mathbf{p}} = -\frac{\delta \mathscr{H}}{\delta \mathbf{x}} \end{cases} \tag{5.3}$$

where

$$\frac{\delta \mathscr{H}}{\delta \mathbf{p}} = \frac{\mathbf{p}}{\rho_0}$$

$$\begin{aligned} \delta \mathscr{H} &= \int_{\Omega_0} \rho_0 \frac{\partial U}{\partial V} \frac{\partial V}{\partial F} \delta \left(\frac{\partial \mathbf{x}}{\partial X} \right) dX \\ &= \int_{\Omega_0} \nabla_X \cdot (pJF^{-T}) \cdot \delta \mathbf{x}. \end{aligned}$$

This gives

$$\frac{\delta \mathscr{H}}{\delta \mathbf{x}} = \nabla_X \cdot (pJF^{-T}).$$

Thus, $\dot{\mathbf{p}} = \frac{\delta \mathscr{H}}{\delta \mathbf{x}}$ is the Euler equation in Lagrangian coordinate.

5.1.2 Poisson Bracket in Lagrangian Variables

1. Given two functionals $\mathscr{F}$ and $\mathscr{G}$ on $\mathcal{T}^*\mathcal{Q}$, we define their Poisson bracket by

$$\boxed{\{\mathscr{F}, \mathscr{G}\} := \int_{\Omega_0} \frac{\delta \mathscr{F}}{\delta \mathbf{x}} \cdot \frac{\delta \mathscr{G}}{\delta \mathbf{p}} - \frac{\delta \mathscr{G}}{\delta \mathbf{x}} \cdot \frac{\delta \mathscr{F}}{\delta \mathbf{p}} \, dX} \tag{5.4}$$

   The Poisson bracket $\{\cdot, \cdot\}$ is bilinear and satisfies

   - non-degenerate: if $\{\mathscr{F}, \mathscr{G}\} = 0$ for all $\mathscr{G}$, then $\mathscr{F} = \text{const.}$,
   - antisymmetry: $\{\mathscr{F}, \mathscr{G}\} = -\{\mathscr{G}, \mathscr{F}\}$,
   - Jacobi identity: [1]

$$\{\{\mathscr{E}, \mathscr{F}\}, \mathscr{G}\} + \{\{\mathscr{F}, \mathscr{G}\}, \mathscr{E}\} + \{\{\mathscr{G}, \mathscr{E}\}, \mathscr{F}\} = 0.$$

2. The Hamilton's equation of motion (5.3) is equivalent to

$$\frac{d\mathscr{F}[\mathbf{x}(t), \mathbf{p}(t)]}{dt} = \{\mathscr{F}, \mathscr{H}\} \tag{5.5}$$

[1] The Jacobi identity is equivalent to the symplectic 2-form being closed, see Symplectic Manifold

for any $\mathscr{F} : \mathcal{T}^*\mathcal{Q} \to \mathbb{R}$. To see this, let X' be an arbitrary point in Ω_0. We choose $\mathscr{F} = x^i\delta(X - X')$, then (5.5) gives

$$\dot{x}^i(t, X') = \frac{\partial H}{\partial p^i}(\mathbf{x}(t), \mathbf{p}(t))(X').$$

Similarly we can recover the momentum equation at X' by choosing $\mathscr{F} = p^i\delta(X - X')$. This shows (5.5) $\Rightarrow$ (5.3). Conversely, given a Hamiltonian flow $(\mathbf{x}(t), \mathbf{p}(t))$ satisfying (5.3) and for any $\mathscr{F} : \mathcal{T}^*\mathcal{Q} \to \mathbb{R}$, we have

$$\begin{aligned}
\frac{d}{dt}\mathscr{F}[\mathbf{x}(t), \mathbf{p}(t)] &= \frac{\delta \mathscr{F}}{\delta \mathbf{x}} \cdot \dot{\mathbf{x}}(t) + \frac{\delta \mathscr{F}}{\delta \mathbf{p}} \cdot \dot{\mathbf{p}}(t) \\
&= \frac{\delta \mathscr{F}}{\delta \mathbf{x}} \cdot \frac{\delta \mathscr{H}}{\delta \mathbf{p}} - \frac{\delta \mathscr{F}}{\delta \mathbf{p}} \cdot \frac{\delta \mathscr{H}}{\delta \mathbf{x}} \\
&= \{\mathscr{F}, \mathscr{H}\}.
\end{aligned}$$

This shows (5.3) $\Rightarrow$ (5.5).

5.2 Hamiltonian Fluid Mechanics in Eulerian Variables

5.2.1 Non-canonical Transformation

1. **Change-of-variables from Lagrangian variables to Eulerian variables.**
   The Eulerian variables are $\rho, \mathfrak{m} := \rho\mathbf{v}$ and $\mathfrak{s} := \rho S$. Notice that there are 5 independent Eulerian variables $(\rho, \mathfrak{m}, \mathfrak{s})$, while there are 6 independent Lagrangian variables $(\mathbf{q}, \mathbf{p})$.

   The mapping
   $$\Phi : (\mathbf{q}, \mathbf{p}) \mapsto (\rho, \mathfrak{s}, \mathbf{m})$$
   is determined by the formulae:
   $$\begin{cases} \rho(\mathbf{x}) &= \int_{\Omega_0} \rho_0(X)\delta(\mathbf{x} - \mathbf{q}(X))\,dX \\ \mathfrak{s}(\mathbf{x}) &= \int_{\Omega_0} \mathfrak{s}_0(X)\delta(\mathbf{x} - \mathbf{q}(X))\,dX \\ \mathbf{m}(\mathbf{x}) &= \int_{\Omega_0} \mathbf{p}(X)\delta(\mathbf{x} - \mathbf{q}(X))\,dX. \end{cases} \tag{5.6}$$

   Proof. Note that $\rho_0(X) = \rho(\mathbf{q}(X))J(X)$. Multiply this by $\delta(\mathbf{x} - \mathbf{q}(X))$ then integrate in X, we get
   $$\begin{aligned}
   \int_{\Omega_0} \rho_0(X)\delta(\mathbf{x} - \mathbf{q}(X))dX &= \int_{\Omega_0} \rho(\mathbf{q}(X))J(X)\delta(\mathbf{x} - \mathbf{q}(X))\,dX \\
   &= \int_{\Omega} \rho(\mathbf{y})\delta(\mathbf{x} - \mathbf{y})\,d\mathbf{y} = \rho(\mathbf{x}).
   \end{aligned}$$

In the last step, we change integration variable from X to $\mathbf{y} = \mathbf{q}(X)$ and use $J(X)\,dX = d\mathbf{y}$. The proofs for $\mathfrak{s}$ and $\mathfrak{m}$ are similar. These formulae only hold for conservative quantities. $\square$

2. **The Jacobian matrix of the change-of-variables** The variations of ρ, $\mathfrak{s}$ and $\mathbf{m}$ can be obtained by taking variation on the transformation formulae (5.6): We get

$$\begin{aligned}
\delta\rho(\mathbf{x}) &= -\int_{\Omega_0} \rho_0(X)\nabla_{\mathbf{x}}\delta(\mathbf{x}-\mathbf{q}(X))\cdot\delta\mathbf{q}(X)\,dX \\
\delta\mathfrak{s}(\mathbf{x}) &= -\int_{\Omega_0} \mathfrak{s}_0(X)\nabla_{\mathbf{x}}\delta(\mathbf{x}-\mathbf{q}(X))\cdot\delta\mathbf{q}(X)\,dX \\
\delta\mathbf{m}(\mathbf{x}) &= \int_{\Omega_0} [-\mathbf{p}(X)\nabla_{\mathbf{x}}\delta(\mathbf{x}-\mathbf{q}(X))\cdot\delta\mathbf{q}(X) + \delta(\mathbf{x}-\mathbf{q}(X))\cdot\delta\mathbf{p}(X)]\,dX
\end{aligned}$$

These give

$$\begin{aligned}
\frac{\delta\rho}{\delta\mathbf{q}} &= -\rho_0(X)\nabla_{\mathbf{x}}\delta(\mathbf{x}-\mathbf{q}(X)) \\
\frac{\delta\mathfrak{s}}{\delta\mathbf{q}} &= -\mathfrak{s}_0(X)\nabla_{\mathbf{x}}\delta(\mathbf{x}-\mathbf{q}(X)) \\
\frac{\delta\mathbf{m}}{\delta\mathbf{q}} &= -\mathbf{p}(X)\nabla_{\mathbf{x}}\delta(\mathbf{x}-\mathbf{q}(X)) \\
\frac{\delta\mathbf{m}}{\delta\mathbf{p}} &= \delta(\mathbf{x}-\mathbf{q}(X)).
\end{aligned}$$

3. **Chain rule formula**
Given a function $\bar{\mathscr{F}}$ defined in $(\rho, \mathfrak{s}, \mathbf{m})$, it induces a functional $\mathscr{F}$ defined on $(\mathbf{q}, \mathbf{p})$ by function composition:

$$\mathscr{F}[\mathbf{q},\mathbf{p}] = \bar{\mathscr{F}}[\Phi(\mathbf{q},\mathbf{p})].$$

Its variation can be represented as

$$\begin{aligned}
\delta\mathscr{F} &= \int_{\Omega_0}\left(\frac{\delta\mathscr{F}}{\delta\mathbf{q}}\delta\mathbf{q} + \frac{\delta\mathscr{F}}{\delta\mathbf{p}}\delta\mathbf{p}\right)dX \\
&= \int_{\Omega}\left(\frac{\delta\bar{\mathscr{F}}}{\delta\rho}\delta\rho + \frac{\delta\bar{\mathscr{F}}}{\delta\mathfrak{s}}\delta\mathfrak{s} + \frac{\delta\bar{\mathscr{F}}}{\delta\mathbf{m}}\delta\mathbf{m}\right)d\mathbf{x}.
\end{aligned}$$

In this expression, $\frac{\delta \bar{\mathscr{F}}}{\delta \rho}$ is a function of $(\rho, \mathbf{m}, \mathfrak{s})$, hence a function of $\mathbf{x}$.

$$
\begin{aligned}
\frac{\delta \mathscr{F}}{\delta \mathbf{q}}(X) &= \int_\Omega \left(\frac{\delta \bar{\mathscr{F}}}{\delta \rho} \frac{\delta \rho}{\delta \mathbf{q}} + \frac{\delta \bar{\mathscr{F}}}{\delta \mathfrak{s}} \frac{\delta \mathfrak{s}}{\delta \mathbf{q}} + \frac{\delta \bar{\mathscr{F}}}{\delta \mathbf{m}} \frac{\delta \mathbf{m}}{\delta \mathbf{q}} \right) d\mathbf{x} \\
&= -\int_\Omega \left(\rho_0(X) \frac{\delta \bar{\mathscr{F}}}{\delta \rho} + \mathfrak{s}_0(X) \frac{\delta \bar{\mathscr{F}}}{\delta \mathfrak{s}} + \mathbf{p}(X) \cdot \frac{\delta \bar{\mathscr{F}}}{\delta \mathbf{m}} \right) \nabla_{\mathbf{x}} \delta(\mathbf{x} - \mathbf{q}(X))\, d\mathbf{x} \\
&= \int_\Omega \left(\rho_0 \nabla_{\mathbf{x}} \frac{\delta \bar{\mathscr{F}}}{\delta \rho} + \mathfrak{s}_0 \nabla_{\mathbf{x}} \frac{\delta \bar{\mathscr{F}}}{\delta \mathfrak{s}} + \mathbf{p} \cdot \nabla_{\mathbf{x}} \frac{\delta \bar{\mathscr{F}}}{\delta \mathbf{m}} \right) \delta(\mathbf{x} - \mathbf{q}(X))\, d\mathbf{x} \\
\frac{\delta \mathscr{F}}{\delta \mathbf{p}}(X) &= \int_\Omega \frac{\delta \bar{\mathscr{F}}}{\delta \mathbf{m}} \delta(\mathbf{x} - \mathbf{q}(X))\, d\mathbf{x} = \frac{\delta \bar{\mathscr{F}}}{\delta \mathbf{m}}|_{\mathbf{x}=\mathbf{q}(X)}.
\end{aligned}
$$

5.2.2 Poisson bracket in Eulerian Conservative Variables

1. **Poisson bracket in Eulerian variables**: We have defined Poisson bracket for functionals defined in Lagrangian variables. This Poisson bracket induces a Poisson bracket for functionals defined in Eulerian variables through the change-of-variable $\Phi : (\mathbf{q}, \mathbf{p}) \mapsto (\rho, \mathfrak{s}, \mathfrak{m})$. Let $\bar{\mathscr{F}}, \bar{\mathscr{G}}$ are two functionals defined in Eulerian variables $(\rho, \mathfrak{s}, \mathfrak{m})$. Let us call the pullback of them by the map Φ by $\bar{\mathscr{F}} \circ \Phi = \mathscr{F}$, $\bar{\mathscr{G}} \circ \Phi = \mathscr{G}$. We have a Poisson structure defined for functionals $\mathscr{F}$ and $\mathscr{G}$. The Poisson structure for $\bar{\mathscr{F}}$ and $\bar{\mathscr{G}}$ is defined as
$$\{\bar{\mathscr{F}}, \bar{\mathscr{G}}\} := \{\mathscr{F}, \mathscr{G}\}.$$
Let us compute the Poisson bracket formula of $\{\mathscr{F}, \mathscr{G}\}$ below. Using the chain-rule formula in the last subsection, we have
$$
\begin{aligned}
\{\bar{\mathscr{F}}, \bar{\mathscr{G}}\} &= \{\mathscr{F}, \mathscr{G}\} \\
&= \int_{M_0} \left(\frac{\delta \mathscr{F}}{\delta \mathbf{q}} \cdot \frac{\delta \mathscr{G}}{\delta \mathbf{p}} - \frac{\delta \mathscr{G}}{\delta \mathbf{q}} \cdot \frac{\delta \mathscr{F}}{\delta \mathbf{p}} \right) dX \\
&= \int_{M_0} \int_M \delta(\mathbf{x} - \mathbf{q}(X)) \left(\rho_0 \nabla_{\mathbf{x}} \frac{\delta \bar{\mathscr{F}}}{\delta \rho} + \mathfrak{s}_0 \nabla_{\mathbf{x}} \frac{\delta \bar{\mathscr{F}}}{\delta \mathfrak{s}} + \mathbf{p} \cdot \nabla_{\mathbf{x}} \frac{\delta \bar{\mathscr{F}}}{\delta \mathbf{m}} \right) \cdot \frac{\delta \bar{\mathscr{G}}}{\delta \mathbf{m}} \\
&\qquad - \delta(\mathbf{x} - \mathbf{q}(X)) \left(\rho_0 \nabla_{\mathbf{x}} \frac{\delta \bar{\mathscr{G}}}{\delta \rho} + \mathfrak{s}_0 \nabla_{\mathbf{x}} \frac{\delta \bar{\mathscr{G}}}{\delta \mathfrak{s}} + \mathbf{p} \cdot \nabla_{\mathbf{x}} \frac{\delta \bar{\mathscr{G}}}{\delta \mathbf{m}} \right) \cdot \frac{\delta \bar{\mathscr{F}}}{\delta \mathbf{m}}\, d\mathbf{x}\, dX
\end{aligned}
$$
Using (5.6) and Lemma 5.4 below, we get the expression of the Poisson bracket formula
$$
\begin{aligned}
\{\bar{\mathscr{F}}, \bar{\mathscr{G}}\} = \int_M & \left(\rho \nabla_{\mathbf{x}} \frac{\delta \bar{\mathscr{F}}}{\delta \rho} + \mathfrak{s} \nabla_{\mathbf{x}} \frac{\delta \bar{\mathscr{F}}}{\delta \mathfrak{s}} + \mathbf{m} \cdot \nabla_{\mathbf{x}} \frac{\delta \bar{\mathscr{F}}}{\delta \mathbf{m}} \right) \cdot \frac{\delta \bar{\mathscr{G}}}{\delta \mathbf{m}} \\
& - \left(\rho \nabla_{\mathbf{x}} \frac{\delta \bar{\mathscr{G}}}{\delta \rho} + \mathfrak{s} \nabla_{\mathbf{x}} \frac{\delta \bar{\mathscr{G}}}{\delta \mathfrak{s}} + \mathbf{m} \cdot \nabla_{\mathbf{x}} \frac{\delta \bar{\mathscr{G}}}{\delta \mathbf{m}} \right) \cdot \frac{\delta \bar{\mathscr{F}}}{\delta \mathbf{m}}\, d\mathbf{x}.
\end{aligned}
$$

Here,

$$\left(\mathbf{m}\cdot\nabla_{\mathbf{x}}\frac{\partial\bar{G}}{\partial\mathbf{m}}\right)\cdot\frac{\partial\bar{F}}{\partial\mathbf{m}} := m_i\left(\frac{\partial}{\partial x^j}\frac{\delta\bar{\mathscr{G}}}{\delta m_i}\right)\frac{\delta\bar{\mathscr{F}}}{\delta m_j}.$$

2. In most cases, the functionals $\bar{\mathscr{F}},\bar{\mathscr{G}}$ have the following expression:

$$\bar{\mathscr{F}}[\rho,\mathfrak{s},\mathfrak{m}] = \int \bar{F}(\rho(\mathbf{x}),\mathfrak{s}(\mathbf{x}),\mathfrak{m}(\mathbf{x}))\,d\mathbf{x}, \quad \bar{\mathscr{G}}[\rho,\mathfrak{s},\mathfrak{m}] = \int \bar{G}(\rho(\mathbf{x}),\mathfrak{s}(\mathbf{x}),\mathfrak{m}(\mathbf{x}))\,d\mathbf{x},$$

In this case, the above functional variation has the following partial derivative form:

$$\frac{\delta\bar{\mathscr{F}}}{\delta\rho} = \frac{\partial\bar{F}}{\partial\rho}, etc.$$

The corresponding Poisson bracket has the following expression

$$\begin{aligned}\{\bar{\mathscr{F}},\bar{\mathscr{G}}\} = \int_M &\left(\rho\nabla_{\mathbf{x}}\frac{\partial\bar{F}}{\partial\rho} + \mathfrak{s}\nabla_{\mathbf{x}}\frac{\partial\bar{F}}{\partial\mathfrak{s}} + \mathbf{m}\cdot\nabla_{\mathbf{x}}\frac{\partial\bar{F}}{\partial\mathbf{m}}\right)\cdot\frac{\partial\bar{G}}{\partial\mathbf{m}} \\ &- \left(\rho\nabla_{\mathbf{x}}\frac{\partial\bar{G}}{\partial\rho} + \mathfrak{s}\nabla_{\mathbf{x}}\frac{\partial\bar{G}}{\partial\mathfrak{s}} + \mathbf{m}\cdot\nabla_{\mathbf{x}}\frac{\partial\bar{G}}{\partial\mathbf{m}}\right)\cdot\frac{\partial\bar{F}}{\partial\mathbf{m}}\,d\mathbf{x},\end{aligned}$$

where

$$\left(\mathbf{m}\cdot\nabla_{\mathbf{x}}\frac{\partial\bar{G}}{\partial\mathbf{m}}\right)\cdot\frac{\partial\bar{F}}{\partial\mathbf{m}} := m_i\left(\frac{\partial}{\partial x^j}\frac{\partial\bar{G}}{\partial m_i}\right)\frac{\partial\bar{F}}{\partial m_j}.$$

The symplectic operator J is a linear in $(\rho,\mathfrak{s},\mathfrak{m})$. Such Poisson bracket is called a Lie-Poisson bracket.

Lemma 5.4.

$$\int_{M_0}\int_M \delta(\mathbf{x}-\mathbf{q}(X))\rho_0(X)\phi(\mathbf{x})\psi(\mathbf{q}(X))\,d\mathbf{x}\,dX = \int_M \rho(\mathbf{x})\phi(\mathbf{x})\psi(\mathbf{x})\,d\mathbf{x}.$$

Proof. Let $\mathbf{y} = \mathbf{q}(X)$. Then the above integral is

$$\begin{aligned}&\int_\Omega\int_\Omega \delta(\mathbf{x}-\mathbf{y})\rho_0(\mathbf{q}^{-1}(\mathbf{y}))\phi(\mathbf{x})\psi(\mathbf{y})\,d\mathbf{x}J^{-1}(\mathbf{q}^{-1}(\mathbf{y}))d\mathbf{y} \\ &= \int_\Omega\int_\Omega \delta(\mathbf{x}-\mathbf{y})\rho(\mathbf{y})\phi(\mathbf{x})\psi(\mathbf{y})\,d\mathbf{x}\,d\mathbf{y} = \int_\Omega \rho(\mathbf{x})\phi(\mathbf{x})\psi(\mathbf{x})\,d\mathbf{x}.\end{aligned}$$

□

3. The Poisson bracket $\{\cdot,\cdot\}$ satisfies

   - bilinear,

- antisymmetry: $\{\bar{\mathscr{F}},\bar{\mathscr{G}}\} = -\{\bar{\mathscr{G}},\bar{\mathscr{F}}\}$,
- Jacobi identity:

$$\{\{\bar{\mathscr{E}},\bar{\mathscr{F}}\},\bar{\mathscr{G}}\} + \{\{\bar{\mathscr{F}},\bar{\mathscr{G}}\},\bar{\mathscr{E}}\} + \{\{\bar{\mathscr{G}},\bar{\mathscr{E}}\},\bar{\mathscr{F}}\} = 0.$$

4. **Hamiltonian dynamics** The Hamiltonian $H[\mathbf{q},\mathbf{p}]$ can be expressed in terms of $(\rho,\mathfrak{s},\mathbf{m})$ as the pull-back of $\mathscr{H}$ by the map Φ:

$$\begin{aligned}\bar{\mathscr{H}}[\rho,\mathfrak{s},\mathbf{m}] &:= \mathscr{H}[\mathbf{q},\mathbf{p}] \\ &= \int_\Omega \frac{|\mathbf{m}|^2}{2\rho} + \rho U(\rho,\frac{\mathfrak{s}}{\rho})\,d\mathbf{x} \\ &= \int_\Omega H(\rho,\mathfrak{s},\mathbf{m})\,d\mathbf{x}\end{aligned}$$

From this expression, we get

$$\begin{aligned}\frac{\delta\bar{\mathscr{H}}}{\delta\rho} &= \frac{\partial H}{\partial\rho} = -\frac{|\mathbf{v}|^2}{2} + U + \frac{p}{\rho} - TS \\ \frac{\delta\bar{\mathscr{H}}}{\delta\mathfrak{s}} &= \frac{\partial H}{\partial\mathfrak{s}} = T \\ \frac{\delta\bar{\mathscr{H}}}{\delta\mathbf{m}} &= \frac{\partial H}{\partial\mathbf{m}} = \mathbf{v}.\end{aligned}$$

By taking

$$\rho(\mathbf{x}') = \bar{\mathscr{F}}[\rho,\mathfrak{s},\mathbf{m}] = \int \rho(\mathbf{x})\delta(\mathbf{x}'-\mathbf{x})\,d\mathbf{x}$$

we get

$$\{\rho(\mathbf{x}'),\mathscr{H}\} = \{\bar{\mathscr{F}},\bar{\mathscr{H}}\} = \int \rho(\mathbf{x})\nabla_{\mathbf{x}}\delta(\mathbf{x}'-\mathbf{x})\cdot\mathbf{v}\,d\mathbf{x} = -\nabla_{\mathbf{x}}\cdot(\rho\mathbf{v})(\mathbf{x}').$$

This is the density equation. Similarly, we get the entropy equation:

$$\{\mathfrak{s}(\mathbf{x}'),\mathscr{H}\} = \int \mathfrak{s}(\mathbf{x})\nabla_{\mathbf{x}}\delta(\mathbf{x}'-\mathbf{x})\cdot\mathbf{v}\,d\mathbf{x} = -\nabla_{\mathbf{x}}\cdot(\mathfrak{s}\mathbf{v}),$$

and the momentum equation:

$$\begin{aligned}\{\mathbf{m}(\mathbf{x}'),\bar{\mathscr{H}}\} = \int &\mathbf{m}\cdot\nabla_{\mathbf{x}}\delta(\mathbf{x}-\mathbf{x}')\cdot\mathbf{v} \\ &-\left(\rho\nabla_{\mathbf{x}}\left(-\frac{|\mathbf{v}|^2}{2}+e+\frac{p}{\rho}-TS\right)+\mathfrak{s}\nabla_{\mathbf{x}}T+\mathbf{m}\cdot\nabla_{\mathbf{x}}\mathbf{v}\right)\delta(\mathbf{x}-\mathbf{x}')\,d\mathbf{x} \\ = &-\nabla_{\mathbf{x}}\cdot(\mathbf{v}\mathbf{m}) - \rho\nabla_{\mathbf{x}}\left(-\frac{|\mathbf{v}|^2}{2}+U+\frac{p}{\rho}-TS\right) - \mathfrak{s}\nabla_{\mathbf{x}}T \\ = &-\nabla_{\mathbf{x}}\cdot(\mathbf{v}\mathbf{m}) - \nabla p.\end{aligned}$$

Thus, we get the equation of the Hamiltonian flow

$$\dot{\rho} = \{\rho, \bar{\mathscr{H}}\}$$
$$\dot{\mathfrak{s}} = \{\mathfrak{s}, \bar{\mathscr{H}}\}$$
$$\dot{\mathbf{m}} = \{\mathbf{m}\bar{\mathscr{H}}\}$$

is the Euler equations.

5.2.3 Poisson bracket in terms of $(\rho, S, \mathbf{v})$

1. We change variables $(\rho, \mathfrak{s}, \mathbf{m})$ to $(\rho, S, \mathbf{v})$ by $S = \mathfrak{s}/\rho$ and $\mathbf{v} = \mathbf{m}/\rho$. Let us use $\mathscr{F}$ and $\mathscr{G}$ for functionals defined on $(\rho, S, \mathbf{v})$ and $\bar{\mathscr{F}}, \bar{\mathscr{G}}$ for functionals defined on $(\rho, \mathfrak{s}, \mathbf{m})$. The chain-rules for this change of variable are

$$\frac{\partial}{\partial \rho}|_{(\mathfrak{s},\mathbf{m})} = \frac{\partial}{\partial \rho}|_{(S,\mathbf{v})} - \frac{S}{\rho}\frac{\partial}{\partial S} - \frac{\mathbf{v}}{\rho}\cdot\frac{\partial}{\partial \mathbf{v}}$$
$$\frac{\partial}{\partial \mathfrak{s}} = \frac{1}{\rho}\frac{\partial}{\partial S}$$
$$\frac{\partial}{\partial \mathbf{m}} = \frac{1}{\rho}\frac{\partial}{\partial \mathbf{v}}.$$

Plug this into the Poisson bracket

$$\{\mathscr{F}, \mathscr{G}\} = \int_\Omega \left(\rho \nabla_{\mathbf{x}} \frac{\delta \bar{\mathscr{F}}}{\delta \rho} + \mathfrak{s}\nabla_{\mathbf{x}} \frac{\delta \bar{\mathscr{F}}}{\delta \mathfrak{s}} + \mathbf{m}\cdot\nabla_{\mathbf{x}}\frac{\delta \bar{\mathscr{F}}}{\delta \mathbf{m}}\right)\cdot\frac{\delta \bar{\mathscr{G}}}{\delta \mathbf{m}}$$
$$- \left(\rho \nabla_{\mathbf{x}} \frac{\delta \bar{\mathscr{G}}}{\delta \rho} + \mathfrak{s}\nabla_{\mathbf{x}} \frac{\delta \bar{\mathscr{G}}}{\delta \mathfrak{s}} + \mathbf{m}\cdot\nabla_{\mathbf{x}}\frac{\delta \bar{\mathscr{G}}}{\delta \mathbf{m}}\right)\cdot\frac{\delta \bar{\mathscr{F}}}{\delta \mathbf{m}}\, d\mathbf{x}.$$

Note that $\frac{\delta \bar{\mathscr{F}}}{\delta \mathbf{m}} = \frac{\partial F}{\partial \mathbf{m}}$. We have

$$\left[\rho\nabla_{\mathbf{x}}\left(\partial_\rho - \frac{\mathbf{v}}{\rho}\cdot\partial_{\mathbf{v}} - \frac{S}{\rho}\partial_S\right)F + \rho S\nabla_{\mathbf{x}}\left(\frac{1}{\rho}\partial_S F\right) + \rho\mathbf{v}\cdot\nabla_{\mathbf{x}}\left(\frac{1}{\rho}\partial_{\mathbf{v}}F\right)\right]\cdot\frac{1}{\rho}\partial_{\mathbf{v}}G$$
$$-\left[\rho\nabla_{\mathbf{x}}\left(\partial_\rho - \frac{\mathbf{v}}{\rho}\cdot\partial_{\mathbf{v}} - \frac{S}{\rho}\partial_S\right)G + \rho S\nabla_{\mathbf{x}}\left(\frac{1}{\rho}\partial_S G\right) + \rho\mathbf{v}\cdot\nabla_{\mathbf{x}}\left(\frac{1}{\rho}\partial_{\mathbf{v}}G\right)\right]\cdot\frac{1}{\rho}\partial_{\mathbf{v}}F$$

We get that

$$\{\mathscr{F}, \mathscr{G}\} = \int_\Omega \Big[(\nabla_{\mathbf{x}}\partial_\rho F)\cdot\partial_{\mathbf{v}}G - (\nabla_{\mathbf{x}}\partial_\rho G)\cdot\partial_{\mathbf{v}}F$$
$$- \frac{\nabla_{\mathbf{x}} S}{\rho}\cdot(\partial_S F\partial_{\mathbf{v}}G - \partial_S G\partial_{\mathbf{v}}F)$$
$$+\frac{1}{\rho}(\partial_{x^i}v^j - \partial_{x^j}v^i)\partial_{v^i}F\partial_{v^j}G\Big]\, d\mathbf{x}$$

The last term can also be expressed as

$$-\frac{1}{\rho}\partial_{x^j} v^i \left(\partial_{v^i} F \partial_{v^j} G - \partial_{v^i} G \partial_{v^j} F\right) = -\frac{\nabla_{\mathbf{x}} \times \mathbf{v}}{\rho} \cdot \frac{\partial F}{\partial \mathbf{v}} \times \frac{\partial G}{\partial \mathbf{v}}.$$

Thus, the Poisson bracket is

$$\begin{aligned} \{\mathscr{F},\mathscr{G}\} &= \int_\Omega \Big[(\nabla_{\mathbf{x}}\partial_\rho F)\cdot\partial_{\mathbf{v}} G - (\nabla_{\mathbf{x}}\partial_\rho G)\cdot\partial_{\mathbf{v}} F \\ &\quad -\tfrac{\nabla_{\mathbf{x}} S}{\rho}\cdot(\partial_S F \partial_{\mathbf{v}} G - \partial_S G \partial_{\mathbf{v}} F) \\ &\quad -\tfrac{\nabla_{\mathbf{x}}\times\mathbf{v}}{\rho}\cdot\tfrac{\partial F}{\partial \mathbf{v}}\times\tfrac{\partial G}{\partial \mathbf{v}}\Big]\, d\mathbf{x}. \end{aligned} \tag{5.7}$$

2. The Poisson bracket $\{\mathscr{F},\mathscr{G}\}$ satisfies

   - Bilinear: $\{\mathscr{F}_1+\mathscr{F}_2,\mathscr{G}\} = \{\mathscr{F}_1,\mathscr{G}\}+\{\mathscr{F}_2,\mathscr{G}\}$,
   - Antisymmetry: $\{\mathscr{F},\mathscr{G}\} = -\{\mathscr{G},\mathscr{F}\}$
   - Jacobi identity:

$$\{\{\mathscr{E},\mathscr{F}\},\mathscr{G}\}+\{\{\mathscr{F},\mathscr{G}\},\mathscr{E}\}+\{\{\mathscr{G},\mathscr{E}\},\mathscr{F}\} = 0.$$

3. With $H(\rho,S,\mathbf{v}) := \frac{1}{2}\rho|\mathbf{v}|^2+\rho U(\rho,S)$ and $\mathscr{H}[\rho,S,\mathbf{v}] = \int H(\rho(\mathbf{x}),S(\mathbf{x}),\mathbf{v}(\mathbf{x}))\,d\mathbf{x}$, we get

$$\frac{\delta\mathscr{H}}{\delta\rho} = \frac{1}{2}|\mathbf{v}|^2+U+\frac{p}{\rho}, \quad \frac{\delta\mathscr{H}}{\delta S} = \rho T, \quad \frac{\delta\mathscr{H}}{\delta \mathbf{v}} = \rho\mathbf{v}.$$

Thus,

$$\{\rho(\cdot-\mathbf{x}'),\mathscr{H}\} = \int \left(\nabla_{\mathbf{x}}\delta(\mathbf{x}-\mathbf{x}')\right)\cdot(\rho\mathbf{v})\,d\mathbf{x} = -\nabla_{\mathbf{x}}\cdot(\rho\mathbf{v})(\mathbf{x}').$$

$$\{S(\cdot-\mathbf{x}'),\mathscr{H}\} = \int -\frac{\nabla_{\mathbf{x}} S}{\rho}\cdot\left(\delta(\mathbf{x}-\mathbf{x}')(\rho\mathbf{v})\right)\,d\mathbf{x} = -\mathbf{v}\cdot\nabla_{\mathbf{x}} S(\mathbf{x}')$$

$$\begin{aligned} \{\mathbf{v}(\cdot-\mathbf{x}'),\mathscr{H}\} &= \int -(\nabla_{\mathbf{x}}\partial_\rho H)\cdot\delta(\mathbf{x}-\mathbf{x}')I + \frac{\nabla_{\mathbf{x}} S}{\rho}\partial_S H\,\delta(\mathbf{x}-\mathbf{x}') \\ &\quad + \frac{1}{\rho}\left(\partial_{x^i} v^j - \partial_{x^j} v^i\right)\delta(\mathbf{x}-\mathbf{x}')\rho v^i\,d\mathbf{x} \\ &= -\nabla_{\mathbf{x}}\left(\frac{1}{2}|\mathbf{v}|^2+U+\frac{p}{\rho}\right)+\frac{\nabla_{\mathbf{x}} S}{\rho}(\rho T)+\left(\partial_{x^i} v^j - \partial_{x^j} v^i\right)v^j \\ &= -v^j\partial_{x^j} v^i - \frac{1}{\rho}\partial_{x^i} p = -\mathbf{v}\cdot\nabla_{\mathbf{x}}\mathbf{v} - \frac{\nabla_{\mathbf{x}} p}{\rho} \end{aligned}$$

These are summarized as

$$\begin{aligned}
\partial_t \rho &= \{\rho, \mathscr{H}\} = -\nabla_{\mathbf{x}} \cdot (\rho \mathbf{v}) \\
\partial_t S &= \{S, \mathscr{H}\} = -\mathbf{v} \cdot \nabla_{\mathbf{x}} S \\
\partial_t \mathbf{v} &= \{\mathbf{v}, \mathscr{H}\} = -\mathbf{v} \cdot \nabla_{\mathbf{x}} \mathbf{v} - \frac{\nabla_{\mathbf{x}} p}{\rho},
\end{aligned}$$

which are the Euler equations.

Homework For Burgers equation $u_t + uu_x = 0$, the corresponding Poisson bracket and the Hamiltonian are

$$\{\bar{\mathscr{F}}, \bar{\mathscr{G}}\} = \int_{\mathbb{R}} u \left\{ \left[\frac{\partial \bar{F}}{\partial u} \right]_x \frac{\partial \bar{G}}{\partial u} - \left[\frac{\partial \bar{G}}{\partial u} \right]_x \frac{\partial \bar{F}}{\partial u} \right\} dx$$

$$H(u) = \frac{1}{2} u^2.$$

5.2.4 Casimir and Conservation of Helicity

1. **Casimirs** There are 5 independent Eulerian variables $(\rho, S, \mathbf{v})$, whereas there are 6 independent Lagrangian variables $(\mathbf{q}, \mathbf{p})$. Thus, the Poisson bracket $\{\cdot, \cdot\}$ in Eulerian variables is expected to be singular. A function $\mathscr{C}(\rho, S, \mathbf{v})$ is called a *Casimir invariant* of the Euler system if

   $$\{\mathscr{C}, \mathscr{F}\} = 0 \text{ for any function } \mathscr{F}(\rho, S, \mathbf{v}).$$

   Using this definition, the Poisson bracket formula (5.7) gives the following equations for $\mathscr{C}(\rho, S, \mathbf{v})$:

   $$\begin{aligned}
   \nabla \cdot \frac{\delta \mathscr{C}}{\delta \mathbf{v}} &= 0, \\
   \frac{1}{\rho} \nabla S \cdot \frac{\delta \mathscr{C}}{\delta \mathbf{v}} &= 0, \\
   \nabla \frac{\delta \mathscr{C}}{\delta \rho} + \frac{\nabla \times \mathbf{v}}{\rho} \times \frac{\delta \mathscr{C}}{\delta \mathbf{v}} - \frac{\nabla S}{\rho} \frac{\delta \mathscr{C}}{\delta S} &= 0.
   \end{aligned}$$

2. **Helicity.** Let us suppose $\mathscr{C}$ depends only on $\mathbf{v}$. Let $\mathbf{w} = \frac{\delta \mathscr{C}}{\delta \mathbf{v}}$. Then $\mathbf{w}$ satisfies

   $$\nabla \cdot \mathbf{w} = 0, \quad (\nabla \times \mathbf{v}) \times \mathbf{w} = 0.$$

   These two imply $\mathbf{w} = Const. \nabla \times \mathbf{v}$ for some constant $Const$. The helicity

   $$\mathscr{C}(\mathbf{v}) := \int \mathbf{v} \cdot \nabla \times \mathbf{v} \, d\mathbf{x}$$

   satisfies $\delta \mathscr{C} / \delta \mathbf{v} = 2 \nabla \times \mathbf{v}$.

3. **Potential vorticity** Let
$$q = \frac{\nabla \times \mathbf{v}}{\rho} \cdot \nabla S$$
be the potential vorticity associated with the advected quantity S. Then
$$\mathscr{C} := \int \rho f(q)\, d\mathbf{x}$$
is a Casimir for any function f.

4. **Thermodynamic Casimirs** Suppose $\mathscr{C}$ only depends on the thermal variables, that is,
$$\mathscr{C}(\rho, S) = \int C(\rho, S)\, d\mathbf{x}.$$
Then the equation for C is
$$\nabla \frac{\partial C}{\partial \rho} - \frac{\nabla S}{\rho} \frac{\partial C}{\partial S} = 0.$$
If, in addition, C is separable, then $C = \rho f(S)$ for an arbitrary function f. The solution $\mathscr{C}$ is
$$\mathscr{C}(\rho, S) = \int \rho f(S)\, d\mathbf{x}.$$

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Chapter 6

Viscous Fluids

6.1 Viscosity

6.1.1 Stress

In fluid dynamics, stress is a surface force, composed with a hydrostatic part $-p\mathbf{I}$ and a viscous part τ:

$$\boxed{\sigma = -p\mathbf{I} + \tau.} \tag{6.1}$$

The first term results from the direct impact of particles to the surface. It represents a thermodynamic force that exists even when the fluid velocity is zero or constant. Assuming the fluid is isotropic (i.e. a property that has the same value in all directions), this thermodynamic stress is $-p\mathbf{I}$.

The second term τ is termed the *viscous stress tensor*. It arises due to the resistance of fluids to the fluid motions, occurring when different fluid parcels move at different velocities. Thus, τ depends on $\nabla\mathbf{v}$, or possibly $\nabla\nabla\mathbf{v}$, and so on. It's noteworthy that $\tau = 0$ when $\mathbf{v}$ is constant. The hypothesis of *Newtonian fluids* posits that τ *is a linear function of* $\nabla\mathbf{v}$.

6.1.2 Strain Rate

Decomposition of train-rate tensor Recall the rat- of-change of the deformation (2.17) is

$$\dot{F} = (\nabla\mathbf{v})F.$$

The term $L := \nabla\mathbf{v}$ measures the changing rate of material deformation and is called rate-of-deformation. We can decompose $\nabla\mathbf{v}$ into two parts:

$$\nabla\mathbf{v} = \frac{1}{2}\left(\nabla\mathbf{v} + (\nabla\mathbf{v})^T\right) + \frac{1}{2}\left(\nabla\mathbf{v} - (\nabla\mathbf{v})^T\right) = D + \omega. \tag{6.2}$$

The symmetric part D can further be decomposition into

$$D_s := D - \frac{1}{3}Tr(D)I, \quad D_b = \frac{1}{3}Tr(D).$$

Here, D_s is called the *shear strain*, describing the rate of shearing, D_b is called the *bulk strain*, the rate of expansion or shrinking, and ω is called the *spin tensor*, charactering the rate of rotation. In summary, the strain rate L is decomposed into

$$L = D_s + D_b + \omega.$$

Examples Let us see two examples of $\nabla \mathbf{v}$ to understand how fluid responds to this deformation rate.

- **Rigid-body rotation** For fluid flows which are undergoing a rigid-body rotation, there is no observed resistance force. The rotation can be expressed as

  $$\mathbf{v} = \alpha \times \mathbf{x}, \quad \alpha = (\alpha_1, \alpha_2, \alpha_3)^T \text{ is the rotation vector.}$$

  This implies:

  $$\nabla \mathbf{v} = \begin{bmatrix} 0 & -\alpha_3 & \alpha_2 \\ \alpha_3 & 0 & -\alpha_1 \\ -\alpha_2 & \alpha_1 & 0 \end{bmatrix},$$

  which is an antisymmetric matrix, i.e.,

  $$\nabla \mathbf{v} + (\nabla \mathbf{v})^T = 0.$$

  For this rotational flow, experimental observations show that the corresponding $\tau = 0$. Thus, we should require $\tau = 0$ when $\nabla \mathbf{v} + (\nabla \mathbf{v})^T = 0$.

- **Simple shear flow** A simple shear flow is given by

  $$v_1 = \dot{\gamma}_{21} x_2, \quad v_2 = 0, \quad v_3 = 0. \tag{6.3}$$

  Here, $\dot{\gamma}_{21}$ is the shear rate, assumed to be a constant. The strain rate is

  $$\nabla \mathbf{v} = \begin{bmatrix} 0 & \dot{\gamma}_{21} & 0 \\ 0 & 0 & 0 \\ 0 & 0 & 0 \end{bmatrix}.$$

  Experimentally, for a wide class of fluids and over a broad range of shear rates, it is found that the pressure p is independent of $\dot{\gamma}_{21}$, and

  $$\tau_{21} = \mu \dot{\gamma}_{21}$$

  for some constant μ. This ratio μ is called the shear viscosity.

6.1.3 The stress and strain-rate relation for Newtonian fluids

Assumptions of isotropic Newtonian fluids

(1) The viscous stress tensor τ is linear in strain rate $\nabla \mathbf{v}$,

(2) τ is isotropic

(3) τ is symmetric

From the assumption that τ is *linear* with respect to $\nabla \mathbf{v}$, it can be expressed as:

$$\tau_{ij} = a_{ijkl} \frac{\partial v^k}{\partial x^l}$$

where a_{ijkl} are constants.

Considering the isotropy of τ, we can show that the constants a_{ijkl} have a specific form:

$$a_{ijkl} = \alpha \delta_{ij} \delta_{kl} + \beta \delta_{ik} \delta_{jl} + \gamma \delta_{il} \delta_{jk} \tag{6.4}$$

for some constants α, β, γ. [1] Further imposing the symmetry of τ, leading to the symmetry of a_{ijkl} in i, j, we find that $\beta = \gamma$, resulting in:

$$a_{ijkl} = \alpha \delta_{ij} \delta_{kl} + \beta \left(\delta_{ik} \delta_{jl} + \delta_{il} \delta_{jk} \right). \tag{6.5}$$

Thus, the viscous stress tensor (τ) takes the form:

$$\begin{aligned}
\tau_{ij} &= a_{ijkl} \frac{\partial v^k}{\partial x^l} \\
&= \left[\alpha \delta_{ij} \delta_{kl} + \beta \left(\delta_{ik} \delta_{jl} + \delta_{il} \delta_{jk} \right) \right] \frac{\partial v^k}{\partial x^l} \\
&= \beta \left(\frac{\partial v^i}{\partial x^j} + \frac{\partial v^j}{\partial x^i} \right) + \alpha \delta_{ij} \frac{\partial v^k}{\partial x^k}
\end{aligned}$$

[1] This is a theorem for isotropic tensor

- A rank 2 tensor $Q = Q_{ij} e_i e_j$ ($\{e_i\}$ is an orthonormal basis) is called isotropic if $Q = Q_{ij} e'_i e'_j$, where $e'_i = R^k_i e_k$ and R^k_i is a rotation matrix.
- A rank 4 tensor $A = a_{ijkl} e_i e_j e_k e_l$ is called isotropic if $A = a_{ijkl} e'_i e'_j e'_k e'_l$ for any $e'_i = R^k_i e_k$ and R^k_i is a rotation matrix.

Lemma 6.5. *(a) A rank-2 isotropic tensor has the form: $Q = \alpha \delta_{ij} e_i e_j$ for some scalar α.*

(b) A rank-4 isotropic tensor has the form: $A = \alpha \delta_{ij} \delta_{kl} + \beta \delta_{ik} \delta_{jl} + \gamma \delta_{il} \delta_{jk}$ for some scalars α, β, γ.

We write it as

$$\tau = 2\beta D + \alpha\,\mathrm{tr}(D) I,$$

where

$$D = \frac{1}{2}\left(\nabla\mathbf{v} + (\nabla\mathbf{v})^T\right) \tag{6.6}$$

is the rate of strain. Let us further decompose D into D_s, the rate of shear strain, and D_b, the rate of bulk strain:

$$D_s := D - \frac{1}{3}Tr(D)I, \quad D_b = \frac{1}{3}Tr(D).$$

We can express τ in terms of D_s and D_b by

$$\boxed{\tau = 2\eta D_s(\mathbf{v}) + 2\zeta D_b(\mathbf{v}).} \tag{6.7}$$

The coefficient η *is called the shear viscosity*, while ζ *the bulk viscosity*. They satisfy

$$\eta > 0, \quad \zeta > 0. \tag{6.8}$$

Homework Show that a rank-4 isotropic tensor has the form: $A = \alpha\delta_{ij}\delta_{kl} + \beta\delta_{ik}\delta_{jl} + \gamma\delta_{il}\delta_{jk}$ for some scalars α, β, γ.

6.1.4 The Momentum Equation and Vorticity Equation for Viscous Flows

Momentum Equation The viscous force is

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

In the above calculation, we have used

$$\begin{aligned}
\partial_j\left[\partial_i v^j + \partial_j v^i - \frac{2}{3}\partial_k v^k\right] &= \partial_j\partial_i v^j + \partial_j^2 v^i - \frac{2}{3}\partial_j(\partial_k v^k) \\
&= \partial_j^2 v^i + \frac{1}{3}\partial_j(\partial_k v^k).
\end{aligned}$$

Thus, for compressible viscous flows, the momentum equation reads

$$\boxed{\rho\left(\partial_t\mathbf{v} + \mathbf{v}\nabla\mathbf{v}\right) + \nabla p = \eta\nabla^2\mathbf{v} + (\zeta + \frac{\eta}{3})\nabla(\nabla\cdot\mathbf{v}).} \tag{6.9}$$

Vorticity equation for compressible viscous flows From (3.2), the momentum equation can also expressed as

$$\left(\mathbf{v}_t+\omega\times\mathbf{v}+\nabla(\frac{1}{2}|\mathbf{v}|^2)\right)+\frac{\nabla p}{\rho}=\frac{\nabla\cdot\tau}{\rho}, \tag{6.10}$$

By taking *curl* on this equation, we obtain the vorticity equation for incompressible viscous flows:

$$\partial_t\omega+\mathbf{v}\cdot\nabla\omega-(\omega\cdot\nabla)\,\mathbf{v}+\omega\,(\nabla\cdot\mathbf{v})=\frac{1}{\rho^2}\nabla\rho\times\nabla p+\nabla\times\left(\frac{\nabla\cdot\tau}{\rho}\right). \tag{6.11}$$

In the case of incompressible flows, we have

$$\partial_t\omega+\mathbf{v}\cdot\nabla\omega-(\omega\cdot\nabla)\,\mathbf{v}+\omega\,(\nabla\cdot\mathbf{v})=\eta\bigtriangleup\omega. \tag{6.12}$$

Note that the bulk viscosity does not effect the diffusion of the vortices.

Boundary condition For a fixed bundary, a natural boundary for viscous flow is

$$\mathbf{v}=0 \quad \text{on boundary.}$$

6.2 Heat Conduction and Energy Equation

The energy equation involves the rate-of-work done by the surface force and body force, which are $\sigma\cdot\mathbf{v}$ and $\mathbf{f}\cdot\mathbf{v}$.

When temperature is not uniform in a media, it generates a heat flux $\mathbf{q}$ due to random motion of particles and causes energy transfer in fluid. This heat flux is a function of ∇T, where T is the temperature. It should be zero when $\nabla T=0$. To the first order, we may assume

$$\boxed{\mathbf{q}=-\kappa\nabla T,} \tag{6.13}$$

where κ is a positive parameter, called heat conductivity. Formula (6.13) is called the Fourier law.

With the above two sources of rate-of-energy, the new energy equation becomes

$$\boxed{\frac{\partial(\rho E)}{\partial t}+\nabla\cdot(\rho E\mathbf{v}-\sigma\mathbf{v}+\mathbf{q})=\mathbf{f}\cdot\mathbf{v},\quad \sigma=-pI+\tau.} \tag{6.14}$$

where $E=\frac{1}{2}|\mathbf{v}|^2+U$ is the total energy density per unit mass.

Boundary condition Since the energy involves 2nd order derivatives of the temperature, natural boundary conditions can be prescribed on T, which is described below. Suppose the boundary is Γ. The boundary Γ is decomposed into $\Gamma_d \cup \Gamma_n \cup \Gamma_0$, where Γ_0 has area 0. We prescribe Dirichlet data T on Γ_d and Neumann data on Γ_n. That is

$$\begin{cases} T(\mathbf{x}) = T_d(\mathbf{x}) & \mathbf{x} \in \Gamma_d \\ \nabla T \cdot \nu(\mathbf{x}) = g(\mathbf{x}) & \mathbf{x} \in \Gamma_n. \end{cases}$$

6.3 Second Law of Thermodynamics for Viscous Fluid Flows

6.3.1 Dissipation of Kinetic Energy

To analyze the evolution of kinetic energy, as that in the classical mechanics, we take dot product of the momentum equation with $\mathbf{v}$, on the left-hand side, we get the time derivative of the kinetic energy:

$$\begin{aligned} \mathbf{v} \cdot [\rho(\mathbf{v}_t + \mathbf{v} \cdot \nabla \mathbf{v})] &= \partial_t \left(\frac{1}{2} \rho |\mathbf{v}|^2 \right) + \nabla \cdot (\rho \mathbf{v}) \frac{|\mathbf{v}|^2}{2} + \mathbf{v} \cdot (\rho \mathbf{v} \cdot \nabla \mathbf{v}) \\ &= \partial_t \left(\frac{1}{2} \rho |\mathbf{v}|^2 \right) + \partial_j (\rho v^j) \frac{v^i v^i}{2} + v^i \rho v^j \partial_j v^i \\ &= \partial_t \left(\frac{1}{2} \rho |\mathbf{v}|^2 \right) + \nabla \cdot (\frac{1}{2} \rho |\mathbf{v}|^2 \mathbf{v}). \end{aligned}$$

The pressure gradient term in the momentum equation contributes the following work:

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

The viscous force contributes the following work: [2]

$$\begin{aligned} \mathbf{v} \cdot (\nabla \cdot \tau) &= \nabla \cdot (\mathbf{v} \cdot \tau) - \nabla \mathbf{v} : \tau \\ &= \nabla \cdot (\mathbf{v} \cdot \tau) - \frac{1}{2} \left(\nabla \mathbf{v} + (\nabla \mathbf{v})^T \right) : \tau \quad \because \tau \text{ is symmetric} \\ &= \nabla \cdot (\mathbf{v} \cdot \tau) - \tau : D \end{aligned}$$

Recall that

$$\tau = 2\eta D_s + 2\zeta D_b, \quad D = D_s + D_b$$

and note that $D_s : D_b = 0$, we get

$$\tau : D = 2\eta |D_s|^2 + 2\zeta |D_b|^2. \tag{6.15}$$

[2] The notation $A:B$ for tensor A and B is $A:B = \sum_{ij} a_{ij} b_{ij}$

Finally, we get the following equation for the kinetic energy:

$$\partial_t(\rho E_k) + \nabla \cdot [(\rho E_k I + pI - \tau) \cdot \mathbf{v}] - p\nabla \cdot \mathbf{v} = -\tau : D.$$

Here,

- $\rho E_k = \rho|\mathbf{v}|^2/2$ is the kinetic energy density per unit volume;
- $\nabla \cdot \mathbf{v} = \frac{1}{V}\frac{dV}{dt}$ is the volume change rate; and $p\nabla \cdot \mathbf{v}$ is the energy rate change due to the work from volume change; If $\frac{dV}{dt} < 0$, then the kinetic energy decreases and transfers to internal energy.
- The term $2\eta|D_s|^2$ and $2\zeta|D_b|^2$ are the dissipation rate of due to viscous shear force and viscous bulk force, respectively. They contribute the decay of the kinetic energy. They are the heat sources generated by viscous terms.

In the case of incompressible flow where $\nabla \cdot \mathbf{v} = 0$, we get that the decay of the total kinetic energy.

6.3.2 Entropy Production and the Clausius-Duhem Inequality

First, we subtract the kinetic energy from the energy equation

$$\partial_t(\rho E) + \operatorname{div}[(\rho E + p)\mathbf{v}] = \nabla \cdot (\tau \cdot \mathbf{v} - \mathbf{q}).$$

to get an equation for internal energy:

$$\boxed{\partial_t(\rho U) + \nabla \cdot (\rho U \mathbf{v}) = -p\nabla \cdot \mathbf{v} - \nabla \cdot \mathbf{q} + \tau : D.}$$

- ρU is the internal energy per unit volume;
- $-p\nabla \cdot \mathbf{v}$ is the rate of change of the work exerted to the fluid parcel from surrounding fluids;
- $-\nabla \cdot \mathbf{q}$ is the heat source from heat conduction;
- $\tau : D$ is the heat source generated from viscosity.

From continuity equation, the above equation can also be expressed as

$$\rho \frac{dU}{dt} = -p\nabla \cdot \mathbf{v} - \nabla \cdot \mathbf{q} + \tau : D. \tag{6.16}$$

From the first law of thermodynamics

$$dU = TdS - pdV,$$

We get

$$\rho\frac{dU}{dt} = \rho T\frac{dS}{dt} - \rho p\frac{dV}{dt} = \rho T\frac{dS}{dt} - p\nabla\cdot\mathbf{v}$$

Thus, we obtain

$$\rho T\frac{dS}{dt} = -\nabla\cdot\mathbf{q} + \tau : D.$$

or

$$\boxed{\rho\frac{dS}{dt} = -\frac{\nabla\cdot\mathbf{q}}{T} + \frac{1}{T}\tau : D,} \tag{6.17}$$

By Adding $S(\partial_t\rho + \nabla\cdot(\rho\mathbf{v})) = 0$ to this equation and express $\frac{\nabla\cdot\mathbf{q}}{T} = \nabla\cdot\left(\frac{\mathbf{q}}{T}\right) + \frac{1}{T^2}\mathbf{q}\cdot\nabla T$, we get

$$\frac{d}{dt}(\rho S) + \nabla\cdot\left(\frac{\mathbf{q}}{T}\right) = -\frac{1}{T^2}\mathbf{q}\cdot\nabla T + \frac{1}{T}\tau : D.$$

$$\boxed{\partial_t(\rho S) + \nabla\cdot(\mathbf{v}\rho S) + \nabla\cdot\left(\frac{\mathbf{q}}{T}\right) = -\frac{1}{T^2}\mathbf{q}\cdot\nabla T + \frac{1}{T}\tau : D.} \tag{6.18}$$

The integral form is

$$\boxed{\frac{d}{dt}\int_{\Omega(t)}\rho S\,d\mathbf{x} + \int_{\partial\Omega(t)}\frac{\mathbf{q}\cdot\mathbf{n}}{T}\,dS = \int_{\Omega(t)}\left(-\frac{1}{T^2}\mathbf{q}\cdot\nabla T + \frac{1}{T}\tau : D\right)d\mathbf{x}} \tag{6.19}$$

- The terms $\frac{1}{T}\tau : D > 0$;
- When $\mathbf{q}$ satisfies the Fourier law: $\mathbf{q} = -\kappa\nabla T$ with $\kappa > 0$, then the term

$$-\frac{1}{T^2}\mathbf{q}\cdot\nabla T = \kappa\frac{|\nabla T|^2}{T^2} > 0.$$

Thus, the increase of entropy is due to the heat dissipation and heat generated from viscosity. The terms D_s and D_b are called the entropy production source.

Clausius-Duhem Inequality The second law of thermodynamics states that

$$\boxed{\frac{d}{dt}\int_{\Omega(t)}\rho S\,d\mathbf{x} + \int_{\partial\Omega(t)}\frac{\mathbf{q}\cdot\mathbf{n}}{T}\,dS - \int_{\Omega(t)}\frac{\rho r}{T}d\mathbf{x} \geq 0,} \tag{6.20}$$

where r is the heat source, $\mathbf{q}$ the heat flux. This is called the *Clausius-Duhem inequality*. Comparing (6.19) and (6.20), and use (6.15), we see the heat source in gas system is

$$\rho r = \kappa\frac{|\nabla T|^2}{T} + 2\left(\eta|D_s|^2 + \zeta|D_b|^2\right).$$

Thus, the second law of thermodynamics, expressed as (6.20) if and only if

$$\kappa \geq 0, \quad \eta \geq 0, \quad \zeta \geq 0. \tag{6.21}$$

Homeworks

1. For viscous flows, the no-slip boundary condition on a solid boundary $\partial\Omega$ is defined to be
$$\mathbf{v} = 0 \quad \text{on } \partial\Omega,$$
the normal stress is defined to be $\tau_N := \tau \cdot \nu$. Show that for incompressible Newtonian viscous flows with no-slip boundary condition, the normal stresses are zero at solid boundary.

2. Derive the entropy production formula in Lagrangian coordinate

Remarks

1. For heat equation $c_v T_t = \nabla \cdot (\kappa \nabla T)$, we divide it by T and integrate it over the whole domain to get
$$\begin{aligned}\int_\Omega c_v \frac{T_t}{T}\, d\mathbf{x} &= \int_\Omega \frac{1}{T} \nabla \cdot (\kappa \nabla T)\, d\mathbf{x} \\ &= \int_\Omega \frac{\kappa}{T^2} |\nabla T|^2\, d\mathbf{x} > 0\end{aligned}$$
Thus, we can define entropy $s = c_v \log T$, then
$$\frac{d}{dt} \int_\Omega s\, d\mathbf{x} > 0.$$

Chapter 7

Mathematical Theory of Fluid Dynamics

7.1 Dimensional Analysis

The incompressible Navier-Stokes equation is given by

$$\rho(\partial_t \mathbf{v} + \mathbf{v} \cdot \nabla \mathbf{v}) = -\nabla p + \mu \triangle \mathbf{v} + \mathbf{f}, \quad \nabla \cdot \mathbf{v} = 0.$$

Let us assume $\rho = constant$. Thus, ρ and μ are parameters. There are 7 dimensional quantities: $[t], [x], [\mathbf{v}], [p], [f], \rho, \mu$. The equation should have equal dimensions for each term. These give 4 relations (3 momentum equations and 1 continuity equation. Therefore, there are only three independent fundamental dimensions. Let us choose them to be

$$[x] = L, \quad , [t] = T, \quad , [\mathbf{v}] = U.$$

Comparing $\mu \triangle \mathbf{v}$ and ∇p gives

$$[p] = \mu \frac{U}{L}.$$

Comparing $\mu \triangle \mathbf{v}$ and $\mathbf{f}$ gives

$$[\mathbf{f}] = \frac{L^2}{\mu U}.$$

Comparing $\mu \triangle \mathbf{v}$ and the convection term $\rho \mathbf{v} \nabla \mathbf{v}$, we get

$$\rho \frac{U^2}{L} = \mu \frac{U}{L}.$$

Finally, comparing $\mu \triangle \mathbf{v}$ and the inertial term $\rho \partial_t \mathbf{v}$, we get

$$\rho \frac{U}{T} = \mu \frac{U}{L}$$

Define dimensionless variables

$$\mathbf{x}^* = \frac{\mathbf{x}}{L}, \quad \mathbf{v}^* = \mathbf{v}/U, \quad t^* = t/T, \quad p^* = p\frac{L}{\mu U}, \quad f^* = \mathbf{f}\frac{L^2}{\mu U}.$$

The incompressible Navier-Stokes equations read

$$Re\,(St\partial_{t^*}\mathbf{v}^* + \mathbf{v}^* \cdot \nabla^* \mathbf{v}) = -\nabla^* p^* + \triangle^* \mathbf{v}^* + \mathbf{f}^*, \tag{7.1}$$

$$\nabla^* \cdot \mathbf{v}^* = 0. \tag{7.2}$$

where the dimensionless parameters

$$Re = \frac{\rho U L}{\mu}, \quad St = \frac{L}{UT}. \tag{7.3}$$

are the Renolds and Strouhal numbers.

Special flows:

- Incompressibility: $\nabla \cdot \mathbf{v} = 0$
- Inviscid flows: $Re = \infty$, or $\mu = 0$.
- Irrotational flows: $\nabla \times \mathbf{v} = 0$.
- Potential flows: there exist a scalar ϕ such that $\mathbf{v} = \nabla\phi$.
- Harmonic flows: $\nabla \cdot \mathbf{v} = 0$ and $\nabla \times \mathbf{v} = 0$.
- Stokes flows: the convection term is neglected.

7.2 Vector Field Decomposition

7.2.1 Hodge-Morrey-Friedrichs Decomposition for Vector Fields

The Helmholtz decomposition states that any smooth and fast decay vector field in $\mathbb{R}^3$ can be decomposed into the sum of an irrotational (curl-free) vector field and a solenoidal (divergence-free) vector field. It is a fundamental theorem in vector calculus and is important in electromagnetism and fluid mechanics. It was published in (1858). Such decomposition was generalized to differential forms by Hodge (1934), to general domains with boundaries by Friedrichs and Morrey (1955,1956), respectively. The theories are termed Helmholtz-Hodge decomposition (without boundaries), and the Hodge-Morrey-Friedrichs decomposition (with boundaries). For details of this decomposition for dofferential forms, we refer to

- Albert Chern's Note on Discrete Differential Geometry.
- Günter Schwarz, Hodge Decomposition—A Method for Solving Boundary Value Problems, Lecture Notes in Mathematics, vol. 1607 (1995).

Helmholtz-Hodge-Morrey-Friedrichs Decomposition Let M be a 3D manifold with boundary ∂M. Let $\mathbf{v} : M \to \mathbb{R}^3$ be a smooth vector field. Then $\mathbf{v}$ can be L^2-orthogonally decomposed into

$$\mathbf{v} = \nabla\varphi + \nabla \times \psi + \mathbf{h}, \tag{7.4}$$

where

- $\varphi : M \to \mathbb{R}$ (potential) satisfies

$$\triangle\varphi = \nabla \cdot \mathbf{v}, \quad \varphi = 0 \text{ on } \partial M, \tag{7.5}$$

- $\psi : M \to \mathbb{R}^3$ (vector potential) satisfies

$$\nabla \times (\nabla \times \psi) = \nabla \times \mathbf{v}, \tag{7.6}$$

$$\psi \perp \partial M, (\mathbb{n}^2(\psi) = 0) \tag{7.7}$$

- $\mathbf{h} : M \to \mathbb{R}^3$ (harmonic vector field) satisfies

$$\nabla \cdot \mathbf{h} = 0, \quad \nabla \times \mathbf{h} = 0. \tag{7.8}$$

Let $V = \{\mathbf{v} : M \to \mathbb{R}^3 \text{ smooth}\}$, the above decomposition is expressed as

$$V = im(grad_D) \oplus im(curl_N) \oplus \mathscr{H}^1(M) \tag{7.9}$$

where

$$\mathscr{H}^1(M) = \{\mathbf{h} : M \to \mathbb{R}^3 | \nabla \cdot \mathbf{h} = 0, \nabla \times \mathbf{h} = 0\}. \tag{7.10}$$

Remarks.

- Note that $\nabla\varphi$ is curl-free, $\nabla \times \psi$ is divergence-free, and $\mathbf{h}$ is both curl-free and divergence-free. Thus, $\nabla \times \psi$ carries the vorticity information, and $\nabla\varphi$ carries the expansion/contraction information.
- Such decomposition is not unique. We need to choose proper boundary conditions and proper gauges to get a unique decomposition. This will be discussed later.

- More precise definition of V is

$$V = \{\mathbf{v} : M \to \mathbb{R}^3 | \int_M |\mathbf{v}|^2 < \infty, \int_M |\nabla \mathbf{v}|^2 < \infty\}.$$

  In mathematical terminology, it is the Sobolov space $H^1(M)$. However, I try to avoid too may mathematical terminology. It is understood that when I say smooth, it means that we can take differentiation and the resulting derivative is still meaningful when we take integration.

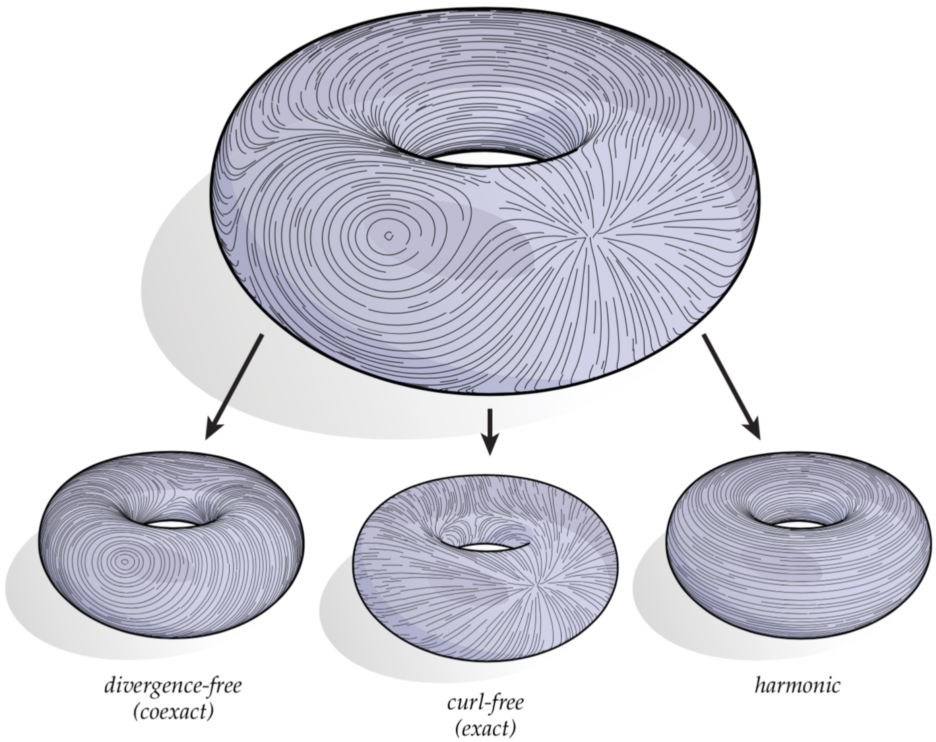


Figure 7.1: Copied from Crane's lecture note

The proof is based on the following Green's theorem and subsequent decomposition.

1. **Green's Identity**

   (a) Let $\varphi : M \to \mathbb{R}$, $\mathbf{w} : M \to \mathbb{R}^3$ be smooth. We have

$$\int_M \nabla\varphi \cdot \mathbf{w}\, d\mathbf{x} = -\int_M \varphi(\nabla \cdot \mathbf{w})\, d\mathbf{x} + \int_{\partial M} \varphi \mathbf{w} \cdot \nu\, dS, \tag{7.11}$$

(b) Let $\psi : M \to \mathbb{R}^3$, $\mathbf{w} : M \to \mathbb{R}^3$ be smooth. We have

$$\int_M (\nabla \times \psi) \cdot \mathbf{w} \cdot d\mathbf{x} = \int_M \psi \cdot (\nabla \times \mathbf{w})\, d\mathbf{x} - \int_{\partial M} (\psi \times \mathbf{w}) \cdot \nu \, dS. \tag{7.12}$$

Remark. In the second Green identity, the vector field ψ is interpreted as a *flux* vector or a *vector potential*.

2. In order to apply the Green theorem for orthogonal decomposition, we need the following boundary restriction operators:

   - Dirichlet and Neumann boundary restriction operators:
     Let ν be an unit outer normal on ∂M. For a vector field $\mathbf{v}$, we can decompose it into $\mathbf{v}_\perp := (\mathbf{v} \cdot \nu)\nu$ and $\mathbf{v}_\parallel := \mathbf{v} - \mathbf{v}_\perp$. We define respectively the following Dirichlet and Neumann boundary restriction operators:

• $\mathtt{t}^0 \phi = \phi\|_{\partial M}$	• $\mathtt{n}^3 \rho = \rho\|_{\partial M}$
• $\mathtt{t}^1 \mathbf{w} = \mathbf{w}_\parallel$	• $\mathtt{n}^1 \mathbf{w} = \mathbf{w}_\perp$
• $\mathtt{t}^2 \psi = \psi_\perp$	• $\mathtt{n}^2 \psi = \psi_\parallel$

   - Kernels:

     $$ker(\mathtt{t}^1) = \{\mathbf{w} | \mathbf{w} \perp \partial M\} \qquad ker(\mathtt{n}^1) = \{\mathbf{w} | \mathbf{w} \parallel \partial M\}$$
     $$ker(\mathtt{t}^2) = \{\psi | \psi \parallel \partial M\} \qquad ker(\mathtt{n}^2) = \{\psi | \psi \perp \partial M\}$$

3. Using the first Green identity, we have

$$im(grad_D)^\perp = ker(div) \tag{7.13}$$
$$im(grad)^\perp = \big(ker(div) \cap ker(\mathtt{n}^1)\big) \tag{7.14}$$

Here, $grad_D$ is the gradient operator restricted to the zero Dirichlet scalar field. That is,

$$grad_D : \{\varphi : M \to \mathbb{R} \text{ smooth }, \varphi|_{\partial M} = 0\}$$

To show this, we see from (1) that

$$\langle \nabla \varphi, \mathbf{w} \rangle = 0 \quad \Leftrightarrow \quad \nabla \cdot \mathbf{w} = 0 \text{ and } \int_{\partial M} \varphi \mathbf{w} \cdot \nu \, dS$$

The last term is zero either $\varphi|_{\partial M} = 0$ or $\mathbf{w} \cdot \nu = 0$. These two correspond to either $\nabla \varphi \in im(grad_D)$ or $\mathbf{w} \in ker(\mathtt{n}^1) \cap ker(div)$.

Note that (7.13) and (7.14) give the decompositions of V:

$$V = im(grad_D) \oplus ker(div) \tag{7.15}$$
$$= im(grad) \oplus \big(ker(div) \cap ker(\mathtt{n}^1)\big)\,. \tag{7.16}$$

4. Using the second Green identity, we have

$$im(curl_N)^{\perp} = ker(curl) \tag{7.17}$$
$$im(curl)^{\perp} = \left(ker(curl) \cap ker(\mathbb{t}^1)\right). \tag{7.18}$$

Here, $curl_N$ means the restriction of the curl operator to the space with Neumann boundary condition:

$$curl_N : \{\psi : M \to \mathbb{R}^3 \text{ smooth, } \mathbb{n}^2(\psi) = 0\}.$$

Note that (7.17) and (7.18) give the decompositions of V:

$$V = im(curl_N) \oplus ker(curl) \tag{7.19}$$
$$= im(curl) \oplus \left(ker(curl) \cap ker(\mathbb{t}^1)\right). \tag{7.20}$$

5. We now successively decompose V into

$$\begin{aligned}V &= im(grad_D) \oplus ker(div)\\ &= im(grad_D) \oplus [ker(div) \cap (im(curl_N) \oplus ker(curl))]\\ &= im(grad_D) \oplus (ker(div) \cap im(curl_N)) \oplus (ker(div) \cap \ker(curl))\\ &= im(grad_D) \oplus im(curl_N) \oplus \mathscr{H}^1(M)\end{aligned}$$

In the last step, we have used $im(curl) \subset ker(div)$.

Decomposition of the Harmonic Vectors The harmonic vector $\mathbf{h}$ can be further decomposed L^2-orthogonally as:

$$\mathbf{h} = \nabla\phi_h + \mathbf{h}_N, \quad \nabla^2\phi_h = 0, \tag{7.21}$$

or

$$\mathbf{h} = \nabla \times \psi_h + \mathbf{h}_D, \quad \nabla \times (\nabla \times \psi_h) = 0, \tag{7.22}$$

Here, $\mathbf{h}_N$ is a harmonic vector satisfying the zero Neumann boundary condition:

$$\mathbf{h}_N \cdot \nu = 0 \text{ on } \partial M, \quad i.e. \quad \mathbf{h}_N \parallel \partial M, \ or\ \mathbb{n}^1(\mathbf{h}_N) = 0, \tag{7.23}$$

and $\mathbf{h}_D$ is a harmonic vector satisfying the zero Dirichlet boundary condition:

$$\mathbf{h}_D \parallel \nu \text{ on } \partial M, \quad i.e. \quad \mathbf{h}_D \perp \partial M, \ or\ \mathbb{t}^1(\mathbf{h}_D) = 0. \tag{7.24}$$

We write this decomposition as

$$\mathscr{H}^1(M) = \left(im(grad) \cap \mathscr{H}^1(M)\right) \oplus \mathscr{H}^1_N(M) \tag{7.25}$$
$$\mathscr{H}^1(M) = \left(im(curl) \cap \mathscr{H}^1(M)\right) \oplus \mathscr{H}^1_D(M) \tag{7.26}$$

Proof. 1. The L^2 orthogonality of the decomposition (7.21) is

$$\int_M \nabla\phi_h \cdot \mathbf{h}_N \, d\mathbf{x} = 0.$$

Taking integration by part and using $\mathbf{h}_N$ being harmonic, we get

$$\int_M \nabla\phi_h \cdot \mathbf{h}_N \, d\mathbf{x} = \int_{\partial M} \phi_h \mathbf{h}_N \cdot \nu \, dS = 0.$$

The Neumann boundary condition (7.23) gives the L^2-orthogonality of $\nabla\phi_h$ and $\mathbf{h}_N$.

2. The L^2-orthogonality of the decomposition (7.22) is

$$\int_M (\nabla \times \psi_h) \cdot \mathbf{h}_D \, d\mathbf{x} = 0.$$

Using Green's theorem, we get

$$\int_M (\nabla \times \psi_h) \cdot \mathbf{h}_D \, d\mathbf{x} = \int_{\partial M} (\psi_h \times \mathbf{h}_D) \cdot \nu \, dS = 0.$$

Thus, the zero Dirichlet boundary condition (7.24) gives the L^2 orthogonality of the decomposition (7.22).

□

Let us summarize the above decomposition as the follows.

$$V = im(grad_D) \oplus im(curl_N) \oplus \left(im(grad) \cap \mathscr{H}^1\right) \oplus \mathscr{H}_N^1 \tag{7.27}$$
$$= im(grad_D) \oplus im(curl_N) \oplus \left(im(curl) \cap \mathscr{H}^1\right) \oplus \mathscr{H}_D^1 \tag{7.28}$$

$$\mathbf{v} = \nabla\varphi + \nabla \times \psi + \nabla\phi_h + \mathbf{h}_N \tag{7.29}$$
$$= \nabla\varphi + \nabla \times \psi + \nabla \times \psi_h + \mathbf{h}_D. \tag{7.30}$$

Harmonic fields and Cohomology

Theorem 7.5. *The spaces of the Dirichlet and Neumann harmonic vector fields are finite dimensional. Indeed,*

1. $\mathscr{H}_N^1 = \{B : M \to \mathbb{R}^3 \text{ harmonic} \mid B \parallel \partial M\} \sim H^1(M)$
2. $\mathscr{H}_D^1 = \{E : M \to \mathbb{R}^3 \text{ harmonic} \mid E \perp \partial M\} \sim H^2(M)$

where $H^k(M)$ is the kth cohomology of M, which is finite dimensional.

Remark

- We interpret E an electric field. ∂M consists of disjoint conductors. $E \perp \partial M$ means that these conductors are perfect conductors. The electric potentials are constants on each conductors. There are finite many such conductors. The number of them minus 1 [1] corresponds to the dimension of $\mathscr{H}_D^1(M)$.

- B is interpreted as a magnetic field. ∂M consists of tubes with constant electric currents. The corresponding B outside these tubes satisfying $B \parallel \partial M$. There are finite many such tubes, which correspond to $\mathscr{H}_N^1(M)$.

Proof. To show these two statement, we regroup the decomposition as

$$V = \underbrace{\underbrace{im(grad_D) \oplus \left(im(grad) \cap \mathscr{H}^1\right)}_{im(grad)} \oplus \mathscr{H}_N^1}_{ker(curl)} \oplus im(curl_D)$$

Thus,

$$\mathscr{H}_N^1(M) \sim ker(curl)/im(grad).$$

The space

$$H^1(M) := ker(curl)/im(grad)$$

is called the first cohomology of M. In the deRham theory, it is equal to a topological quantity: the homology $H_1(M)$.

Similarly, we regroup the decomposition as

$$V = \underbrace{\underbrace{im(curl_N) \oplus \left(im(curl) \cap \mathscr{H}^1\right)}_{im(curl)} \oplus \mathscr{H}_D^1(M)}_{ker(div)} \oplus im(grad_D)$$

We get

$$\mathscr{H}_D^1(M) \sim ker(div)/im(curl) = H^2(M).$$

□

7.2.2 Extract Each Component of the Decomposition

We need to choose proper boundary conditions and gauges to get a unique decomposition.

[1] One can normalize the potential on a specific conductor to be 0.

Solving the scalar potential φ By taking *div* of the decomposition

$$\mathbf{v} = \nabla\varphi + \nabla\times\psi + \mathbf{h}$$

we get the governing equation for φ:

$$\begin{cases} \triangle\varphi = \nabla\cdot\mathbf{v} & \text{in } M \\ \varphi = 0 & \text{on } \partial M. \end{cases} \tag{7.31}$$

It is a standard Poisson problem. It has a unique solution.

Solving the vector potential ψ

1. By taking *curl* of the decomposition

$$\mathbf{v} = \nabla\varphi + \nabla\times\psi + \mathbf{h}$$

we get the governing equation for ψ:

$$\nabla\times(\nabla\times\psi) = \omega, \quad \text{where} \quad \omega = \nabla\times\mathbf{v}, \tag{7.32}$$

with boundary condition:

$$\psi \perp \partial M. \tag{7.33}$$

2. The solution is not unique. Adding any Dirichlet closed vector ξ (i.e. $\nabla\times\xi = 0$ and $\xi \parallel \partial M$, denoted by $ker(curl)\cap ker(\mathbb{t}^2)$) to ψ does not change $\nabla\times\psi$ and $\psi\perp\partial M$.

Note that V can be decomposed orthogonally into

$$V = im(curl)\oplus\left(ker(curl)\cap ker(\mathbb{t}^2)\right),$$

To get a unique solution, we should select

$$\psi \perp ker(curl)\cap ker(\mathbb{t}^2).$$

We also note that

$$ker(curl) = im(curl)\oplus\mathscr{H}^2_D(M).$$

These two lead to

$$\nabla\cdot\psi = 0 \quad \text{in } M \tag{7.34}$$

$$\langle\psi,\chi\rangle = 0, \quad \text{for all } \chi\in\mathscr{H}^2_D(M). \tag{7.35}$$

Adding these two conditions is called fixing a gauge. There are many ways to fix a gauge. The gauge we select is called the Coulomb gauge.

3. The variational approach to (7.32) and (7.34) is

$$\min_{\psi} \int_M \frac{1}{2}\left(|\nabla \times \psi|^2 + |\nabla \cdot \psi|^2\right) - \langle \omega, \psi \rangle \, d\mathbf{x}. \tag{7.36}$$

The admissible ψ satisfies the boundary conditions:

$$\psi \perp \partial M \tag{7.37}$$

$$\nabla \cdot \psi = 0 \text{ on } \partial M, \tag{7.38}$$

and the orthogonal condition:

$$\langle \psi, \chi \rangle = 0 \quad \text{ for all } \chi \in \mathscr{H}_D^2(M). \tag{7.39}$$

Note that the boundary condition (7.38) comes from the null boundary condition in the variation of $\int |\nabla \cdot \psi|^2 \, d\mathbf{x}$:

$$\delta \int_M \frac{1}{2}|\nabla \cdot \psi|^2 \, d\mathbf{x} = \int_M (-\nabla(\nabla \cdot \psi)) \cdot (\delta \psi) \, d\mathbf{x} + \int_{\partial M} (\nabla \cdot \psi) \delta \psi \cdot \nu dS.$$

We should require $\nabla \cdot \psi) = 0$ on ∂M.
Note that the boundary condition (7.37) is

$$\psi_{\parallel} = 0. \tag{7.40}$$

Because of this, the boundary condition (7.38) is equivalent to

$$\partial_\nu \psi_{\perp} = 0. \tag{7.41}$$

Thus, the admissible class for the variational problem is

$\mathscr{A} = \{ \psi : M \to \mathbb{R}^3 |\ \psi$ satisfies (7.40) (7.41) on ∂M and the orthogonal condition (7.39) $\}$

4. One can show that the Euler-Lagrange equation the above variational problem is equivalent to

$$\begin{cases} -\nabla(\nabla \cdot \psi) + \nabla \times (\nabla \times \psi) = \omega & \text{in } M \\ \quad \psi_{\parallel} = 0, \quad \partial_\nu \psi_{\perp} = 0 & \text{on } \partial M \\ \langle \psi, \chi \rangle = 0 \quad \text{for all } \chi \in \mathscr{H}_D^2(M) & \end{cases}$$

The the operator: $-\nabla(\nabla \cdot \psi) + \nabla \times (\nabla \times \psi)$ is called the *Hodge-Laplacian operator*, which has nice property (coerciveness) in the space $\mathscr{A}$. Standard Lax-Milgram Theorem can be applied for existence and uniqueness.

7.2.3 Hodge-Morrey-Friedrichs Decomposition for Differential Forms

Ref.

- This subsection is copied from Albert Chern's Note on Discrete Differential Geometry, Chapter 11, UCSD.
- Günter Schwarz, Hodge Decomposition—A Method for Solving Boundary Value Problems, Lecture Notes in Mathematics, vol. 1607 (1995).

The purpose in this subsection is to orthogonally decompose a k-form ω into

$$\omega = d^{k-1}\alpha + \delta^{k+1}\beta + d^{k-1}\phi + h_N$$
$$\omega = d^{k-1}\alpha + \delta^{k+1}\beta + \delta^{k+1}\psi + h_D,$$

where d and δ are the exterior derivative and codifferential for differential forms. $d\phi$, $\delta\psi$, h_N and h_D are harmonic differential forms. I will explain these notation below. I will also make a correspondence between the notations in differential geometry and those in vector calculus for the case $\dim M = 3$.

1. **Differential forms** Let $\Omega^k(M)$ be the space of differential k-forms on an n-dimensional manifold M.
   - $\Omega^0(M) = \{\phi \in M \to \mathbb{R}\}$, the space of scalar potentials.
   - $\Omega^1(M) = \{\eta = v_1dx^1 + v_2dx^2 + v_3dx^3\}$. This corresponds to the space of vector fields $\{\mathbf{v} : M \to \mathbb{R}^3\}$. We write $\eta^\sharp = \mathbf{v}$.
   - $\Omega^2(M) = \{\sigma = \sigma_1dx^2 \wedge dx^3 + \sigma_2dx^3 \wedge dx^1 + \sigma_3dx^1 \wedge dx^2\}$. This corresponds to the space of fluxes: $\{\mathbf{w} : M \to \mathbb{R}^3\}$. We write
   $$\star\sigma = \sigma_1dx^1 + \sigma_2dx^2 + \sigma_3dx^3, \quad \mathbf{w} = (\star\sigma)^\sharp.$$
   - $\Omega^3(M) = \{m = \rho dx^1 \wedge dx^2 \wedge dx^3\}$. It corresponds to the space of density $\{\rho : M \to \mathbb{R}^3\}$. We write $\star m = \rho$.
2. **Boundary restriction operators** There are two kinds of boundary restriction operators we will use. Below, a vector $\mathbf{v}$ on the boundary, we can decompose it into $\mathbf{v}_{\|}$ and $\mathbf{v}_{\perp}$, the components parallel to the boundary and orthogonal to the boundary, respectively. The differential forms below are in $\Omega^k(M)$.
   - Dirichlet and Neumann boundary restriction:

• $\mathbb{t}^0\phi = \phi\|_{\partial M}$	• $\mathbb{n}^3 m = (\star m)\|_{\partial M}$
• $\mathbb{t}^1\eta = (\eta^\sharp)_{\|}$	• $\mathbb{n}^1\eta = (\star\eta)^\sharp_{\perp}$
• $\mathbb{t}^2\sigma = (\star\sigma)^\sharp_{\perp}$	• $\mathbb{n}^2\sigma = (\star\sigma)^\sharp_{\|}$

- Kernels:

$$\begin{array}{ll} ker(\mathbb{t}^1) = \{\eta | \eta^\sharp \perp \partial M\}, & ker(\mathbb{n}^1) = \{\eta | \eta^\sharp \parallel \partial M\} \\ ker(\mathbb{t}^2) = \{\sigma | \sigma^\sharp \parallel \partial M\}, & ker(\mathbb{n}^2) = \{\sigma | \sigma^\sharp \perp \partial M\} \end{array}$$

- $\Omega_D^k(M) = \{\alpha \in \Omega^k(M) | \mathbb{t}^k \alpha = 0 \text{ on } \partial M\}$
- $\Omega_N^k(M) = \{\alpha \in \Omega^k(M) | \mathbb{n}^k \alpha = 0 \text{ on } \partial M\}$

3. **Differential** d **and Codifferential** δ This is the exterior derivative: $\Omega^k(M) \to \Omega^{k+1}(M)$. The codifferential δ is the dual of d:

$$\Omega^{k-1}(M) \underset{\delta^k}{\overset{d^{k-1}}{\rightleftarrows}} \Omega^k(M) \underset{\delta^{k+1}}{\overset{d^k}{\rightleftarrows}} \Omega^{k+1}(M) \ ,$$

- d exterior derivative, $d : \Omega^k \to \Omega^{k+1}$, We also write it as d^k.
- d_D is the restriction of d on Ω^k with zero Dirichlet boundary condition. That is,

$$d_D^k = d|_{ker(\mathbb{t}^k)}.$$

- d_N is the restriction of d on Ω^k with zero Neumann boundary condition.

$$d_N^k := d|_{ker(\mathbb{n}^k)}.$$

- δ is the co-differential, $\delta : \Omega^{k+1} \to \Omega^k$.
- The correspondence are

$$\begin{array}{ll} \bullet\ d^0 \longleftrightarrow grad & \bullet\ \delta^3 \longleftrightarrow -grad \\ \bullet\ d^1 \longleftrightarrow curl & \bullet\ \delta^2 \longleftrightarrow curl \\ \bullet\ d^2 \longleftrightarrow div & \bullet\ \delta^1 \longleftrightarrow -div \end{array}$$

$$\Omega^0(M) \underset{\delta^1}{\overset{d^0}{\rightleftarrows}} \Omega^1(M) \underset{\delta^2}{\overset{d^1}{\rightleftarrows}} \Omega^2(M) \underset{\delta^3}{\overset{d^2}{\rightleftarrows}} \Omega^3(M) \ ,$$

4. **Green's identity**: for $\alpha \in \Omega^{k-1}$, $\beta \in \Omega^k$, we have

$$\langle\langle d\alpha, \beta \rangle\rangle = \langle\langle \alpha, \delta\beta \rangle\rangle + \int_{\partial M} (\mathbb{t}^{k-1}\alpha) \cdot (\mathbb{n}^k \beta).$$

Here, let $\alpha^\sharp$ denote the vector corresponding to α. The notation

$$\langle\langle d\alpha, \beta \rangle\rangle := \int_M (d\alpha) \wedge (\star\beta) = \int (d\alpha)^\sharp \cdot (\star\beta)^\sharp d\mathbf{x}$$

$$\int_{\partial M} \mathbb{t}\,(\alpha \wedge (\star\beta)) = \int_{\partial M} (\mathbb{t}\alpha) \wedge (\mathbb{t}(\star\beta)) = \int_{\partial M} (\mathbb{t}\alpha) \wedge \star(\mathbb{n}\beta) = \int_{\partial M} (\mathbb{t}\alpha)^\sharp \cdot (\mathbb{n}\beta)^\sharp.$$

5. **Decomposition via d**

$$\begin{aligned}\Omega^k(M) &= im(d_D^{k-1}) \oplus ker(\delta^k) \\ &= im(d^{k-1}) \oplus \Big(ker(\delta^k) \cap ker(\mathtt{n}^k)\Big)\end{aligned}$$

For $k = 1$, this is the decomposition of the vector field space V:

$$\begin{aligned}V &= im(grad_D) \oplus ker(div) \\ &= im(grad) \oplus \big(ker(div) \cap ker(\mathtt{n}^1)\big)\end{aligned}$$

where

$$ker(\mathtt{n}^1) = \{\mathbf{v} : M \to \mathbb{R}^3 | \mathbf{v}_\perp = 0\}$$

6. **Decomposition via δ**

$$\begin{aligned}\Omega^k(M) &= im(\delta_N^{k+1}) \oplus ker(d^k) \\ &= im(\delta^{k+1}) \oplus \Big(ker(d^k) \cap ker(\mathtt{t}^k)\Big)\end{aligned}$$

For $k = 1$, this is the decomposition of the vector field space V:

$$\begin{aligned}V &= im(curl_N) \oplus ker(curl) \\ &= im(curl) \oplus \big(ker(curl) \cap ker(\mathtt{t}^1)\big)\end{aligned}$$

where

$$ker(\mathtt{t}^1) = \{\mathbf{v} : M \to \mathbb{R}^3 | \mathbf{v}_\| = 0\}$$

7. There are many ways to further decompose Ω^k orthogonally:

$$\begin{aligned}\Omega^k(M) &= im(d_D^{k-1}) \oplus ker(\delta^k) \\ &= im(d_D^{k-1}) \oplus im(\delta_N^k) \oplus \underbrace{\Big(ker(d^k) \cap ker(\delta^k)\Big)}_{\mathscr{H}^k \text{ harmonic}}\end{aligned}$$

   - $im(d_D)$: Dirichlet exact, $im(\delta_N)$ Neumann coexact, $\mathscr{H}^k$ harmonic.

8. The harmonic forms can be decomposed into Neumann harmonic and those in $im(d)$, or Dirichlet harmonic and those in $im(\delta)$:

$$\mathscr{H}^k = \Big(im(d) \cap \mathscr{H}^k\Big) \oplus \mathscr{H}_N^k = \Big(im(\delta) \cap \mathscr{H}^k\Big) \oplus \mathscr{H}_D^k \tag{7.42}$$

where

$$\mathscr{H}_N^k(M) := \mathscr{H}^k(M) \cap ker(\mathtt{n}^k), \quad \mathscr{H}_D^k(M) := \mathscr{H}^k(M) \cap ker(\mathtt{t}^k).$$

Its proof is the follows. Using $im(d) \subset ker(d)$ and $(im(d))^\perp = ker(\delta) \cap ker(\mathtt{n})$, we have

$$ker(d) = im(d) \oplus (im(d)^\perp \cap ker(d)) = im(d) \oplus (ker(\delta) \cap ker(\mathtt{n}) \cap ker(d))$$

Thus,

$$\begin{aligned} \mathscr{H}^k &= ker(d) \cap ker(\delta) = [im(d) \oplus (ker(\delta) \cap ker(\mathtt{n}) \cap ker(d))] \cap ker(\delta) \\ &= [im(d) \cap ker(d)] \cap [\mathscr{H}^k \cap ker(\mathtt{n})]. \end{aligned}$$

9. We can regroup them as

$$\Omega^k(M) = \underbrace{im(d_D) \oplus (im(d) \cap \mathscr{H}^k)}_{im(d) \text{ exact}} \oplus \underbrace{\mathscr{H}_N^k \oplus im(\delta_N)}_{ker(\delta) \cap \mathrm{ker}(\mathtt{n}) \text{ Neumann coclosed}}$$

$$\Omega^k(M) = \underbrace{im(\delta_N) \oplus (im(\delta) \cap \mathscr{H}^k)}_{im(\delta) \text{ exact}} \oplus \underbrace{\mathscr{H}_D^k \oplus im(d_D)}_{ker(d) \cap ker(\mathtt{t}) \text{ Dirichlet closed}}$$

or

$$\Omega^k(M) = \underbrace{\underbrace{im(d_D) \oplus (im(d) \cap \mathscr{H}^k)}_{im(d) \text{ exact}} \oplus \mathscr{H}_N^k}_{ker(d) \text{ closed}} \oplus im(\delta_N)$$

$$\Omega^k(M) = \underbrace{\underbrace{im(\delta_N) \oplus (im(\delta) \cap \mathscr{H}^k)}_{im(\delta) \text{ exact}} \oplus \mathscr{H}_D^k}_{ker(\delta) \text{ closed}} \oplus im(d_D)$$

Thus, we get

$$\mathscr{H}_N^k = \frac{ker(d^k)}{im(d^{k-1})} = H^k_{\text{deRham}}(M), \quad \mathscr{H}_D^k = \frac{ker(\delta^k)}{im(\delta^{k+1})} = H^{n-k}_{\text{deRham}}(M).$$

They are called the (absolute) cohomology of M. Note that both $\mathscr{H}_N^k(M)$ and $\mathscr{H}_D^k(M)$ are finite dimensional and

$$\mathscr{H}_N^k \equiv \mathscr{H}_D^{n-k}.$$

7.2.4 Extraction of each component

Let $\omega \in \Omega^k(M)$. We will decompose ω into either one of the following two:

$$\omega = d^{k-1}\alpha + \delta^{k+1}\beta + d\phi + h_N \tag{7.43}$$

$$\omega = d^{k-1}\alpha + \delta^{k+1}\beta + \delta\psi + h_D, \tag{7.44}$$

where

$$\alpha \in \Omega_D^{k-1}(M), \quad \beta \in \Omega_N^{k+1}(M),$$

$$\phi \in \Omega^{k-1} \text{ with } \delta d\phi = 0, \quad (\because d\phi \text{ is harmonic })$$

$$\psi \in \Omega^{k+1} \text{ with } d\delta\psi = 0, \quad (\because \delta\psi \text{ is harmonic })$$

$$h_N \in \mathscr{H}_N^k(M), \quad h_D \in \mathscr{H}_D^k(M).$$

Extraction of α

1. We look for the inverse map of the Dirichlet differential

   $$d_D^{k-1} : \Omega^{k-1}(M) \to \Omega^k(M)$$

   By taking δ^k on (7.43), we get an equation for α:

   $$\begin{cases} \delta^k d^{k-1}\alpha = \delta^k\omega & \text{in } M \\ \hat{t}^{k-1}\alpha = 0 & \text{on } \partial M \end{cases} \tag{7.45}$$

2. This equation is not unique. Adding any Dirichlet closed form ($ker(d) \cap ker(\mathbb{t})$) to α yields the same $d\alpha$. Therefore, we look for the least L^2 norm solution, which gives

   $$\alpha \perp [ker(d) \cap ker(\mathbb{t})] \text{ in } \Omega^{k-1}.$$

   Note that

   $$[ker(d) \cap ker(\mathbb{t})]^\perp = im(\delta).$$

   and

   $$ker(\delta) = im(\delta) \oplus \mathscr{H}_D^{k-1}(M),$$

   we get

   $$\delta\alpha = 0,$$

   $$\text{and} \quad \langle\langle \alpha, \chi \rangle\rangle = 0, \quad \text{for all } \chi \in \mathscr{H}_D^{k-1}(M).$$

3. Solving
$$\begin{cases} \delta d\alpha = \delta\omega & \text{in } M \\ \delta\alpha = 0 & \text{in } M \\ \mathbb{t}^{k-1}\alpha = 0 & \text{on } \partial M \\ \langle\langle \alpha, \chi \rangle\rangle = 0, & \text{for all } \chi \in \mathscr{H}_D^{k-1}(M). \end{cases} \tag{7.46}$$
is equivalent to
$$\begin{cases} -\triangle\,\alpha = \delta\omega & \text{in } M \\ \mathbb{t}\alpha = 0, \quad \mathbb{t}(\delta\alpha) = 0 & \text{on } \partial M \\ \langle\langle \alpha, \chi \rangle\rangle = 0, & \text{for all } \chi \in \mathscr{H}_D^{k-1}(M) \end{cases} \tag{7.47}$$
where $-\triangle := \delta d + d\delta$.

4. We denote $\alpha = d_D^+(\omega)$, the pseudo inverse of d_D. That is,
$$d_D d_D^+ = id_{\Omega^k}, \quad d_D^+ d_D \text{ is a projection to } im(d_D^+).$$
The image and kernel of d_D^+ are
$$im(d_D^+) = im(\delta) \cap ker(\mathbb{t}), \quad ker(d_D^+) = ker(\delta).$$
The space $im(d_D^+)$ is not closed. Indeed,
$$(im(d_D^+))^\perp = ker(d_D) = ker(d) \cap ker(\mathbb{t}),$$
$$\overline{im(d_D^+)} = (im(d_D^+))^{\perp\perp} = (ker(d) \cap ker(\mathbb{t}))^\perp = im(\delta).$$
We have
$$\frac{ker(\delta)}{im(\delta)} = \frac{ker(\delta)}{im(\delta) \cap ker(\mathbb{t})} = \frac{ker(d_D^+)}{im(d_D^+)} = \frac{ker(d_D^+)}{\overline{im(d_D^+)}}$$

Extraction of β

1. We look for the pseudo inverse of δ_N. By taking d on both sides of (7.43), we get that β satisfies
$$d\delta\beta = d\omega, \quad \beta \in ker(\mathbb{n}).$$

2. The solution is not unique because adding any Neumann coclosed $(k+1)$-form to β results in the same $\delta\beta$. Thus, we choose $\beta \in (ker(\delta) \cap ker(\mathbb{n}))^\perp$. This is the Coulomb gauge. Note that
$$(ker(\delta) \cap ker(\mathbb{n}))^\perp = im(d) = \frac{ker(d)}{H_N^{k+1}(M)}$$

Thus,

$$\begin{cases} d\delta\beta = d\omega \\ \mathbb{n}\beta|_{\partial M} = 0 \\ \beta \in im(d) \end{cases} \quad \Leftrightarrow \quad \begin{cases} d\delta\beta = d\omega \\ d\beta = 0 \\ \beta \perp H_N^{k+1}(M) \\ \mathbb{n}\beta|_{\partial M} = 0 \end{cases}$$

3. This is equivalent to the following Poisson problem:

$$\begin{cases} -\triangle\beta = d\omega & \text{in } M \\ \mathbb{n}\beta = 0 & \text{on } \partial M \\ \mathbb{n}d\beta = 0 & \text{on } \partial M \\ \langle\langle\beta,\chi\rangle\rangle = 0 & \text{for all } \chi \in H_N^{k+1}(M). \end{cases}$$

4. We denote the operator $\omega \mapsto \beta$ by δ_N^+. We have

$$\delta_N\delta_N^+ = id_{\Omega^{k+1}(M)}, \qquad \delta_N^+\delta_N : \text{ projection operator onto } im(\delta_N^+).$$

$$im(\delta_N^+) = im(d) \cap ker(\mathbb{n}), \quad ker(\delta_N^+) = ker(d).$$

7.3 Flow Field Decomposition

7.3.1 Velocity Field Decomposition

7.3.2 Force Field Decomposition

Ref.

- Force/Moment Partition Method
- Force/Moment Partition in Experiment

Consider the potential Φ_i, $i = 1,2$:

$$\triangle\Phi_i = 0 \text{ in } \partial\Omega$$
$$\mathbf{n}\cdot\nabla\Phi_i = \begin{cases} n_i & \text{on body} \\ 0 & \text{elsewhere} \end{cases}$$

The projections of $\nabla\Phi_1$ gives *drag*, $\nabla\Phi_2$ give *lift*:

$$\int_\Omega \nabla p\cdot\nabla\Phi_i = \int_\Omega \left(-\rho\mathbf{v}_t - \rho\mathbf{v}\cdot\nabla\mathbf{v} + \mu\nabla^2\mathbf{v}\right)\cdot\nabla\Phi_i\,d\mathbf{x}.$$

7.4 2D Potential Flows

References

- Graebel, Advanced Fluid Mechanics

1. A flow is called a potential flow if there exists a scalar function φ such that $\mathbf{v} = \nabla\varphi$. The function φ is called the *velocity potential*.

2. If a flow is irrotational (i.e., $\nabla \times \mathbf{v} = 0$) and the domain is *simply connected*, then we can find a scalar function φ such that

$$\mathbf{v} = \nabla\varphi$$

3. If, in addition, the flow is *incompressible*, i.e.,

$$\nabla \cdot \mathbf{v} = 0,$$

then we have

$$\triangle\varphi = 0. \tag{7.48}$$

On the boundary, we should apply slip boundary condition, i.e.

$$\nabla\varphi \cdot \nu = 0.$$

4. In this case, the *potential theory* can be adopted. In particular, complex variable methods can be used for 2D potential flows.

7.4.1 Examples of 2D Potential Flows

Here are examples of 2D potential flows along with their mathematical formulations using complex potential, where the complex potential w is related to the velocity potential φ by $w = \varphi + \psi$, where ψ is the stream function.

1. **Uniform Flow:** Constant velocity U in one direction, representing a stream of fluid with uniform flow. $w = Ue^{i\theta}$.

2. **Source Flow:** Radial flow outward from a point source, representing fluid emanating from a single point.

$$w = m \ln z$$

m is the source strength, $z = x + iy$ represents the coordinate.

3. **Sink Flow:** Radial flow towards a point sink, representing fluid converging towards a single point.
$$w = -m \ln z.$$

4. **Dipole Flow:**

5. **Doublet Flow:** Combination of a source and a sink, resulting in a dipole-like flow pattern.
$$w = \frac{m}{z}.$$

6. **Jets**

7. **Potential flow around a circular cylinder**: Uniform Flow + Doublet.

8. See more pictures on websites: Examples of 2D Potential Flows

7.4.2 Axisymmetric Potential Flows

In three-dimensional potential flows, the complex potential approach is extended to include axial symmetry. Here are examples of 3D potential flows along with their mathematical formulations using cylindrical coordinates:

1. **Axisymmetric Source:** Radial flow outward in three dimensions from an axisymmetric source.
$$w = \frac{m}{2\pi} \ln r + mz.$$
Here, r is the radial coordinate, and z is the axial coordinate.

2. **Axisymmetric Sink:** Radial flow towards an axisymmetric sink.
$$w = -\frac{m}{2\pi} \ln r - mz.$$

3. **Axisymmetric Doublet:** Combination of an axisymmetric source and sink, creating an axisymmetric dipole.
$$w = -\frac{m}{2\pi} \frac{z}{r}.$$

4. **Helical Flow:** Combination of axial and azimuthal flows, resulting in a helical flow pattern.
$$w = Ue^{i\theta} + \frac{m}{2\pi} \ln r + im\theta + mz.$$
Here, U is the axial velocity, m the azimuthal circulation, r radial coordinate, θ the azimuthal angle, z the axial coordinate.

5. **Dipole in 3D:** Three-dimensional combination of a source and sink, producing a dipole flow.

$$w = -\frac{m}{z}.$$

m is the dipole strength.

Here are ChatGPT's answer to the examples of axisymmetric potential flows.
ChatGPT: Axisymmetric potential flows are those where the flow variables (velocity, pressure, etc.) are independent of the azimuthal angle (θ), meaning that the flow is symmetric around an axis of rotation. Here are a few examples of axisymmetric potential flows:

Flow around a Sphere: In this case, the flow variables (velocity, pressure, etc.) remain the same as we rotate around the axis passing through the center of the sphere. This symmetry is due to the geometric symmetry of the sphere.

Flow past a Blunt Body: When a fluid flows past a blunt body, such as a circular cylinder with a rounded nose, the flow can be axisymmetric if the Reynolds number is low and turbulence effects are negligible. The flow variables exhibit symmetry around the axis of the cylinder.

Flow through a Pipe: In the case of laminar flow through a straight pipe, the flow can be treated as axisymmetric. This is because the flow velocity and pressure distributions are uniform along the cross-section of the pipe, and they do not vary with the azimuthal angle.

Flow past a Spheroid: A spheroid is a three-dimensional shape that is formed by rotating an ellipse about one of its principal axes. When a fluid flows past a spheroid with its symmetry axis aligned with the flow direction, the resulting flow can be axisymmetric.

Flow around a Cone: In certain conditions, such as low Reynolds numbers or idealized flow, the flow around a cone can be considered axisymmetric. This is particularly true for symmetric cones where the flow variables remain invariant as we rotate around the axis of symmetry.

In each of these examples, the flow variables can be described using cylindrical coordinates (r, θ, z), and the governing equations, such as the Laplace equation for potential flow, can be simplified due to the axisymmetric nature of the flow. These examples find applications in various fields such as aerodynamics, fluid mechanics, and engineering. These formulations are based on cylindrical coordinates and the complex potential approach extended to three dimensions. They describe various types of 3D potential flows, including source, sink, doublet, helical flow, dipole, and flow past a sphere.

7.5 Incompressible Irrotational Flows in 3D

The velocity field of incompressible and irrotational flows are harmonic. It must be steady. The governing equation is

$$\begin{cases} \nabla \times \mathbf{v} = 0 & \text{in } M \\ \nabla \cdot \mathbf{v} = 0 & \text{in } M \\ \mathbf{v} \cdot \nu = 0 & \text{on } \partial M. \end{cases} \tag{7.49}$$

7.6 Compressible Irrotational Flows

7.6.1 Compressible Potential Flows

Potential flows are those flows whose velocity is determined by a potential function φ:

$$\mathbf{v} = \nabla \varphi.$$

For irrotational flows in simply connected domain, such potential function exists.

1. With the assumption $\mathbf{v} = \nabla \varphi$, we have to abandon the energy equation. Thus, the governing equations for compressible potential flow are the continuity equation, the momentum equation, plus $\mathbf{v} = \nabla \varphi$. The pressure p is obtained from the Bernoulli principle.

   The unknowns are (ρ, φ).

7.7 Incompressible Rotational flows

7.7.1 Examples of incompressible rotational flows

2D Cases Here is a link for 2D incompressible inviscid flow.

1. **Single Point Vortex Flow:** Circulation around a point without a radial flow, creating a vortex.

   $$w = \frac{\Gamma}{2\pi} \ln z.$$

   Γ is the vortex strength.

2. **Point vortex Dipole**

3. **Lamb-Chaplygin Dipole**

4. **Dynamics of point vortices**

5. **Flow around a Circular Cylinder:** Flow around a circular cylinder, producing a combination of source and sink flows along with a vortex.

$$w = Ue^{i\theta} + \frac{K}{z}.$$

where U is the uniform velocity, K the doublet strength, $z = re^{i\theta}$ the complex position.

6. **Flow around the Joukowski Airfoil**

7. **von Kármán Vortex Street**

8. **Vortex Patches**

9. **Vortex Sheet**

3D Cases

1. **Flow past a Sphere:** Flow around a sphere exhibits a combination of radial and circumferential flow.

$$w = U\left(\frac{R^2}{z} + z\right) + iU\left(R^2 + z^2\right)\cos\theta.$$

Here, U is the uniform velocity, R is the sphere radius, z is the axial coordinate, and θ is the polar angle.

2. **Vortex filament and binormal equation**

3. **Helical Vertex**

4. **Vortex ring**:

   - Solitary waves on a vortex ring.
   - Leap-flog motion of a pair of vortex rings,
   - Impact of two vortex rings.

5. **Vortex reconnection**

6. **Vortex sheet**

7.8 One Dimensional Compressible Flows

References

- Courant and Friedrichs, Supersonic Flow and Shock Wave.

7.8.1 Riemann problems for hyperbolic conservation laws

Hyperbolicity We consider the following systems of PDEs:

$$u_t + f(u)_x = 0, \tag{7.50}$$

$$u = \begin{bmatrix} u_1 \\ u_2 \\ \vdots \\ u_n \end{bmatrix}, \quad f : \mathbb{R}^n \to \mathbb{R}^n.$$

The system (7.50) is called *hyperbolic* if the $n \times n$ matrix $f'(u)$ can be diagonalized with real eigenvalues $\lambda_1(u) \le \lambda_2(u) \le \cdots \le \lambda_n(u)$ for all u under consideration. The system is called strictly hyperbolic if $\lambda_1(u) < \lambda_2(u) < \cdots < \lambda_n(u)$ for all u. Let us denote corresponding left/right eigenvectors by $\ell_i(u)/r_i(u)$, respectively. Let us normalize them by requiring

$$\|r_i(u)\| \equiv 1, \quad \ell_i(u) \cdot r_j(u) \equiv \delta_{ij}.$$

Self-similar solutions It is important to notice that the system is Galilean invariant, meaning that the equation is unchanged under the transformation:

$$t \to \lambda t, \;\; x \to \lambda x, \qquad \forall \lambda > 0.$$

This suggests that we can look for special solutions of the form $u(\frac{x}{t})$. Such a solution is called a self-similar solution. Suppose $u(\frac{x}{t})$ is such a solution. Let us plug it into (7.50) and yield

$$u' \cdot (-\frac{x}{t^2}) + f'(u)u' \cdot \frac{1}{t} = 0$$
$$\Longrightarrow \quad f'(u)u' = \frac{x}{t}u'.$$

This means that there exists a field i such that $u' \parallel r_i(u)$ and $\frac{x}{t} = \lambda_i(u(\frac{x}{t}))$. Thus, to construct such self-similar solution, we first construct the integral curve of $r_i(u)$. Let $R_i(u_0, s)$ be the integral curve of $r_i(u)$ passing through u_0 parameterized by its arc length. That is

$$\frac{d}{ds} R_i(u_0, s) = r_i(R_i(u_0, s)), \quad R_i(u_0, 0) = u_0.$$

Along R_i, the speed λ_i has the variation:

$$\frac{d}{ds}\lambda_i(R_i(u_0,s)) = \nabla\lambda_i \cdot R_i' = \nabla\lambda_i \cdot r_i.$$

We have the following definitions.

Definition 7.3. *The i-th characteristic field is called*

- *genuinely nonlinear if* $\nabla\lambda_i(u)\cdot r_i(u) \neq 0\ \forall u$*;*
- *linearly degenerate if* $\nabla\lambda_i(u)\cdot r_i(u) \equiv 0\ \forall u$*;*
- *non-genuinely nonlinear if* $\nabla\lambda_i(u)\cdot r_i(u) = 0$ *on isolated hypersurface in* $\mathbb{R}^n$*.*

For scalar conservation laws, the genuine nonlinearity is equivalent to the convexity (or concavity) of the flux f, linear degeneracy is $f(u) = au$, while non-genuine nonlinearity is non-convexity of f.

Rarefaction Waves When the i-th field is genuinely nonlinear, we define the rarefaction curve in the state space as

$$R_i^+(u_0) = \{u \in R_i(u_0) |\ \lambda_i(u) \geq \lambda_i(u_0)\}.$$

Now suppose $u_1 \in R_i^+(u_0)$, we construct the *centered rarefaction wave*, denoted by (u_0,u_1), as below:

$$(u_0,u_1)\left(\frac{x}{t}\right) = \begin{cases} u_0 & \text{if } \frac{x}{t} \leq \lambda_i(u_0) \\ u_1 & \text{if } \frac{x}{t} \geq \lambda_i(u_1) \\ u & \text{if } \lambda_i(u_0) \leq \frac{x}{t} \leq \lambda_i(u_1) \text{ and } \lambda_i(u) = \frac{x}{t}. \end{cases}$$

It is easy to check that this is a solution. We call (u_0,u_1) an *i-rarefaction wave*.

Shock Waves The shock wave is expressed as:

$$u\left(\frac{x}{t}\right) = \begin{cases} u_0 & \text{for } \frac{x}{t} < \sigma \\ u_1 & \text{for } \frac{x}{t} > \sigma, \end{cases}$$

where σ is the shock speed. Here, (u_0,u_1,σ) need to satisfy the jump condition:

$$f(u_1) - f(u_0) = \sigma(u_1 - u_0). \tag{7.51}$$

Lemma 7.6. *(Local structure of shock curves)*

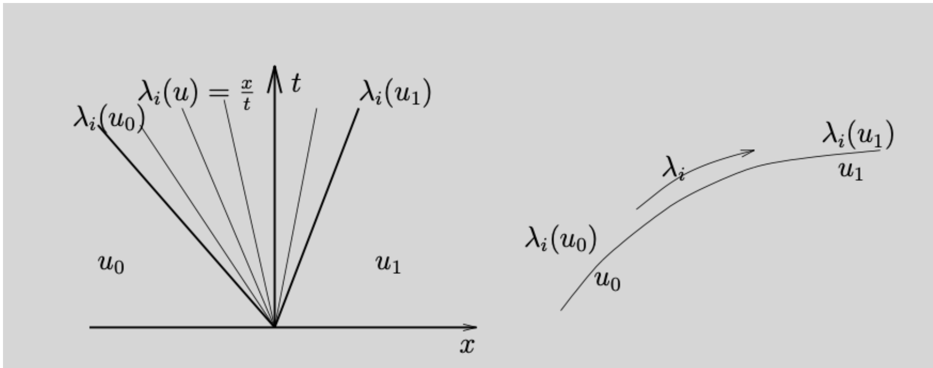


Figure 7.2: (Left) The rarefaction wave. (Right) The integral curve of $u' = r_i(u)$.

1. *The solution of (7.51) for (u,σ) consists of n algebraic curves passing through u_0 locally, named them by $S_i(u_0), i = 1,\cdots,n$.*

2. *$S_i(u_0)$ is tangent to $R_i(u_0)$ up to second order. i.e., $S_i^{(k)}(u_0) = R_i^{(k)}(u_0), k = 0,1,2.$ Here the derivatives are arclength derivatives.*

3. *$\sigma_i(u_0,u) \to \lambda_i(u_0)$ as $u \to u_0$, and $\sigma_i'(u_0,u_0) = \frac{1}{2}\lambda_i'(u_0)$*

Proof. 1. Let $S(u_0) = \{u | f(u) - f(u_0) = \sigma(u-u_0) \text{ for some } \sigma \in \mathbb{R}\}$. We claim that $S(u_0) = \bigcup_{i=1}^{n} S_i(u_0)$, where each $S_i(u_0)$ is a smooth curve passing through u_0 with tangent $r_i(u_0)$ at u_0. When u is on $S(u_0)$, rewrite the jump condition as

$$\begin{aligned} f(u) - f(u_0) &= \left[\int_0^1 f'(u_0 + t(u-u_0)\,dt\right](u-u_0) \\ &= \tilde{A}(u_0,u)(u-u_0) \end{aligned}$$

Thus,

$$\therefore \quad u \in S(u_0) \Longleftrightarrow (u-u_0) \text{ is an eigenvector of } \tilde{A}(u_0,u).$$

Assuming $A(u) = f'(u)$ has real and distinct eigenvalues $\lambda_1(u) < \cdots < \lambda_n(u)$, then, from perturbation theory (or the implicit function theorem), for $u \sim u_0$, $\tilde{A}(u_0,u)$ also has real and distinct eigenvalues $\tilde{\lambda}_1(u_0,u) < \cdots < \tilde{\lambda}_n(u_0,u)$ with left/right eigenvectors $\tilde{\ell}_i(u_0,u)$ and $\tilde{r}_i(u_0,u)$, respectively, and they converge to $\lambda_i(u_0), \ell_i(u_0), r_i(u_0)$ as $u \to u_0$, respectively. We normalize theses eigenvectors by

$$\|\tilde{r}_i\| = 1, \quad \tilde{\ell}_i \tilde{r}_j = \delta_{ij}.$$

The vector which is parallel to $\tilde{r}_i$ can be determined by the $n-1$ equations:

$$\tilde{\ell}_k(u_0,u)(u-u_0) = 0, \quad k = 1,\cdots,n,\ k \neq i,$$

Thus, we define

$$S_i(u_0) = \{u \mid \tilde{\ell}_k(u_0,u)(u-u_0) = 0,\ k = 1,\cdots,n,\ k \neq i\}.$$

We claim that this is a smooth curve passing through u_0. First, we choose the coordinate frame $r_1(u_0),\cdots,r_n(u_0)$. Differential the equation $\tilde{\ell}_k(u_0,u)(u-u_0) = 0$ in $r_j(u_0)$ direction to get

$$\left.\frac{\partial}{\partial r_j}\right|_{u=u_0} (\tilde{\ell}_k(u_0,u)(u-u_0)) = \tilde{\ell}_k(u_0,u_0)\cdot r_j(u_0) = \delta_{jk}.$$

Thus, $(\frac{\partial \tilde{\ell}_k}{\partial r_j})$ is a full rank matrix. By the implicit function theorem, $S_i(u_0)$ is a smooth curve passing through u_0. Since any $u \in S(u_0)$ must satisfy $\tilde{\ell}_k(u_0,u)(u-u_0) = 0$ for $k = 1,\ldots,n,\ k \neq i$ for some i. This means that $u \in S_i(u_0)$ for some i. Hence, $S(u_0) = \bigcup_{i=1}^{n} S_i(u_0)$.

2. First, clearly we have $R_i(u_0) = u_0 = S_i(u_0)$ from construction. Next, we compute first and second derivatives of S_i at u_0. We take arclength derivative along $S_i(u_0)$:

$$f(u) - f(u_0) = \sigma_i(u_0,u)(u-u_0) \quad \forall u \in S_i(u_0)$$

to get

$$f'(u)u' = \sigma_i'(u-u_0) + \sigma_i u' \text{ and } u' = S_i'.$$

When $u \to u_0$

$$\begin{aligned} & f'(u_0)S_i'(u_0) = \sigma_i(u_0,u_0)S_i'(u_0) \\ \Longrightarrow \qquad & S_i'(u_0) = r_i(u_0) \text{ and } \sigma_i(u_0,u_0) = \lambda_i(u_0). \end{aligned}$$

Now we compute the second derivative of the jump condition:

$$(f''(u)u',u') + f'(u)u'' = \sigma_i''(u-u_0) + 2\sigma_i'\cdot u' + \sigma_i u''.$$

At $u = u_0$, $u' = S_i'(u_0) = R_i'(u_0) = r_i(u_0)$ and $u'' = S_i''(u_0)$. These imply

$$(f''r_i,r_i) + f'S_i'' = 2\sigma_i' r_i + \sigma_i S_i''. \tag{7.52}$$

On the other hand, we differentiate $f'(u)r_i(u) = \lambda_i(u)r_i(u)$ along $R_i(u_0)$, then evaluate at $u = u_0$ to get

$$(f''r_i,r_i) + f'(\nabla r_i\cdot r_i) = \lambda_i' r_i + \lambda_i \nabla r_i\cdot r_i, \tag{7.53}$$

where $\nabla r_i \cdot r_i = R_i''$. Comparing (7.52) and (7.53), we get that

$$(f' - \lambda_i)(S_i'' - R_i'') = (2\sigma_i' - \lambda_i')r_i \text{ and } 2\sigma_i' = \lambda_i' \text{ at } u_0.$$

Since $\{r_k(u_0)\}$ are independent, we can express $S_i'' - R_i'' = \sum_k \alpha_k r_k(u_0)$. Plug this into the above equation, we get

$$\sum_{k \neq i} (\lambda_k - \lambda_i)\alpha_k r_k = (2\sigma_i' - \lambda_i')r_i.$$

Since $\lambda_k \neq \lambda_i$ for $k \neq i$ and $\{r_k\}$ are independent, we get

$$\alpha_k = 0 \ \forall k \neq i \text{ and } \lambda_i' = 2\sigma_i' \text{ at } u_0.$$

Hence $(R'' - S'') \parallel r_i$ at u_0. To show that $R_i'' = S_i''$ at u_0, we first notice that $(R_i'', R_i') = 0$ and $(S_i'', S_i') = 0$ which can be derived by differentiate the equations $(R_i', R_i') = 1, (S_i', S_i') = 1$. From these and $S_i'(u_0) = R_i'(u_0) = r_i(u_0)$, we get

$$(R_i'' - S_i'') \perp r_i \text{ at } u_0.$$

Hence $R_i'' = S_i''$ at u_0.

□

Let $S_i^-(u_0) = \{u \in S_i(u_0) | \lambda_i(u) \leq \lambda_i(u_0)\}$. If $u_1 \in S-_i(u_0)$, define

$$(u_0, u_1) = \begin{cases} u_0 & \text{for } \frac{x}{t} < \sigma_i(u_0, u_1) \\ u_1 & \text{for } \frac{x}{t} > \sigma_i(u_0, u_1) \end{cases}$$

(u_0, u_1) is a weak solution. Let $\mathfrak{S}_i^-(u_0) = \{u \in \mathfrak{S}_i(u_0) | \lambda_i(u) \leq \lambda_i(u_0)\}$.
If $u_1 \in \mathfrak{S}_i^-(u_0)$, define

$$(u_0, u_1) = \begin{cases} u_0 & \text{for } \frac{x}{t} < \sigma_i(u_0, u_1) \\ u_1 & \text{for } \frac{x}{t} > \sigma_i(u_0, u_1) \end{cases}$$

u_0 $\mathfrak{R}_i^+$

$\mathfrak{R}_i$

$\mathfrak{S}_i$

$\mathfrak{S}_i^-$

(u_0, u_1) is a weak solution.
We propose the following entropy condition: (Lax entropy condition)

$$\lambda_i(u_0) > \sigma_i(u_0, u_1) > \lambda_i(u_1). \tag{7.54}$$

If the i-th characteristic field is genuinely nonlinear, then for $u_1 \in S_i^-(u_0)$, and $u_1 \sim u_0$, (7.54) is always valid. This follows easily from $\lambda_i = 2\sigma_i'$ and $\sigma_i(u_0, u_0) = \lambda_i(u_0)$. For $u_1 \in S_i^-(u_0)$, we call the solution (u_0, u_1) *i-shock*.

Contact Discontinuity (Linear Wave) If $\nabla\lambda_i(u)\cdot r_i(u)\equiv 0$, we call the i-th characteristic field *linearly degenerate (ℓ. dg.)*. In the case of scalar equation, this correspond $f''=0$. We claim

$$R_i(u_0)=S_i(u_0) \text{ and } \sigma_i(u_0,u)=\lambda_i(u_0) \text{ for } u\in S_i(u_0) \text{ or } R_i(u_0).$$

Indeed, along $R_i(u_0)$, we have

$$f'(u)u'=\lambda_i(u)u'.$$

and $\lambda_i(u)$ is a constant $\lambda_i(u_0)$ from the linear degeneracy. We integrate the above equation from u_0 to u along $R_i(u_0)$, we get

$$f(u)-f(u_0)=\lambda_i(u_0)(u-u_0).$$

This gives the shock condition. Thus, $S_i(u_0)\equiv R_i(u_0)$ and $\sigma(u,u_0)\equiv\lambda_i(u_0)$.

Homeworks

$$(u_0,u_1)=\begin{cases} u_0 & \frac{x}{t}<\sigma_i(u_0,u_1) \\ u_1 & \frac{x}{t}>\sigma_i(u_0,u_1) \end{cases}$$

Riemann Problems Let $T_i(u_0)=R_i^+(u_0)\cup S_i^-(u_0)$ be called the *i-th wave curve*. For $u_1\in T_i(u_0),(u_0,u_1)$ is either a rarefaction wave, a shock, or a contact discontinuity.

Theorem 7.6. *(Lax) For strictly hyperbolic system (7.50), if each field is either genuinely nonlinear or linear degenerate, then for $u_L\sim u_R$, the Riemann problem with two end states (u_l,u_R) has unique self-similar solution which consists of n elementary waves. Namely, there exist $u_0=u_L,\cdots,u_n=u_R$ such that (u_{i-1},u_i) is an i-wave.*

Proof. Given $(\alpha_1,\cdots,\alpha_n)\in\mathbb{R}^n$, define u_i inductively $u_i\in T_i(u_{i-1})$, and the arclength of (u_{i-1},u_i) on $T_i=\alpha_i$.

$$u_i=f(u_0,\alpha_1,\cdots,\alpha_i)$$

We want to find $\alpha_1,\cdots,\alpha_n$ such that

$$u_R=f(u_L,\alpha_1,\cdots,\alpha_n).$$

First $u_L=f(u_L,0,\cdots,0)$, as $u_R=u_L,(\alpha_1,\cdots,\alpha_n)=(0,\cdots,0)$ is a solution. When $u_R\sim u_L$ and $\{r_i(u_0)\}$ are independent,

$$\left.\frac{\partial}{\partial\alpha_i}\right|_{\alpha=0} f(u_L,0,\cdots,0)=r_i(u_0) \text{ and } f\in C^2$$

By Inverse function theorem, for $u_R\sim u_L$, there exists unique α such that $u_R=f(u_L,\alpha)$. Uniqueness leaves as an exercise. $\square$

7.8.2 Riemann Problems for Gas Dynamics

Reference This subsection mainly comes from Courant and Friedrichs' book: Supersonic Flow and Shock Waves.

Hyperbolicity of the equations of gas dynamics We use (ρ, u, S) as our unknown variables. The equations of gas dynamics can be expressed as

$$\begin{bmatrix}\rho\\ u\\ S\end{bmatrix}_t + \begin{bmatrix} u & \rho & 0\\ \frac{c^2}{\rho} & u & \frac{P_S}{\rho}\\ 0 & 0 & u\end{bmatrix}\begin{bmatrix}\rho\\ u\\ S\end{bmatrix}_x = 0$$

Here, $P(\rho,S) = A(S)\rho^\gamma$, $\gamma > 1$, and $c^2 = \frac{\partial P}{\partial \rho}\Big|_S$. This system is *hyperbolic*. The eigenvalues and eigenvectors are

$$\begin{aligned}
&\lambda_1 = u - c, \quad \lambda_2 = u, \quad \lambda_3 = u + c,\\
&r_1 = \begin{bmatrix}\rho\\ -c\\ 0\end{bmatrix}, \quad r_2 = \begin{bmatrix}-P_S\\ 0\\ c^2\end{bmatrix}, \quad r_3 = \begin{bmatrix}\rho\\ c\\ 0\end{bmatrix},\\
&\ell_1 = [c, -\rho, \frac{P_S}{c}], \quad \ell_2 = [0,0,1], \quad \ell_3 = [c, \rho, \frac{P_S}{c}].
\end{aligned}$$

Note that

$$\begin{aligned}
\nabla\lambda_1 \cdot r_1 &= \frac{1}{c}(\frac{1}{2}\rho P_{\rho\rho} + c^2) > 0,\\
\nabla\lambda_3 \cdot r_3 &= \frac{1}{c}(\frac{1}{2}\rho P_{\rho\rho} + c^2) > 0,\\
\nabla\lambda_2 \cdot r_2 &\equiv 0.
\end{aligned}$$

These show that the 1st and 3rd characteristic fields are genuinely nonlinear, while the 2nd is linearly degenerate.

Rarefaction curves The rarefaction curve $\mathfrak{R}_1$ is the integral curve of the vector field r_1, that is, $(d\rho, du, dS)^T \parallel r_1$. Note that $\ell_2 r_1 = 0$, $\ell_3 r_1 = 0$. Thus, the differential equations for $\mathfrak{R}_1$ are govern by

$$\begin{cases} (d\rho, du, dS)\cdot(0,0,1) = 0\\ (d\rho, du, dS)\cdot(c, \rho, \frac{P_S}{c}) = 0.\end{cases}$$

$$\Longrightarrow \quad \begin{cases} dS = 0\\ c\,d\rho + \rho\,du + \frac{P_S}{c}dS = 0\end{cases}$$

Thus, $\mathfrak{R}_1$ can be expressed as

$$\begin{cases} dS = 0 \\ \frac{c}{\rho} d\rho + du = 0 \end{cases}$$

Similarly, $\mathfrak{R}_3$ is expressed as

$$\begin{cases} dS = 0 \\ \frac{c}{\rho} d\rho - du = 0. \end{cases}$$

Since $S = S_0$, a constant, on $\mathfrak{R}_1$ and $\mathfrak{R}_3$, it is convenient to project the rarefaction curves $\mathfrak{R}_1$ and $\mathfrak{R}_3$ onto the u-P plane. The rarefaction curves $\mathfrak{R}_1$ and $\mathfrak{R}_3$ are given by

$$\begin{cases} \mathfrak{R}_1 : u - u_0 = -\ell + \ell_0 \\ \mathfrak{R}_3 : u - u_0 = \ell - \ell_0. \end{cases}$$

where

$$\ell(P,S) := \int \frac{c(\rho,S)}{\rho}\, d\rho.$$

Below, we express ℓ in terms of (P,S). From $P = A(S)\rho^\gamma$, $c = \sqrt{P_\rho} = \sqrt{A(S)\gamma\rho^{\gamma-1}}$, we obtain

$$\ell := \int \frac{c}{\rho}\, d\rho = \sqrt{\gamma A(S)}\frac{2}{\gamma-1}\rho^{\frac{\gamma-1}{2}} = \frac{2}{\gamma-1}\sqrt{\frac{\gamma P}{\rho}}.$$

Note that

$$P\rho^{-\gamma} = A(S) = A(S_0) = P_0\rho_0^{-\gamma}.$$

We can express ρ in terms of P, P_0, ρ_0:

$$\rho^{-1} = \rho_0^{-1}\left(\frac{P_0}{P}\right)^{1/\gamma}.$$

Hence,

$$\begin{aligned} \ell - \ell_0 &= \frac{2}{\gamma-1}\left(\sqrt{\gamma P\left(\frac{P_0}{P}\right)^{1/\gamma}\rho_0^{-1}} - \sqrt{\frac{\gamma P_0}{\rho_0}}\right) \\ &= \frac{2\sqrt{\gamma}}{\gamma-1}\rho_0^{-\frac{1}{2}}P_0^{\frac{1}{2\gamma}}\left(P^{\frac{\gamma-1}{2\gamma}} - P_0^{\frac{\gamma-1}{2\gamma}}\right) := \psi_0(P). \end{aligned}$$

$$\begin{aligned} \therefore\quad \mathfrak{R}_1 :&\quad u = u_0 - \psi_0(P) \\ \mathfrak{R}_3 :&\quad u = u_0 + \psi_0(P). \end{aligned}$$

The contact discontinuity On $\mathfrak{R}_2$, $(d\rho, du, dS) \perp \ell_1, \ell_3$, which gives

$$\Longrightarrow \quad \begin{cases} c^2 d\rho + c\rho du + P_S dS = 0 \\ c^2 d\rho - c\rho du + P_S dS = 0 \end{cases}$$
$$\Longrightarrow \quad \begin{cases} dP + c\rho du = 0 \\ dP - c\rho du = 0 \end{cases}$$

Thus, $\mathfrak{R}_2$ is given by

$$\begin{cases} dP = 0 \\ du = 0 \end{cases}$$

For any $(u_1, P_1) \in \mathfrak{R}_2$, we have $u_1 = u_0$, $P_1 = P_0$, and $((u_0, P_0, S_0), (u_0, P_0, S_1))$ constitutes a contact discontinuity.

Note that $\mathfrak{R}_2 = \mathfrak{S}_2$ because the 2-characteristic field is linearly degenerate.

Shock curves Let us consider a 1-shock (resp. 3-shock) with left state (resp. right state) $(0) := (\rho_0, u_0, P_0)$ and shock speed σ. We want to find the shock curves $\mathfrak{S}_1$ (resp. $\mathfrak{S}_3$) passing through the state (0). Indeed, we want to find the projection of $\mathfrak{S}_1$ (resp. $\mathfrak{S}_3$) on the u-P plane.

Let $v := u - \sigma$. The jump conditions are

$$\begin{cases} [\rho v] = 0 \\ [\rho v^2 + P] = 0 \\ [(\frac{1}{2}\rho v^2 + \rho e + P)v] = 0. \end{cases}$$

Let

$$m := \rho v.$$

From the first jump condition, we have

$$m = m_0.$$

The second jump condition is

$$\rho_0 v_0^2 + P_0 = \rho v^2 + P \quad \Longrightarrow \quad m v_0 + P_0 = m v + P.$$

This gives

$$m = -\frac{P - P_0}{v - v_0} = -\frac{P - P_0}{mV - mV_0},$$

where $V = \frac{1}{\rho}$ is the specific volume. Note that $m \neq 0$. [2]

$$\therefore \quad m^2 = -\frac{P - P_0}{V - V_0}, \quad v - v_0 = -\frac{P - P_0}{m}$$

[2] The case $m = 0$ corresponds to the contact discontinuity.

These give

$$(u-u_0)^2 = (v-v_0)^2 = -(P-P_0)(V-V_0). \tag{7.55}$$

The third jump condition is

$$\left(\frac{1}{2}\rho_0 v_0^2 + \rho_0 e_0 + P_0\right) v_0 = \left(\frac{1}{2}\rho v^2 + \rho e + P\right) v.$$

We want to remove the kinetic energy part and only remain an internal energy relation. From $\rho_0 v_0 = \rho v$, we get

$$\frac{1}{2}v_0^2 + U_0 + P_0 V_0 = \frac{1}{2}v^2 + U + PV.$$

By $v_0^2 = m^2 V_0^2, v^2 = m^2 V^2$, and $m^2 = -\frac{P-P_0}{V-V_0}$, we arrive at

$$H(P,V) := U - U_0 + \frac{P+P_0}{2}(V-V_0) = 0$$

Using $U = \frac{PV}{\gamma-1}$, we get

$$\frac{PV}{\gamma-1} - \frac{P_0 V_0}{\gamma-1} + (\frac{P+P_0}{2})(V-V_0) = 0.$$

We use this equation to express V in terms of P, P_0, V_0:

$$V = \frac{\left(\frac{P+P_0}{2}\right)V_0 + \frac{P_0 V_0}{\gamma-1}}{\frac{P+P_0}{2} + \frac{P}{\gamma-1}}$$

then plug it into

$$(u-u_0)^2 = -(P-P_0)(V-V_0).$$

We get an expression of $\mathfrak{S}_1$ and $\mathfrak{S}_3$ on the u-P plane:

$$\begin{array}{rrcl} \mathfrak{S}_1: & u & = & u_0 - \varphi_0(P) \\ \mathfrak{S}_3: & u & = & u_0 + \varphi_0(P) \end{array}$$

$$\varphi_0(P) = (P-P_0)\sqrt{\frac{\frac{2}{\gamma+1}V_0}{P + \frac{\gamma-1}{\gamma+1}P_0}} = \frac{(P-P_0)}{Z_0},$$

$$Z_0 = \sqrt{\frac{P_0}{V_0}}\Phi\left(\frac{P}{P_0}\right), \quad \Phi(w) = \sqrt{\frac{\gamma+1}{2}w + \frac{\gamma-1}{2}}.$$

Admissible rarefaction curves and shock curves On $\mathfrak{R}_1$, only the portion where λ_1 is increasing is admissible, because the rarefaction fan requires the characteristic speed of the left end of the fan should be smaller than that of the right end of the fan. Therefore, we define the admissible rarefaction curves and shock curves for the left state (ℓ) as

$$\mathfrak{R}_1^+(\ell) = u_0 - \psi_0(P) \text{ for } P < P_0$$
$$\mathfrak{S}_1^-(\ell) = u_0 - \phi_0(P) \text{ for } P > P_0$$

and the admissible rarefaction curves and shock curves for the right state (r) as

$$\mathfrak{R}_3^-(r) = u_0 + \psi_0(P) \text{ for } P < P_0$$
$$\mathfrak{S}_3^+(r) = u_0 + \phi_0(P) \text{ for } P > P_0.$$

The admissible wave curves are defined to be

$$T_1^{(\ell)} := \mathfrak{R}_1^+(\ell) \cup \mathfrak{S}_1^-(\ell)$$
$$T_3^{(r)} := \mathfrak{R}_3^-(r) \cup \mathfrak{S}_3^+(r).$$

Solving Riemann problems Now we are ready to solve the Riemann Problem with initial states (ρ_L, P_L, u_L) and (ρ_R, P_R, u_R). The solution to this Riemann problem consists of three elementary waves:

$$\text{1-wave} :((\rho_L, P_L, u_L), (\rho_I, P_I, u_I)),$$
$$\text{2-wave} :((\rho_I, P_I, u_I), (\rho_{II}, P_{II}, u_{II})),$$
$$\text{3-wave} :((\rho_{II}, P_{II}, u_{II}), (\rho_R, P_R, u_R)).$$

Recall that the second wave is a contact discontinuity, on which $[u] = 0$, $[P] = 0$. Thus, we have

$$u_I = u_{II} = u_*,$$
$$P_I = P_{II} = P_*.$$

Finding the mid states (u_*, P_*) Given a left state $U_L := (\rho_L, P_L, u_L)$ and a right state $U_R := (\rho_R, P_R, u_R)$, we want to find two mid states U_I and U_{II} such that (U_L, U_I) forms an 1-wave, and (U_{II}, U_R) forms a 3-wave and (U_I, U_{II}) forms a 2-wave. From the jump condition of the 2-wave, we have $U_I = (\rho_I, P_*, u_*)$ and $U_{II} = (\rho_{II}, P_*, u_*)$. With this, then

ρ_I and ρ_{II} can be determined the equation on $T_1^{(\ell)}(U_L)$ and $T_3^{(r)}(U_R)$, respectively. The mid state (u_*, P_*) is the intersection of $T_1^{(\ell)}(U_L)$ and $T_3^{(r)}(U_R)$ on the u-P plane.

Godunov gives a procedure to find the mid state (u_*, P_*). The algorithm to find P_* is to solve

$$\begin{aligned} u_L - f_L(P) &= u_I = u_{II} = u_R + f_R(P) \\ f_0(P) &= \begin{cases} \psi_0(P) & P < P_0 \\ \phi_0(P) & P \geq P_0 \end{cases} \quad 0 = L, \text{ or } R. \end{aligned}$$

This is equivalent to

$$\begin{cases} -Z_L(u_* - u_L) &= P_* - P_L \\ Z_R(u_* - u_R) &= P_* - P_R, \end{cases} \tag{7.56}$$

where

$$Z_L = \sqrt{\frac{P_L}{V_L}} \Phi\left(\frac{P_*}{P_L}\right), \quad Z_R = \sqrt{\frac{P_R}{V_R}} \Phi\left(\frac{P_*}{P_R}\right)$$

and

$$\Phi(w) = \begin{cases} \sqrt{\frac{\gamma+1}{2} w + \frac{\gamma-1}{2}} & w > 1 \text{ (shock)}, \\ \frac{\gamma-1}{2\sqrt{\gamma}} \frac{1-w}{1-w^{\frac{\gamma-1}{2\gamma}}} & w \leq 1 \text{ (rarefaction)}. \end{cases}$$

System (7.56) is an equation for (u_*, P_*). It can be solved by Newton's method.

The state ρ_{II} can be obtained from (ρ_R, p_R, u_R) and (u_*, P_*) by similar way.

Wave structures Given (ρ_L, P_L, u_L) and (ρ_R, P_R, u_R). Let us define

- raref $:= \frac{2}{\gamma-1} c_L \left(1 - \left(\frac{p_R}{p_L}\right)^{\frac{\gamma-1}{2\gamma}}\right)$,
- shk $:= c_L \left(\frac{P_R}{P_L} - 1\right) \sqrt{\frac{2}{\gamma\left((\gamma-1)+(\gamma+1)\frac{P_R}{P_L}\right)}}$,
- $du := u_R - u_L$.

We have the following cases:

(1) $(P_R < P_L)$ & $(du \geq \text{raref})$ or $(p_R \geq P_L)$ & $(du \geq \text{shk}) \Rightarrow R_1 + R_3$.

(2) $(p_R \geq P_L)$ & $(-\text{shk} < du < \text{shk}) \Rightarrow S_1 + R_3$

(3) $(p_R < P_L)$ & $(-\text{shk} < du < \text{shk}) \Rightarrow R_1 + S_3$

(4) $(P_R < P_L)$ & $(du \leq -\text{raref})$ or $(p_R \geq P_L)$ & $(du < -\text{shk}) \Rightarrow S_1 + S_3$.

Note that the transition from (1) to (2) (i.e. $R_1 + R_3$ to $S_1 + R_3$ happens when the left state $(\ell) \in R_3^-(r)$.

Once (u_*, P_*) is found, the full mid state can be obtained by the follows:

- If the 1-wave is a rarefaction wave, then ρ_I can be determined by

$$P_* \rho_I^{-\gamma} = A(S_I) = A(S_L) = P_L \rho_L^{-\gamma}$$

  In the region: $\lambda_1(U_L) < x/t < \lambda_1(U_I)$, the state $U = (\rho, u, S_L)$ is determined by

$$\begin{cases} u - c = \frac{x}{t} \\ u - u_L = \phi_L(P). \end{cases}$$

- If the 1-wave is a shock, then $1/\rho_I = V_I$ can be determined by

$$(u_* - u_L)^2 = -(P_* - P_L)(V_I - V_L).$$

The vacuum State The mid state should satisfy $P_* > 0$. There are situations that the mid state $P_* < 0$. In such cases, we say the mid state contains a vacuum state. The intersections of the admissible wave curves and the axis where $P = 0$ are the vacuum states. Usually, this happens when the two sides of gases running in opposite directions too fast.

7.9 Viscous Flows

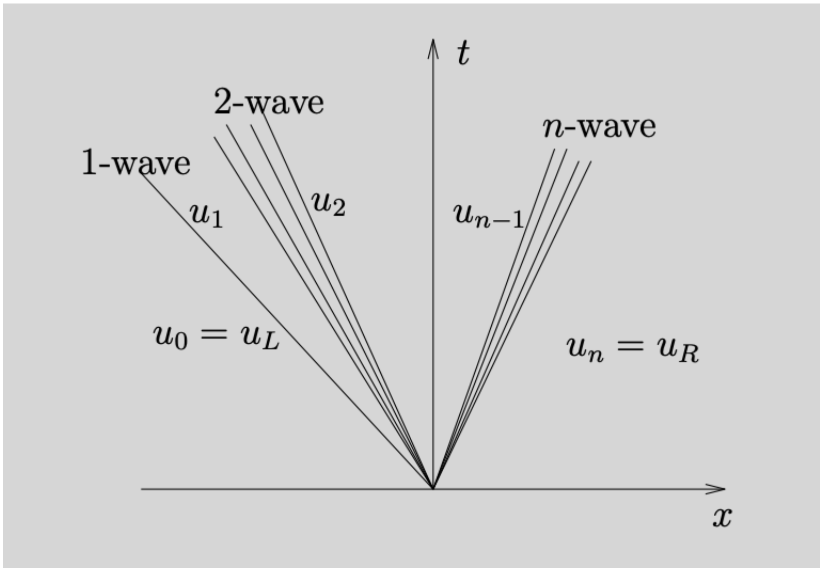
7.9.1 Stokes Flows

Shear flows

- Poiseuille Flow (Laminar flow in a tube)
- Stability/Instability of Shear Flows.

7.9.2 Bifurcation of fluid flows

- Flow past a cylinder
- Flow Separation
- Taylor-Couette flow
- Rayleigh-Bénard Convection



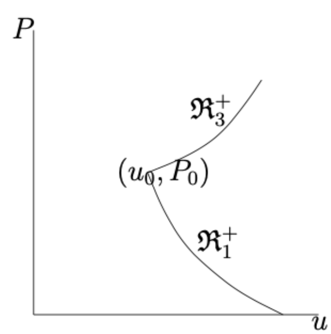


Figure 7.3: The integral curve of the rarefaction curves $\mathfrak{R}_1$ and $\mathfrak{R}_3$ on the u-P plane. Here (u_0,P_0) is a left state. For any point (u_1,P_1) on $\mathfrak{R}_1^+$, $((u_0,P_0),(u_1,P_1))$ forms a 1-rarefaction wave. Note that the entropy $S = S_0$ along a rarefaction curve.

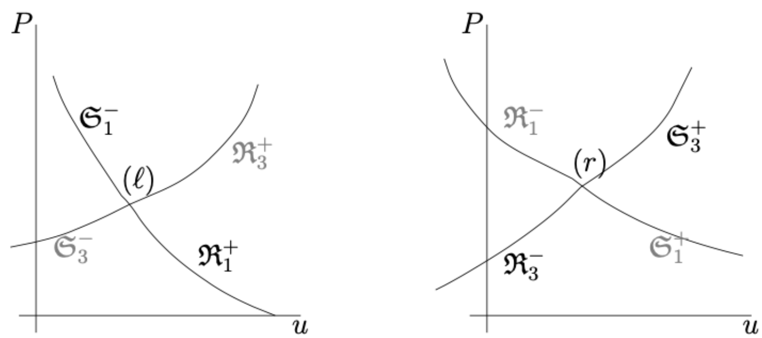


Figure 7.4: The admissible rarefaction curves and shock curves on the u-P plane with left/right states.

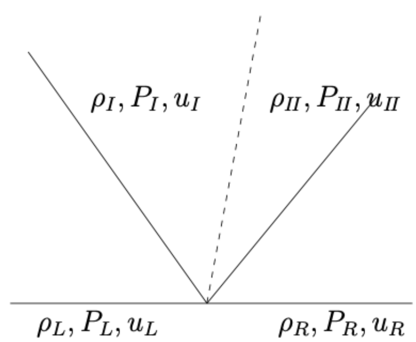


Figure 7.5: The three elementary waves with the left state (ρ_L, P_L, u_L) and the right state (ρ_R, P_R, u_R). The states (ρ_I, P_I, u_I) and $(\rho_{II}, P_{II}, u_{II})$ are called the mid states, which forms a contact discontinuity.

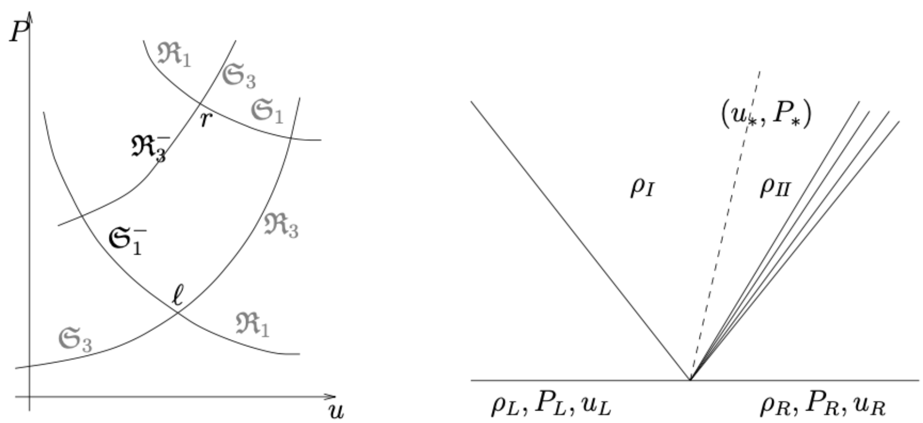


Figure 7.6: This is a solution of the Riemann problem with $p_L < p_R$. In this case, from the left state (ℓ), we follow $\mathfrak{S}_1^-$; and from the right state (r), we follow $\mathfrak{R}_3^-$. Their intersection gives the mid state (u_*, P_*).

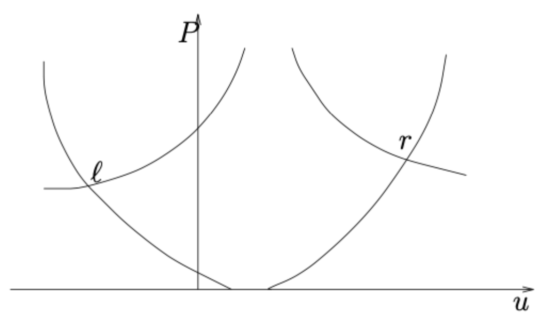


Figure 7.7: The vacuum state appears when $P_* < 0$.

Part II

Elasticity

Chapter 8

Kinematics of Elasticity

Brief History of Elasticity The following historical notes are copied from Love's book: A Treatise on the Mathematical Theory of Elasticity (1926).

- Galileo Galilei, Discorsi e Dimostrazioni matematiche, Leiden (1638)
- Robert Hookes, De Potentia restitutiva, London (1678)
- E. Mariotte, Traité du mouvement des eaux, Paris (1686)
- Euler
- Coulomb and Young
- Navier
- Fresnel
- Cauchy, Poisson
- Green
- Kelvin
- Saint-Venant
- Kirchhoff
- Clebsch

References

- Landau and Lifshitz, Theory of Elasticity, 3rd Edition, 1986.
- J. Ball, Mathematical Foundations of Elasticity Theory (Oxford Lecture slides).
- Ciarlet, Mathematical Elasticity, Vol. 1, Three dimensional elasticity.
- Marsden and Hughes, Mathematical Foundations of Elasticity (1983)
- Drozdov, Finite Elasticity and Viscoelasticity.
- Beris and Edwards, Thermodynamics of Flowing Systems (1994).
- Vlado A. Lubarda, Elastoplasticity Theory.

Contents Solid mechanics includes elasticity, plasticity, viscoelasticity, visco-plasticity, etc. The deformation of solid material is described by the flow map of the material. The geometric change (deformation) of the material involves forces in the internal molecular structure or from the external world. There are two kinds of forces: conservative and non-conservative. The conservative force gives reversible physical process, while the physical process is irreversible for nonconservative forces. In the first few chapters, we study mechanics of simple elasticity. Its content includes

- the geometry of the deformation (strain);
- the response of the material to the deformation (stress-strain relation);
- the dynamics of a simple elastic material.

8.1 Deformation and Strain

8.1.1 Flow Map and Deformation Gradient

Flow maps and velocity fields Let us imagine an elastic material deforms from a domain M_0 at time 0 to M_t at time t. The domain M_t is a manifold, called the configuration space or the observor's space. The initial region M_0 is called the reference space or the material space. We denote such a deformation or flow map by [1]

$$\varphi_t : X \mapsto \mathbf{x}(t,X).$$

[1] In later chapters, the flow map will also be denoted by $\mathbf{x} = \varphi_t(X)$ in differential geometry, and by $\mathbf{x} = \mathbf{q}(t,X)$ in Hamilton mechanics.

That is, a position with coordinate X is deformed to a position $\mathbf{x}$ at time t. The coordinate X is called the Lagrange coordinate (or the material coordinate, or the reference coordinate), while $\mathbf{x}$ the Euler coordinate (or the world coordinate, or the observer's coordinate). We shall assume the flow map $\mathbf{x}(\cdot,\cdot)$ is Lipschitz continuous and the map $\varphi_t : X \mapsto \mathbf{x}(t,X)$ invertible for almost all t. [2] The velocity $\mathbf{v}(t,\mathbf{x})$ is defined to be

$$\mathbf{v}(t,\mathbf{x}(t,X)) = \dot{\mathbf{x}}(t,X).$$

Here, the dot is the differentiation in t with fixed X. Conversely, given a vector field $\mathbf{v} : \cup_{t\ge 0}\{t\}\times M_t \to \mathbb{R}^3$, one can obtain a flow map $\mathbf{x}(t,X)$ by solving the ODE

$$\dot{\mathbf{x}}(t,X) = \mathbf{v}(t,\mathbf{x}), \quad \mathbf{x}(0,X) = X.$$

Thus, the dynamics of the material is described by either the flow map $\mathbf{x}(t,X)$ or the velocity field $\mathbf{v}(t,\mathbf{x})$.

Deformation gradient The gradient

$$\boxed{F(t,X) := \nabla_X \mathbf{x}(t,X) = \frac{\partial \mathbf{x}}{\partial X}(t,X)} \tag{8.1}$$

is called the *deformation gradient*. [3] It is clear that $F(0,X) = I$. Its component expression is

$$dx^i = F^i_\alpha dX^\alpha := \frac{\partial x^i}{\partial X^\alpha} dX^\alpha.$$

Let us denote the Jacobian by

$$J(t,X) := \det F(t,X).$$

We require $J(t,X) > 0$ for all time from physical consideration. That means that the flow map φ_t is orientation preserving.

Rate of deformation By differentiating the equation $\dot{\mathbf{x}}(t,X) = \mathbf{v}(t,\mathbf{x}(t,X))$ in X, we get

$$\frac{\partial \dot{\mathbf{x}}}{\partial X} = \frac{\partial \mathbf{v}}{\partial X}(t,\mathbf{x}(t,X)) = \frac{\partial \mathbf{v}}{\partial \mathbf{x}}\frac{\partial \mathbf{x}}{\partial X}.$$

In component form, it is

$$\frac{\partial}{\partial X^\alpha}\frac{\partial}{\partial t}x^i(t,X) = \frac{\partial v^i}{\partial x^k}\frac{\partial x^k}{\partial X^\alpha}.$$

[2] The flow map $\mathbf{x}(t,\cdot)$ may not be differentiable everywhere. $\partial \mathbf{x}/\partial X$ may have discontinuity.

[3] In differential geometry, we express F as $d\varphi_t$.

Using commuting property of ∂_t and ∂_X, we obtain

$$\frac{\partial}{\partial t}\frac{\partial x^i}{\partial X^\alpha} = \frac{\partial v^i}{\partial x^k}\frac{\partial x^k}{\partial X^\alpha},$$

or

$$\boxed{\dot{F} = (\nabla \mathbf{v})F = LF.} \tag{8.2}$$

The term

$$L^i_k := \frac{\partial v^i}{\partial x^k}, \quad \text{or} \quad L = \nabla \mathbf{v}$$

is called the *rate-of-deformation*. [4]

8.1.2 Examples

1. Rigid body motion A trivial flow motion is the rigid-body motion defined by

$$\mathbf{x} = \mathbf{x}_0(t) + Q(t)X$$

where $Q(t)$ is an orthogonal matrix, i.e. $QQ^T = \mathbf{I}$. We have

$$X = Q^T(\mathbf{x} - \mathbf{x}_0(t)).$$

The deformation gradient $F = Q$. From

$$\mathbf{v} = \dot{\mathbf{x}} = \dot{\mathbf{x}}_0(t) + \dot{Q}(t)X = \dot{\mathbf{x}}_0(t) + \dot{Q}(t)Q^T(t)(\mathbf{x} - \mathbf{x}_0(t)).$$

Thus,

$$\nabla \mathbf{v} = \dot{Q}(t)Q^T(t).$$

Note that

$$\nabla \mathbf{v} + (\nabla \mathbf{v})^T = \dot{Q}Q^T + Q\dot{Q}^T = 0, \quad \because Q^TQ = I.$$

Let us characterize the rigid-body motion without proof.

Proposition 8.4. *Let $\varphi_t : \Omega \to \mathbb{R}^3$ be a flow map in $\mathbb{R}^3$. Then $\varphi_t(X)$ is a rigid-body motion if and only if $F^TF \equiv I$, where $F := \nabla_X \varphi_t$.*

[4] Note that $(\nabla \mathbf{v})^i_k := \partial v^i/\partial \mathbf{x}^k$, which is different from the notation of ordinary tensor product. There, $(\nabla \otimes \mathbf{v})^i_k := \partial_{x^i} v^j$. In terms of the notation of tensor product, our $\nabla \mathbf{v}$ is the tensor product $\mathbf{v} \otimes \nabla$.

2. Shear flow A simple shear flow is given by

$$v_1 = \dot{\gamma}_{21} x_2, \quad v_2 = 0, \quad v_3 = 0. \tag{8.3}$$

Here, $\dot{\gamma}_{21}$ is a constant, called the shear rate. The corresponding flow map is

$$x_1 = X_1 + \dot{\gamma}_{21} t X_2, \quad x_2 = X_2, \quad x_3 = X_3.$$

The deformation gradient and rate-of-deformation are

$$F = \begin{bmatrix} 1 & \dot{\gamma}_{21} t & \\ & 1 & \\ & & 1 \end{bmatrix}, \quad \nabla \mathbf{v} = \begin{bmatrix} 0 & \dot{\gamma}_{21} & \\ & 0 & \\ & & 0 \end{bmatrix}.$$

3. Simple shearless flow [5] is given by

$$\begin{aligned} v_1 &= -\frac{1}{2}\dot{\varepsilon}(1+b)x_1 \\ v_2 &= -\frac{1}{2}\dot{\varepsilon}(1-b)x_2 \\ v_3 &= \dot{\varepsilon} x_3. \end{aligned} \tag{8.4}$$

Here, $0 \le b \le 1$ and $\dot{\varepsilon}$ are two constants, called the elongation rates. We have

$$\nabla \mathbf{v} = \begin{bmatrix} -\frac{1}{2}\dot{\varepsilon}(1+b) & & \\ & -\frac{1}{2}\dot{\varepsilon}(1-b) & \\ & & \dot{\varepsilon} \end{bmatrix},$$

It satisfies

$$\nabla \cdot \mathbf{v} = 0.$$

Thus, this flow map is volume preserving. The flow map is given by

$$\begin{bmatrix} x^1 \\ x^2 \\ x^3 \end{bmatrix} = \begin{bmatrix} \exp(-\frac{1}{2}\dot{\varepsilon}(1+b)t) & & \\ & \exp(-\frac{1}{2}\dot{\varepsilon}(1-b)t) & \\ & & \exp(\dot{\varepsilon} t) \end{bmatrix} \begin{bmatrix} X^1 \\ X^2 \\ X^3 \end{bmatrix}.$$

Special cases are

- Elongational flow: $b = 0, \dot{\varepsilon} > 0$. It elongates in x^3 direction and shrinks in x^1 and x^2 cross-section plane.
- Bi-axial stretching flow: $b = 0, \dot{\varepsilon} < 0$. It stretches in x^3 direction and expands in x^1-x^2 cross section plane.
- Planar elongational flow: $b = 1$. A flow with motion only in x^1-x^3 plane.

[5] This part of note mainly comes from Bird's book, Vol. I, Chapter 3.

4. Linear Deformation Consider an elastic motion satisfying $\nabla \mathbf{v} = constant$. That is,

$$\mathbf{v} = A\mathbf{x}, \quad A \text{ is a constant matrix.}$$

We can compute the corresponding flow map

$$\dot{\mathbf{x}} = \mathbf{v} = A\mathbf{x}, \quad \mathbf{x}(0, X) = X.$$

The flow map is

$$\mathbf{x}(t, X) = e^{tA}X.$$

The deformation gradient and rate of deformation are

$$F = e^{tA}, \quad \nabla \mathbf{v} = A.$$

We see that

1. From $\det(e^{tA}) = e^{tTr(A)}$, we get $J(t) = \det F(t) = 1$ iff $Tr(A) = 0$.

2. If A is anti-symmetric, i.e. $A + A^T = 0$, then A can be expressed as

$$A = \begin{bmatrix} & -\omega_3 & \omega_2 \\ \omega_3 & & -\omega_1 \\ -\omega_2 & \omega_1 & \end{bmatrix},$$

   and $Q = e^{tA}$ satisfies [6]

$$QQ^T = e^{tA}e^{tA^T} = e^{t(A+A^T)} = I.$$

   That is, Q is a rotation. Thus, the flow is a rigid-body motion.

3. If $A = \lambda I$, then $\mathbf{x}(t, X) = e^{tA}X$ is an isotropic expansion/shrinking.

4. Suppose A is symmetric and $Tr(A) = 0$. We can diagonalize A, say $A = \mathrm{diag}(\lambda_1, \lambda_2, \lambda_3)$ with $\sum_i \lambda_i = 0$. Then

$$e^{tA} = \mathrm{diag}(e^{t\lambda_1}, e^{t\lambda_2}, e^{t\lambda_3}).$$

   It expands in those directions where $\lambda_i > 0$ and shrinks in those where $\lambda_i < 0$.

[6] Note that for any two constant square matrices A and B, we have $\exp(A)\exp(B) = exp(A+B)$ if and only if $AB = BA$. This can be proven by using Taylor expansion and mutual diagonalization. For antisymmetric matrix A, we have $A^T = -A$. Thus, $AA^T = -A^2 = A^T A$.

5. A symmetric matrix A can be expressed as

$$A = (A - \frac{1}{3}Tr(A)I) + \frac{1}{3}Tr(A)I$$

The first term is trace free and the second term is isotropic.

$$e^{tA} = e^{t(A-\frac{1}{3}Tr(A)I)} e^{\frac{t}{3}Tr(A)}.$$

6. A general matrix A can be decomposed into

$$A = \frac{1}{2}(A + A^T) + \frac{1}{2}(A - A^T) = S + \Omega.$$

Its exponential map $e^{\Delta t A}$ in a short period of time Δt can be approximated by

$$e^{\Delta t A} = e^{\Delta t S} e^{\Delta t \Omega} + O((\Delta t)^2) = e^{\Delta t \Omega} e^{\Delta t S} + O((\Delta t)^2) \quad \text{for small time } \Delta t.$$

The reason why this is only an approximation is because S and Ω may not commute to each other.

Homework Let A, B be two $n \times n$ matrices. Show that

$$e^{\Delta t(A+B)} = e^{\Delta t A} e^{\Delta t B} + O((\Delta t)^2).$$

Hint: Use the definition $e^{tA} = \sum_n \frac{1}{n!}(tA)^n$.

8.1.3 Geometric Meaning of Deformation Gradient

Singular Value Decomposition of F.

Proposition 8.5. *The deformation gradient F has the following representation:*

$$\boxed{F = O_{\mathbf{n}} \Lambda O_{\mathbf{N}}^T} \tag{8.5}$$

where

$$\Lambda = diag(\lambda_1, \lambda_2, \lambda_3), \quad \lambda_i \geq 0,$$

and

$$O_{\mathbf{n}} = [\mathbf{n}_1, \mathbf{n}_2, \mathbf{n}_2], \quad O_{\mathbf{N}} = [\mathbf{N}_1, \mathbf{N}_2, \mathbf{N}_3]$$

are two orthogonal matrices in the world space and material space, respectively.

Remark The representation (8.5) is called the singular value decomposition of F; where λ_i are the singular values of F. We can also express F as

$$F = \sum_k \lambda_k \mathbf{n}_k \mathbf{N}_k^T.$$

In component form, it reads

$$F_\alpha^i = \sum_k \lambda_k \mathbf{n}_k^i N_k^\alpha.$$

The matrix $\mathbf{n}_k \mathbf{N}_k^T$ is a rank-1 matrix. It is a projectionon to $\mathbf{n}_k$.

Proof. 1. Consider the matrix $F^T F$, which is symmetric and non-negative. It has eigenvalues/eigenvectors: λ_k^2 and $\mathbf{N}_k$, $k = 1,2,3$. These eigenvectors are orthonormal. That is,

$$\langle \mathbf{N}_k, \mathbf{N}_\ell \rangle = \delta_{k\ell}.$$

We choose $\lambda_k \geq 0$. They are called the singular values of F. [7]

2. For those k with $\lambda_k \neq 0$, we define $\mathbf{n}_k := F\mathbf{N}_k/\lambda_k$, then $\|\mathbf{n}_k\|^2 = 1$. For

$$\langle \mathbf{n}_k, \mathbf{n}_k \rangle = \frac{1}{\lambda_k^2} \langle F\mathbf{N}_k, F\mathbf{N}_k \rangle = \frac{1}{\lambda_k^2} \langle F^T F\mathbf{N}_k, \mathbf{N}_k \rangle = \langle \mathbf{N}_k, \mathbf{N}_k \rangle = 1.$$

If $\lambda_k \neq \lambda_\ell$, then $\langle \mathbf{n}_k, \mathbf{n}_\ell \rangle = 0$. This is because

$$\langle \mathbf{n}_k, \mathbf{n}_\ell \rangle = \frac{1}{\lambda_k \lambda_\ell} \langle F\mathbf{N}_k, F\mathbf{N}_\ell \rangle = \frac{1}{\lambda_k \lambda_\ell} \langle F^T F\mathbf{N}_k, \mathbf{N}_\ell \rangle = \frac{\lambda_k^2}{\lambda_k \lambda_\ell} \langle \mathbf{N}_k, \mathbf{N}_\ell \rangle = 0.$$

3. If there are $\lambda_\ell = 0$ for some ℓ, then the set $\{\mathbf{n}_k |$ the corresponding $\lambda_k \neq 0\}$ can not form a basis in $\mathbb{R}^3$. We extend the set $\{\mathbf{n}_k | \lambda_k \neq 0\}$ to its orthogonal complement such that the extended set $\{\mathbf{n}_k\}_{k=1}^3$ constitutes an orthonormal basis in $\mathbb{R}^3$. That is,

$$\langle \mathbf{n}_k, \mathbf{n}_\ell \rangle = \delta_{k\ell}, \quad 1 \leq k, \ell \leq 3.$$

The above construction of $\{\mathbf{n}_k\}$ satisfies

$$F\mathbf{N}_k = \lambda_k \mathbf{n}_k, k = 1,2,3. \tag{8.6}$$

[7] The eigenvalues are nonnegative because

$$0 \leq \langle F\mathbf{N}_k, F\mathbf{N}_k \rangle = \langle F^T F\mathbf{N}_k, \mathbf{N}_k \rangle = \lambda_k^2 \langle \mathbf{N}_k, \mathbf{N}_k \rangle = \lambda_k^2.$$

4. Let $O_{\mathbf{n}} := [\mathbf{n}_1, \mathbf{n}_2, \mathbf{n}_3]$, $O_{\mathbf{N}} := [\mathbf{N}_1, \mathbf{N}_2, \mathbf{N}_3]$ and $\Lambda = \operatorname{diag}(\lambda_1, \lambda_2, \lambda_3)$. Then $O_{\mathbf{n}}$ and $O_{\mathbf{N}}$ are orthogonal matrices, and (8.6) can be expressed as

$$F[\mathbf{N}_1, \mathbf{N}_2, \mathbf{N}_3] = [\mathbf{n}_1, \mathbf{n}_2, \mathbf{n}_3]\operatorname{diag}(\lambda_1, \lambda_2, \lambda_3),$$

or in matrix form:

$$F = O_{\mathbf{n}} \Lambda O_{\mathbf{N}}^T.$$

$\square$

Remarks

1. Let $\{E_\alpha := \partial_{X^\alpha} | \alpha = 1,2,3\}$ be the basis in the material space, and $\{e_i := \partial_{x^i} | i = 1,2,3\}$ be the basis in the observer's space. The representations of $O_{\mathbf{N}} = [\mathbf{N}_1, \mathbf{N}_2, \mathbf{N}_3]$ and $O_{\mathbf{n}} = [\mathbf{n}_1, \mathbf{n}_2, \mathbf{n}_3]$ are

$$\mathbf{N}_k = N_k^\alpha E_\alpha, \quad \mathbf{n}_k = \mathbf{n}_k^i e_i.$$

2. Suppose we choose $[\mathbf{N}_1, \mathbf{N}_2, \mathbf{N}_3]$ as an orthonormal frame in material space and $[\mathbf{n}_1, \mathbf{n}_2, \mathbf{n}_3]$ an orthonormal frame in observer's space. Let X' be the coordinate of X in the frame $[\mathbf{N}_1, \mathbf{N}_2, \mathbf{N}_3]$, then we have $dX' = O_{\mathbf{N}}^T dX$. Similarly, let $\mathbf{x}'$ be the coordinate of $\mathbf{x}$ in the frame $[\mathbf{n}_1, \mathbf{n}_2, \mathbf{n}_3]$, we also have $d\mathbf{x}' = O_{\mathbf{n}}^T d\mathbf{x}$. Under these two frames, the deformation gradient F has the representation:

$$d\mathbf{x}' = O_{\mathbf{n}}^T d\mathbf{x} = O_{\mathbf{n}}^T F dX = O_{\mathbf{n}}^T (O_{\mathbf{n}} \Lambda O_{\mathbf{N}}^T) dX = \Lambda dX'.$$

This means that in the coordinate systems X' and $\mathbf{x}'$, the deformation is an elongation/stretching.

3. Let us restate the above argument by investigating the deformation of a small ball. Consider a small ball $\{|\Delta X|^2 = \varepsilon^2\}$ in the tangent space of material space TM_0. Let us represent the tangent ΔX in terms of N_k as $\Delta X = \Delta X'^k \mathbf{N}_k$. The deformation gradient F maps ΔX to $\Delta \mathbf{x}$, which has the representation:

$$\Delta \mathbf{x} = F(\Delta X) = F(\Delta X'^k \mathbf{N}_k) = \lambda_k \Delta X'^k \mathbf{n}_k.$$

On the other hand, $\Delta \mathbf{x} = \Delta x'^k \mathbf{n}_k$. Thus, the small ball $\|\Delta X\|^2 = \varepsilon^2$ is deformed to an ellipsoid

$$\sum_k \frac{(\Delta x^k)^2}{\lambda_k^2} = \varepsilon^2$$

with axes $\mathbf{n}_1, \mathbf{n}_2, \mathbf{n}_3$.

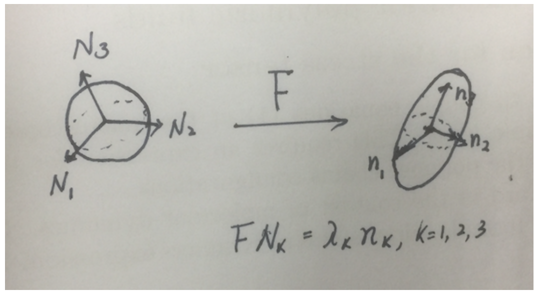


Figure 8.1: Singular value decomposition of F. $FN_k = \lambda_k \mathbf{n}_k$

Polar decomposition of F

1. **Right polar decomposition**

   - Let $F = O_{\mathbf{n}}\Lambda O_{\mathbf{N}}^T$ be the singular value decomposition of F. Then
   $$F = O_{\mathbf{n}}\Lambda O_{\mathbf{N}}^T = (O_{\mathbf{n}}O_{\mathbf{N}}^T)(O_{\mathbf{N}}\Lambda O_{\mathbf{N}}^T) = OS_r, \quad F^i_\alpha = O^i_\beta S^\beta_{r,\alpha}.$$
   $$O := O_{\mathbf{n}}O_{\mathbf{N}}^T, \quad S_r := O_{\mathbf{n}}\Lambda O_{\mathbf{N}}^T.$$
   This is called the right polar decomposition of F, where O is a rotation and S_r is a self-adjoint semi-positive definite operator.

   - There is a geometric interpretation for the polar decomposition of a deformation gradient. The rotation O is an isometry map (metric preserving) from material space to the world space (an Eulerian space), while S_r is a self-adjoint operator from material space to itself. It is called *right stretching tensor. The decomposition of an infinitesimal deformation F means that we perform an elongation or stretching (i.e. S_r) in the material space first, then map to the world space by an isometry (i.e. O).* We shall see in a later section that the isometry contributes no energy. Thus, the internal energy W corresponding to the deformation gradient F is only a function of S_r, or equivalently, only a function of $S_r^2 = C = F^T F$, the right Cauchy-Green strain. We shall see this in the material response to the deformation in the Chapter of Stress-Strain relation.

2. **Left polar decomposition** Alternatively, we can have left polar decomposition:
   $$F = O_{\mathbf{n}}\Lambda O_{\mathbf{N}}^T = (O_{\mathbf{n}}\Lambda O_{\mathbf{n}}^T)(O_{\mathbf{n}}O_{\mathbf{N}}^T) = S_l O^T, \quad F^i_\alpha = S^i_{l,k} O^k_\alpha,$$
   $$O = O_{\mathbf{n}}O_{\mathbf{N}}, \quad S_l := O_{\mathbf{n}}\Lambda O_{\mathbf{n}}^T.$$
   We notice that
   $$S_r = O^T S_l O.$$
   Thus they have the same eigenvalues λ_i. The corresponding eigenvectors are $\mathbf{N}_i$ for S_r and $\mathbf{n}_i$ for S_l.

8.1.4 Deformation Tensors and Strain Tensors

There are many ways to measure the deformation of a material. The basic one is the deformation gradient F. Others are various forms of F, which encode necessary information of F needed in the stress-strain relation. They are tensors, called the strain tensors. These deformation tensors and the strain tensors are dimensionless quantities.

Deformation Tensors

1. There are many ways to measure the deformation of a material. Some are naturally defined in the material space M_0, some are naturally defined in the world space M_t. We shall assume both spaces are Euclidean. These deformation tensors are also called the *strain tensors*. [8]

   - Strain tensors defined on M_0:
     - Deformation gradient $F^i_\alpha(t,X) = \frac{\partial x^i}{\partial X^\alpha}$.
     - Right Cauchy-Green deformation tensor: $C = F^T F$, or $C_{\alpha\beta} = (F^T)^\alpha_i F^i_\beta = F^i_\beta F^i_\alpha$. Note that C is symmetric.
     - Right stretch tensor $S_r := (F^T F)^{1/2}$.
   - Strain tensors defined on M_t:
     - Inverse deformation gradient: $(F^{-1})^\alpha_i(t,\mathbf{x}) = \frac{\partial X^\alpha}{\partial x^i}$.
     - Left Cauchy-Green deformation tensor: $B := FF^T$, or $B^{ij} = F^i_\alpha (F^T)^\alpha_j = F^i_\alpha F^j_\alpha$. Note that B is also symmetric.
     - Left stretch tensor $S_l := (FF^T)^{1/2}$.

2. The right Cauchy-Green deformation tensor is also the first fundamental form of the domain M_t. The tangent vector $g_\alpha := \frac{\partial \mathbf{x}}{\partial X^\alpha}$ and the first fundamental form is defined to be
$$C_{\alpha\beta} := \langle g_\alpha, g_\beta \rangle = \sum_{ij} g_{ij} \frac{\partial x^i}{\partial X^\alpha} \frac{\partial x^j}{\partial X^\beta}.$$
   Here, (g_{ij}) is the metric of the world space. Thus, C is the pullback of the metric (g_{ij}).

3. Deformation of an infinitesimal ellipsoid. Suppose M_0 has a metric g_0. (Let us denote the corresponding inner product by $\langle \cdot, \cdot \rangle_0$.) Consider an infinitesimal sphere

[8] Some textbooks use the following names: Finger's tensor (FF^T), Cauchy ($F^T F$), Piola ($F^{-1}F^{-T}$), and Almansi ($F^{-T}F^{-1}$)

at $t = 0$. It can be expressed as

$$\langle dX, dX \rangle_0 = 1.$$

At time t, it is deformed to

$$\langle d\mathbf{x}, B^{-1} d\mathbf{x} \rangle = \langle dX, dX \rangle_0 = 1.$$

This is an infinitesimal ellipsoid with three axes $\mathbf{n}_1, \mathbf{n}_2, \mathbf{n}_3$ and length λ_k.

8.1.5 Advection of Strains

Let the dot represent $d/dt := \partial_t + \mathbf{v} \cdot \nabla_{\mathbf{x}}$, the material derivative.

1. We have seen that
$$\dot{F} = LF, \quad L = \nabla \mathbf{v}.$$
In component form, it is
$$\frac{d}{dt}\left(\frac{\partial x^i}{\partial X^\alpha}\right) = \frac{\partial v^i}{\partial x^k}\frac{\partial x^k}{\partial X^\alpha}.$$
The term $L = \nabla \mathbf{v}$ is the rate of deformation.

2. For F^{-1}, we have
$$\frac{d}{dt}F^{-1} = -F^{-1}\dot{F}F^{-1} = -F^{-1}LFF^{-1} = -F^{-1}L.$$

3. For the right Cauchy-Green tensor,
$$\begin{aligned}\dot{C} = \frac{d}{dt}(F^T F) &= \dot{F}^T F + F^T \dot{F} = F^T L^T F + F^T LF \\ &= F^T L^T F^{-T} F^T F + F^T F F^{-1} LF = R^T C + CR,\end{aligned}$$
where $R = F^{-1}LF$.

4. For the left Cauchy-Green tensor,
$$\begin{aligned}\dot{B} = \frac{d}{dt}(FF^T) &= \dot{F}F^T + F\dot{F}^T \\ &= LFF^T + FF^T L^T = LB + BL^T.\end{aligned}$$
That is,
$$B_{(1)} := \dot{B} - LB - BL^T = 0,$$
The notation $B_{(1)}$ is called first-order *upper-convected derivative* for tensor B. We will see this again in the theory of viscoelasticity.

5. We can decompose L into symmetric part and antisymmetric part:

$$L = D + \Omega, \quad D = \frac{1}{2}\left(\nabla\mathbf{v} + (\nabla\mathbf{v})^T\right), \quad \Omega = \frac{1}{2}\left((\nabla\mathbf{v})^T - \nabla\mathbf{v}\right).$$

   Since B is symmetric, the upper-convected derivative can be re-expressed as

$$B_{(1)} = \dot{B} - LB - BL^T = (\dot{B} - \Omega B + B\Omega) + (DB + BD).$$

   The part $B^{\nabla} := \dot{B} - \Omega B + B\Omega$ is also called Jaumann tensor derivative.

6. For C^{-1}, we have

$$\frac{d}{dt}C^{-1} = -C^{-1}\dot{C}C^{-1} = -C^{-1}(CR + R^T C)C^{-1} = -RC^{-1} - C^{-1}R^T.$$

7. For B^{-1}, we have

$$\frac{d}{dt}B^{-1} = -B^{-1}\dot{B}B^{-1} = -B^{-1}(LB + BL^T)B^{-1} = -B^{-1}L - L^T B^{-1}.$$

8.2 Infinitesimal Strain

Many material such as steel only performs small deformation. In this case, infinitesimal strain theory can be applied. Below, we shall assume both the material space and the world space are the Euclidean space with Euclidean metric.

8.2.1 Displacement and Relative Strains

- **Displacement:** Instead of using the absolute flow map, we use the relative motion, which is the displacement

$$\mathbf{u}(t, X) := \mathbf{x}(t, X) - X.$$

  In the Eulerian frame, we use

$$\bar{\mathbf{u}}(t, \mathbf{x}) = \mathbf{x}(t, X) - X, \text{ with } \mathbf{x}(t, X) = \mathbf{x}.$$

- Lagrangian (relative) strain tensor:

$$E := \frac{1}{2}(C - I) = \frac{1}{2}((I + \nabla_X \mathbf{u})^T (I + \nabla_X \mathbf{u}) - I).$$

- Eulerian strain tensor:
$$e := \frac{1}{2}(I - B^{-1}).$$
Note that both E and e are symmetric.

- **Geometric Meaning** Let $ds^2 := d\mathbf{x} \cdot d\mathbf{x}$ and $dS^2 = dX \cdot dX$ be the Euclidean metric in the world space and the material space, respectively. We have
$$d\mathbf{x} \cdot d\mathbf{x} - dX \cdot dX = dX \cdot F^T F \cdot dX - dX \cdot dX = dX \cdot (2E) \cdot dX$$
$$d\mathbf{x} \cdot d\mathbf{x} - dX \cdot dX = d\mathbf{x} \cdot d\mathbf{x} - d\mathbf{x} \cdot (F^{-T} F^{-1}) \cdot d\mathbf{x} = d\mathbf{x} \cdot (2e) \cdot d\mathbf{x}.$$
Sometimes, we write them as
$$E = \frac{ds^2 - dS^2}{2dS^2}, \quad e = \frac{ds^2 - dS^2}{2ds^2}.$$

8.2.2 Infinitesimal Strains

Lagrangian infinitesimal strain We can also express strains in terms of displacement gradients. Note that
$$F = I + \nabla_X \mathbf{u}.$$
Define the following infinitesimal Lagrangian strain tensor
$$\mathbf{e} := \frac{1}{2}\left(\nabla_X \mathbf{u} + \nabla_X \mathbf{u}^T\right) = \frac{1}{2}(F + F^T) - I.$$
That is,
$$e_{ij} = \frac{1}{2}\left(\frac{\partial u^i}{\partial X^j} + \frac{\partial u^j}{\partial X^i}\right).$$
We have
$$E = \frac{1}{2}\left((I + \nabla_X \mathbf{u})^T (I + \nabla_X \mathbf{u}) - I\right) = \mathbf{e} + o(\mathbf{e}). \tag{8.7}$$

Eulerian infinitesimal strain We also define the infinitesimal Eulerian strain tensor
$$\varepsilon := \frac{1}{2}\left(\nabla_{\mathbf{x}} \bar{\mathbf{u}} + \nabla_{\mathbf{x}} \bar{\mathbf{u}}^T\right).$$
Note that
$$\bar{\mathbf{u}}(t, \mathbf{x}) := \mathbf{u}(t, X) \quad \text{when } \mathbf{x} = \mathbf{x}(t, X).$$
In terms of infinitesimal strain tensor, C and B can be expressed as
$$C = (I + \nabla_X \mathbf{u})^T (I + \nabla_X \mathbf{u}) = I + 2\mathbf{e} + (\nabla_X \mathbf{u})^T (\nabla_X \mathbf{u})$$

$$B = (I + \nabla_{\mathbf{x}} \bar{\mathbf{u}})(I + \nabla_{\mathbf{x}} \bar{\mathbf{u}})^T = I + 2\varepsilon + (\nabla_{\mathbf{x}} \bar{\mathbf{u}})(\nabla_{\mathbf{x}} \bar{\mathbf{u}})^T.$$

When the deformation variation is small (i.e. $|\nabla_X \mathbf{u}| << 1$), then we may treat

$$\partial_X \approx \partial_{\mathbf{x}}, \quad \mathbf{e} \approx \varepsilon,$$

$$C \approx I + 2\mathbf{e}, \quad B \approx I + 2\varepsilon,$$

with

$$\varepsilon_{ij} = \frac{1}{2}\left(\frac{\partial u^i}{\partial x^j} + \frac{\partial u^j}{\partial x^i}\right).$$

Symmetry Both $\mathbf{e}$ and ε are symmetric.

Geometric meaning of infinitesimal strain. To understand the physical meaning of ε_{11}, let us consider an infinitesimal vector $dX_1 := (d\ell_1, 0, 0)^T$. The vector is deformed to

$$d\mathbf{x}_1 = (1 + \frac{\partial u^1}{\partial X^1}, \frac{\partial u^2}{\partial X^1}, \frac{\partial u^3}{\partial X^1})^T d\ell_1.$$

Its length square

$$(d\tilde{\ell}_1)^2 = \langle d\mathbf{x}_1, d\mathbf{x}_1 \rangle \approx \left(1 + 2\frac{\partial u^1}{\partial X^1}\right)(d\ell_1)^2.$$

Here, we have neglected the hight order terms. Thus,

$$d\tilde{\ell}_1 \approx \sqrt{1 + 2\frac{\partial u^1}{\partial X^1}}\, d\ell_1 \approx \left(1 + \frac{\partial u^1}{\partial X^1}\right) d\ell_1 \tag{8.8}$$

That is

$$e_{11} \approx \frac{d\tilde{\ell}_1 - d\ell_1}{d\ell_1}.$$

Thus, the physical meaning of e_{11} is the relative change of $d\ell$ in the direction e_1. Similarly, to understand the physical meaning of e_{12}, we consider two infinitesimal vectors

$$\begin{aligned} dX_1 &= (d\ell_1, 0, 0)^T \\ dX_2 &= (0, d\ell_2, 0)^T. \end{aligned}$$

The corresponding deformed vectors are

$$\begin{aligned} d\mathbf{x}_1 &= (1 + \frac{\partial u^1}{\partial X^1}, \frac{\partial u^2}{\partial X^1}, \frac{\partial u^3}{\partial X^1})^T d\ell_1 \\ d\mathbf{x}_2 &= (\frac{\partial u^1}{\partial X^2}, 1 + \frac{\partial u^2}{\partial X^2}, \frac{\partial u^3}{\partial X^2})^T d\ell_2. \end{aligned}$$

The inner product

$$\langle d\mathbf{x}_1, d\mathbf{x}_2\rangle \approx \left(\frac{\partial u^1}{\partial X^2} + \frac{\partial u^2}{\partial X^1}\right) d\ell_1 d\ell_2.$$

Hence, we get

$$d\tilde{\ell}_1 d\tilde{\ell}_2 \cos\theta = 2e_{12} d\ell_1 d\ell_2$$

where θ is the angle between $d\mathbf{x}_1$ and $d\mathbf{x}_2$. Using (8.8) and neglecting higher order terms, we get

$$e_{12} = \frac{1}{2}\cos\theta.$$

Thus, the physical meaning of e_{12} is the half of the cosine of the relative angle between the two deformed orthogonal vectors e_1 and e_2 directors.

8.3 Geometric View of Strain

8.3.1 Tensor Types of Strains

Let $\varphi_t : M_0 \to M_t \subset \mathcal{S}$ be the flow map. We denote it by $\varphi_t(X) = \mathbf{x}(t,X)$. We will call M_0 the material space and M_t the world space.

- Let $\{X^\alpha\}$ be a coordinate in M_0. The material space has basis $\{\partial_{X^\alpha}\}$ in the tangent space TM_0 and dual basis $\{dX^\alpha\}$ in the cotangent space T^*M_0. The material space needs not have a Riemannian metric.

- The world space is assumed to be a Riemannian manifold with metric g (which is a non-degenerate symmetric type-$(0,2)$ tensor. Let $\{\partial_{x^i}\}$ be a basis in TM_t. Let $\{dx^i\}$ be its dual bass in the cotangent space T^*M_t. The metric g has the representation

  $$g = g_{ij} dx^i \otimes dx^j,$$

  where $g_{ij} = g_{ji}$. The metric g_t induces a map (*flat*)

  $$\flat : TM_t \to T^*M_t, \quad \flat\partial_{x^i} = g_{ij} dx^j.$$

  The inverse map of $\flat$ is called $\sharp$ (the sharp operator).

  $$\sharp : T^*M_t \to TM_t, \quad \sharp\partial_{x^i} = g^{ij}\partial_{x^j}, \qquad \text{where } (g^{ij}) = (g_{ij})^{-1}.$$

- The deformation gradient F is $d\varphi_t$:

  $$d\varphi_t = d\mathbf{x}(t,X) = \frac{\partial x^i}{\partial X^\alpha} dX^\alpha \otimes \partial_{x^i}. \tag{8.9}$$

We can say that the matrix $(F^i_\alpha(X))$ is the matrix representation of $d\varphi_t(X)$ under the bases $\{\partial_{X^\alpha}\}$ and $\{\partial_{x^i}\}$. In this section, we just write

$$F(X) = d\varphi_t(X) = F^i_\alpha(X) dX^\alpha \otimes \partial_{x^i}.$$

- A tangent vector $V = V^\alpha \partial_{X^\alpha} \in T_X M_0$ is mapped to a tangent vector $\mathbf{v} = v^i \partial_{x^i} \in T_{\mathbf{x}} M_t$ by F:
$$\mathbf{v} = F(V) = F^i_\alpha \langle dX^\alpha | V^\beta \partial_{X^\beta} \rangle \otimes \partial_{x^i} = F^i_\alpha V^\alpha \partial_{x^i}.$$
We say that F is a TM_t-valued 1-form in M_0, denoted by $\Omega^1(M_0, TM_t)$. This is equivalent to say $F \in \Gamma(\mathrm{Hom}(TM_0, TM_t))$ is the space of all section maps from M_0 to $\mathrm{Hom}(TM_0, TM_t)$. Here, $\mathrm{Hom}(V,W)$ is the space of all linear maps from vector space V to vector space W. Note that $\mathrm{Hom}(V,W) \cong V^* \otimes W$, see Appendix C2 (3.1). Thus, F can be treated as a section map from M to $T^*M_0 \otimes TM_t$ with $F(X) \in T^*_X(M_0) \otimes T_{\mathbf{x}} M_t$ and $\mathbf{x} = \mathbf{x}(t,X)$. [9]

- Inverse deformation gradient F^{-1} maps a vector ∂_{x^i} in TM_t to a vector $(F^{-1})^\alpha_i \partial_{X^\alpha}$ in TM_0. Thus,
$$(F^{-1})(\mathbf{x}) \in Hom(T_{\mathbf{x}} M_t, T_X M_0) \cong T^*_{\mathbf{x}} M_t \otimes T_X(M_0) \quad with\ \mathbf{x} = \mathbf{x}(t,X).$$
The coordinate representation of (F^{-1}) is
$$\boxed{(F^{-1})(\mathbf{x}) = (F^{-1})^\alpha_i dx^i \otimes \partial_{X^\alpha} = \frac{\partial X^\alpha}{\partial x^i} dx^i \otimes \partial_{X^\alpha}.}$$

- The adjoint map F^*: The mapping $F : TM_0 \to TM_t$ induces a dual map
$$F^* : T^*M_t \to T^*M_0, \quad F^* = F^i_\alpha \partial_{X^\alpha} \otimes dx^i.$$

- The dual map (transpose) F^T: The transpose of F is $F^* \flat$
$$F^T : TM_t \xrightarrow{\flat} T^*M_t \xrightarrow{F^*} T^*M_0.$$
In component form
$$F^T(\mathbf{x}) = (F^T)^\alpha_i dx^i \otimes dX^\alpha = g_{ij} F^j_\alpha dx^i \otimes dX^\alpha.$$

- The map $F^{-T} := (F^T)^{-1}$, which is the inverse of F^T.
$$F^{-T} : T^*M_0 \xrightarrow{(F^*)^{-1}} T^*M_t \xrightarrow{\sharp} TM_t,$$
$$\boxed{F^{-T} = (F^{-1})^\alpha_j g^{ij} \partial_{X^\alpha} \otimes \partial_{x^i} = \frac{\partial X^\alpha}{\partial x^j} g^{ij} \partial_{X^\alpha} \otimes \partial_{x^i}.}$$

[9] In Marsden & Hughes's book, F is called a two-point tensor of type $(0,1;1,0)$.

- Right Cauchy-Green tensor: $C = F^T F$: Then $C : TM_0 \to T^*M_0$ with coordinate representation:

$$\boxed{C(X) = C_{\alpha\beta} dX^\alpha \otimes dX^\beta = F^j_\beta g_{ij} F^i_\alpha dX^\alpha \otimes dX^\beta}$$

  Note that C is symmetric. C is the pullback metric of g by φ_t from M_t to M_0. That is, $C = \varphi_t^*(g)$.

- Left Cauchy-Green tensor $B := F\sharp_0 F^* \flat$:

$$B : TM_t \xrightarrow{\flat} T^*M_t \xrightarrow{F^*} T^*M_0 \xrightarrow{\sharp_0} TM_0 \xrightarrow{F} TM_t.$$

  Here, $\sharp_0$ operator is the sharp operatot in M_0. The coordinate representation of B reads:

$$\boxed{B(\mathbf{x}) = B_{ij} dx^i \otimes dx^j = F^i_\alpha (g^0)^{\alpha\beta} F^k_\beta g_{jk} dx^i \otimes dx^j}$$

  Note that B is symmetric.

- $B^{-1} : T^*M_t \to TM_t$

$$B^{-1}(\mathbf{x}) = (B^{-1})^{ij} \partial_{x^i} \otimes \partial_{x^j}.$$

- We summarize the tensor types of various forms of strains by
  - $F \in \Gamma(T^*M_0 \otimes TM_t) \cong \Gamma(Hom(TM_0, TM_t))$
  - $F^{-1} \in \Gamma(T^*M_t \otimes TM_0) \cong \Gamma(Hom(T_{\mathbf{x}}M_t, T_X M_0))$
  - $C \in \Gamma(T^*M_0 \otimes T^*M_0) \cong \Gamma(Hom(TM_0, T^*M_0))$

8.3.2 Advection of Strain in terms of Lie Derivatives

- Let us treat F as $F = F^i_\alpha dX^\alpha \otimes \partial_{x^i}$. The advection of F: the Lie derivative of F (w.r.t. the second argument) is unchanged. That is,

$$\boxed{(\partial_t + \mathscr{L}_{\mathbf{v}}) F = 0.}$$

  See Appendix D3 (4.4).

- If we write F^{-1} as

$$(F^{-1})(\mathbf{x}) = (F^{-1})^\alpha_i \frac{\partial}{\partial X^\alpha} \otimes dx^i.$$

  The advection of F^{-1} is also the Lie derivative w.r.t. the second argument is unchanged:

$$\boxed{(\partial_t + \mathscr{L}_{\mathbf{v}})(F^{-1}) = 0.}$$

  See Appendix D3 (4.5).

- Left Cauchy-Green Strain: $B = B_{ij} dx^i \otimes dx^j$

$$\boxed{(\partial_t + \mathscr{L}_{\mathbf{v}}) B = 0.}$$

  See Appendix D3 (4.6).

- $B^{-1} = (B^{-1})^{ij} \partial_{x^i} \otimes \partial_{x^j}$:

$$\boxed{(\partial_t + \mathscr{L}_{\mathbf{v}}) (B^{-1}) = 0.}$$

  Homework. Check this.

8.4 Stress

The approach of stress in this section starts with the stress in the Eulerian coordinate system, called the Cauchy stress. Then we pull it back to the Lagrangian coordinate system, called the Piola-Kirchhoff stress. In the last subsection, we take the differential geometry approach. We define the Piola-Kirchhoff stress as the variation of an energy functional with respect to the deformation gradient. The Cauchy stress is the pull-back of the Piola-Kirchhoff stress by the inverse of the flow map.

8.4.1 The Stress Tensor in Eulerian Coordinate – Cauchy Stress

The stress is a surface force. It is a restoration force in response to material deformation. Imagine an elastic bar being stretched. You can measure a force on the cross-section opposite to the direction of the stretching. This is the stress. It is the surface force measured per unit area. The existence of the stress is based on the following Cauchy stress principle.

Axiom of Cauchy Stress Principle For an elastic material occupying Ω_t under a body force $\mathbf{f}$ and surface force $\mathbf{g}$, it holds that for any $\mathbf{x} \in \Omega_t$, any small surface $dS \subset \Omega_t$ with normal ν, *there exists a surface force* $\mathbf{t}(\mathbf{x}, \nu)$ *on* dS such that $\mathbf{t} = \mathbf{g}$ on the boundary $\partial\Omega_t$. We call $\mathbf{t}(\mathbf{x}, \nu)$ the Cauchy stress vector, or a tensile force. The Cauchy stress vector is characterized by the following Cauchy theorem.

Theorem 8.7 (Cauchy)**.** *Assuming the Cauchy stress principle.*

- *In addition, assuming Principle of linear momentum:*

$$\int_G \rho \dot{\mathbf{v}} \, d\mathbf{x} = \int_{\partial G} \mathbf{t} \, dS + \int_G \mathbf{f} \, d\mathbf{x}$$

  for any domain $G \subset \Omega_t$*. Then, there exists a tensor* $\sigma(\mathbf{x})$ *such that*

$$\mathbf{t}(\mathbf{x}, \nu) = \sigma(\mathbf{x}) \cdot \nu. \tag{8.10}$$

- *In addition, assuming Principle of angular momentum:*

$$\int_G \rho\, \mathbf{x} \times \frac{d\mathbf{v}}{dt}\, d\mathbf{x} = \int_{\partial G} \mathbf{x} \times \sigma \cdot \nu\, dS + \int_G \mathbf{x} \times \mathbf{f}\, d\mathbf{x}$$

for any $G \subset \Omega_t$, then

$$\sigma(\mathbf{x}) \textit{ is symmetric.} \tag{8.11}$$

Proof. 1. To show (8.10), given ν, we consider a plane with normal ν. The plane intersects the coordinate axes $\mathbf{e}_1, \mathbf{e}_2, \mathbf{e}_3$ at A_1, A_2, A_3, respectively. Let us consider the pyramid $OA_1A_2A_3$, call it ΔG. The surface $A_1A_2A_3$ is denoted by ΔS, and the three sides of the pyramid are denoted by ΔS_i. The conservation of linear momentum on ΔG reads

$$\int_{\Delta G} \rho \frac{d\mathbf{v}}{dt}\, d\mathbf{x} = \int_{\Delta S} \mathbf{t}(\mathbf{x}, \nu)\, dS + \sum_{i=1}^{3} \int_{\Delta S_i} \mathbf{t}(\mathbf{x}, -\mathbf{e}_i)\, dS + \int_{\Delta G} \mathbf{f}\, d\mathbf{x}.$$

By dividing both sides by ΔS then take $\Delta S \to 0$, we can get

$$\int_{\Delta G} \rho \frac{d\mathbf{v}}{dt}\, d\mathbf{x} \to 0, \quad \int_{\Delta G} \mathbf{f}\, d\mathbf{x} \to 0$$

because $\Delta G / \Delta S \to 0$, and

$$\mathbf{t}(\mathbf{x}, \nu) = -\sum_{i=1}^{3} \nu_i \mathbf{t}(\mathbf{x}, -\mathbf{e}_i)$$

because

$$\nu \Delta S = (\Delta S_1, \Delta S_2, \Delta S_3).$$

On the other hand, from Newton's third law, we can get $\mathbf{t}(\mathbf{x}, -\mathbf{e}_i) = -\mathbf{t}(\mathbf{x}, \mathbf{e}_i)$. We conclude that $\mathbf{t}$ is linear in ν.

2. The principle of moments (conservation of angular momentum) reads

$$\int_G \rho \left(\mathbf{x} \times \frac{d\mathbf{v}}{dt} \right) d\mathbf{x} = \int_{\partial G} (\mathbf{x} \times \sigma \cdot \nu) dS + \int_G \mathbf{x} \times \mathbf{f}\, d\mathbf{x},$$

where the left-hand side is the change of the total angular momentum. The first term on the right-hand side is the total surface torque, the second term is the total body toque. In terms of differential equation, it reads:

$$\rho \mathbf{x} \times \frac{d\mathbf{v}}{dt} = \nabla_{\mathbf{x}} \cdot (\mathbf{x} \times \sigma) + \mathbf{x} \times \mathbf{f}.$$

On the other hand, from linear momentum equation:

$$\rho \frac{d\mathbf{v}}{dt} = \nabla_{\mathbf{x}} \cdot \sigma + \mathbf{f},$$

we take cross product of it with $\mathbf{x}$ to get

$$\rho \mathbf{x} \times \frac{d\mathbf{v}}{dt} = \mathbf{x} \times (\nabla_{\mathbf{x}} \cdot \sigma) + \mathbf{x} \times \mathbf{f}.$$

This leads to

$$\nabla_{\mathbf{x}} \cdot (\mathbf{x} \times \sigma) = \mathbf{x} \times (\nabla_{\mathbf{x}} \cdot \sigma). \tag{8.12}$$

The left-hand term in coordinate form is

$$\begin{aligned} \partial_l (\varepsilon_{ijk} x^j \sigma^{kl}) &= \varepsilon_{ijk} \delta_l^j \sigma^{kl} + \varepsilon_{ijk} x^j \partial_l \sigma^{kl} \\ &= \varepsilon_{ijk} \sigma^{kj} + \varepsilon_{ijk} x^j \partial_l \sigma^{kl} \end{aligned}$$

The right-hand term $\mathbf{x} \times (\nabla_{\mathbf{x}} \cdot \sigma)$ in coordinate form is $\varepsilon_{ijk} x^j \partial_l \sigma^{kl}$. Comparing both sides of (8.12), we get

$$\varepsilon_{ijk} \sigma^{kj} = 0.$$

That is,

$$\sigma^{ij} = \sigma^{ji}.$$

□

Thus, by assuming the conservation of linear momentum, the conservation of angular momentum is equivalent to the symmetry of the stress tensor.

Remarks

- If there is no internal torque, then the principle of moment is valid. In general, the Cauchy stress is not necessarily symmetric for complex fluids. For instance, the liquid crystal looks like fluids with rods. In equilibrium and below certain critical temperature, the rods align with each other. The corresponding stress is symmetric. However, *in non-equilibrium, rods may not align to the same direction. There is an internal torque try to align them to reach equilibrium.* This internal torque is the source of asymmetry of the Cauchy stress.

- *The symmetry of the Cauchy is a property of equilibrium state.* If the relaxation time of the material response to the deformation is very short as compared with the macroscopic time dt, we can treat the deformation process is in equilibrium at every instance. In this case, we treat the Cauchy stress to be symmetric.

8.4.2 Geometric View of the Cauchy Stress Tensors

1. **The tensor type of the Cauchy stress tensor** We recall that the Cauchy stress tensor σ is a representation of the tensile force $\mathbf{t}(\mathbf{x},\nu)$ on the area dS with normal ν:

$$\sigma : \nu \mapsto (\mathbf{t} \text{ on } \nu dS)$$

- The force is treated as a covector, because for conservative force $\mathbf{f} = -dV$ for some potential V. The type of $\mathbf{f}$ is a covector (i.e. it is in T^*M_t). Thus, we express this tensile force as $\mathbf{t} = t_j dx^j$.
- We claim that the tensor σ is a covector-valued 2-form:

$$\boxed{\sigma = \sigma^i_j(\star dx^i) \otimes dx^j.} \tag{8.13}$$

We recall that the tensor $\mathbf{t}(\mathbf{x},\nu)$ is a surface force on the area dS. In the Language of differential geometry, νdS is the vector valued 2-form:

$$\nu dS = (dx^2 \wedge dx^3, dx^2 \wedge dx^3, dx^2 \wedge dx^3).$$

This is also expressed as $(\star dx^1, \star dx^2, \star dx^3)$, or $\star d\mathbf{x}$. It reads two two tangent vector $\mathbf{v},\mathbf{w} \in T_{\mathbf{x}}M_t$ with output

$$\star d\mathbf{x}(\mathbf{v},\mathbf{w}) = \mathbf{v} \times \mathbf{w},$$

which is a directed surface area. Its area is $\|\mathbf{v}\times\mathbf{w}\|$, and its direction is the normal $(\mathbf{v}\times\mathbf{w})/\|\mathbf{v}\times\mathbf{w}\|$, which we denoted by ν. Thus, the stress $\mathbf{t}$ on the surface spanned by two vectors $\mathbf{v},\mathbf{w}$ is

$$\mathbf{t} = \sigma(\mathbf{v},\mathbf{w}) = \sigma^i_j(\star dx^i)(\mathbf{v},\mathbf{w})dx^j.$$

In other words,

$$\sigma : T_{\mathbf{x}}M_t \otimes T_{\mathbf{x}}M_t \to T_{\mathbf{x}}^*M_t, \quad \text{or} \quad \sigma \in \Omega^2(M_t) \otimes T^*(M_t).$$

- Note that $\Omega^2(M_t)$ has basis $dx^2 \wedge dx^3, dx^3 \wedge dx^1, dx^1 \wedge dx^2$. They are also expressed as $\star dx^i$, $i = 1,2,3$ by using the Hodge star operator. This shows that the dual space of $\left(\Omega^1(M_t)\right)^*$ is $\Omega^2(M_t)$ by using the Hodge star operator. By using Hodge star operator again, we get

$$\left(\Omega^2(M_t)\right)^* = \Omega^1(M_t) = T^*M_t.$$

Thus, we can also treat

$$\sigma \in Hom(T^*M_t, T^*M_t).$$

2. **Change tensor type of the Cauchy stress** Since we have a metric g in the world space M_t, we can change σ from covector valued two-form to a vector-valued two-form:
$$\bar{\sigma} = \sharp\sigma.$$
$$\bar{\sigma}^{ij} := g^{ik}\sigma^i_k.$$
Then
$$\bar{\sigma} \in \Omega^2(M_t)\otimes TM_t \cong Hom(\Omega^1(M_t), TM_t) = Hom(T^*M_t, TM_t).$$
From the definition of the adjoint operation, $\bar{\sigma}^* \in Hom(T^*M_t, TM_t)$. In this case, we can argue that
$$\bar{\sigma}^* = \bar{\sigma}, \quad \bar{\sigma}^{ji} = \bar{\sigma}^{ij}.$$
Thus, the stress discussed in the last section is indeed $\bar{\sigma}$.

8.4.3 The Stress Tensor in Lagrangian Coordinate – Piola-Kirchhoff Stress

The Cauchy stress is defined in the Eulerian coordinate system. We can pull it back to the Lagrange coordinate system. The corresponding stress is called the Piola-Kirchhoff stress.

There are two kinds of Piola-Kirchhoff stress tensors:

- The first Piola-Kirchhoff stress P is the pullback of the Cauchy stress σ via φ_t only in the first argument:
$$\begin{aligned} P &= P^\alpha_i(\partial_{X^\alpha}\otimes\hat{\mu})\otimes dx^i \\ &= (\varphi_t^{-1})^*\left(\sigma^j_i(\partial_{x^j}\otimes\mu)\right)\otimes dx^i \\ &= J\sigma^j_i(F^{-1})^\alpha_j(\partial_{X^\alpha}\otimes\hat{\mu})\otimes dx^i \\ &= J\sigma^j_i\frac{\partial X^\alpha}{\partial x^j}(\partial_{X^\alpha}\otimes\hat{\mu})\otimes dx^i, \end{aligned}$$
$$P = J\sigma F^{-T}.$$
- The second Piola-Kirchhoff stress is the pullback of the first Piola-Kirchhoff stress P via φ_t for the second argument:
$$\begin{aligned} \Sigma &= \Sigma^{\alpha\beta}(\partial_{X^\alpha}\otimes\hat{\mu})\otimes dX^\beta \\ &= P^\alpha_i(\partial_{X^\alpha}\otimes\hat{\mu})\otimes(\varphi_t^{-1})^*(dx^i) \\ &= P^\alpha_i(\partial_{X^\alpha}\otimes\hat{\mu})\otimes(F^{-1})^\beta_i dX^\beta \\ &= (F^{-1})^\beta_i P^\alpha_i(\partial_{X^\alpha}\otimes\hat{\mu})\otimes dX^\beta. \end{aligned}$$

which has range in material space, not in the world space. On the other hand, P has its range in world space. Note that Σ is the pullback of P for its second argument (from world space to material space. That is

$$\Sigma = F^{-1}P.$$

8.4.4 Geometric View of Stress

In this subsection, we shall assume that there is a stored energy density W which is a function of the deformation gradient. The stress is a derived quantity.

1. **From a vector $\mathbf{v} \in TM_0$ to an $(n-1)$-form (flux)**: Let $\mathbf{v} \in TM_0$, we define an $(n-1)$-form by
$$\mathbf{v} \otimes \hat{\mu} \mapsto i_{\mathbf{v}}(\hat{\mu})$$
$i_{\mathbf{v}} : \Omega^k(M) \to \Omega^{k-1}(M)$ is called an interior product.
$$i_{\mathbf{v}}\omega[\mathbf{v}_1, ..., \mathbf{v}_{k-1}] = \omega[\mathbf{v}, \mathbf{v}_1, ..., \mathbf{v}_{k-1}].$$
The $(n-1)$-form $i_{\mathbf{v}}(\hat{\mu})$ is called a *flux*. Thus, with the help of $\hat{\mu}$, we have
$$TM_0 \otimes \Lambda^n(T^*M_0) \cong \Lambda^{n-1}(T^*M_0).$$

2. **The first Piola-Kirchhoff stress:**

   - Derivation of Piola stress from internal energy. Given a constitutive equation of state (the internal energy or Helmholtz free energy):
   $$\mathscr{U}(F) = \int_{\hat{M}} W(F)\hat{\mu},$$
   define
   $$P(F) := \frac{\delta \mathscr{U}(F)}{\delta F} = \frac{\partial W}{\partial F^i_\alpha}(\partial_{X^\alpha} \otimes \hat{\mu}) \otimes dx^i, \quad P_i^\alpha := \frac{\partial W}{\partial F^i_\alpha}.$$
   Thus, the first Piola-Kirchhoff stress is derived from the variation of the energy functional with respective to the deformation gradient.
   - Tensor form of a Piola stress. The first Piola stress P is defined so that it is paired with a deformation gradient and form an energy density. That is $F \wedge P(F) = W(F)\hat{\mu}$. Since we express $F = F^i_\alpha dX^\alpha \otimes \partial_{x^i}$, P must have the form
   $$P(F) = P_i^\alpha(F)(\partial_{X^\alpha} \otimes \hat{\mu}) \otimes dx^i. \tag{8.14}$$

This means that $P \in \Omega^{n-1}(M_0) \otimes T^*M_t$ (i.e. a two-point tensor of type $(0,2;0,1)$), or a covector-valued $(n-1)$-form (i.e. $\Omega^2(M_0, T^*M_t)$). Recall that F is a vector-valued 1-form. The pairing of P and F is

$$W(F)\hat{\mu} := F \wedge P = F^i_\alpha P^\alpha_i dX^\alpha \wedge (\partial_{X^\alpha} \otimes \hat{\mu}) \langle \partial_{x^i} | dx^i \rangle = F^i_\alpha P^\alpha_i \hat{\mu}. \tag{8.15}$$

3. **The second Piola-Kirchhoff stress Σ:** The stress Σ is defined as

$$\Sigma := \frac{\delta \mathscr{U}(C)}{\delta C} = \frac{\partial W}{\partial C^\beta_\alpha} (\partial_{X^\alpha} \otimes \hat{\mu}) \otimes dX^\beta, \quad \Sigma^\alpha_\beta := \frac{\partial W}{\partial C^\beta_\alpha}$$

where $C = F^T F$ is the right Cauchy-Green strain. We shall see in the Chapter of Stress-Strain relation, the stored energy density can be written as a function of C (instead of F). Since C is symmetric, we conclude that Σ is also symmetric.[10]

4. **Cauchy stress.** The Cauchy stress has the form

$$\sigma = \sigma^j_i (\partial_{x^j} \otimes \mu) \otimes dx^i.$$

It is a covector-valued $(n-1)$-form (i.e. $\Omega^{n-1}(M_t, T^*M_t)$). It is the pullback of P by φ_t^{-1}.

$$\begin{aligned} \sigma = \left(\varphi_t^{-1}\right)^* (P) &= P^\alpha_i \left(\varphi_t^{-1}\right)^* (\partial_{X^\alpha} \otimes \hat{\mu}) \otimes dx^i \\ &= P^\alpha_i J^{-1} \frac{\partial x^j}{\partial X^\alpha} (\partial_{x^j} \otimes \mu) \otimes dx^i, \end{aligned}$$

$$\sigma^j_i = P^\alpha_i J^{-1} \frac{\partial x^j}{\partial X^\alpha}.$$

Or equivalently, P is the pullback of σ with respective to its first argument:

$$\begin{aligned} \varphi_t^*(\sigma) &= \sigma^j_i \varphi_t^* (\partial_{x^j} \otimes \mu) \otimes dx^i \\ &= \sigma^j_i J (F^{-T})^\alpha_j (\partial_{X^\alpha} \otimes \hat{\mu}) \otimes dx^i \\ &= P^\alpha_i (\partial_{X^\alpha} \otimes \hat{\mu}) \otimes dx^i \\ &= P. \end{aligned}$$

5. σ is also the pullback of Σ by φ_t^{-1} with respective to its both argument.

[10] The symmetry of Σ is from the symmetry of C and the fact that W is a function of C. This is based on the frame-indifference and isotropic assumption of the material. We will study this property in the chapter of stress-strain relation.

Or equivalently, Σ is the pull-back of σ with respect to both arguments to M_0: That is

$$\begin{aligned}\Sigma = \varphi_t^*(\sigma) &= \sigma_i^j \varphi_t^*(\partial_{x^j} \otimes \mu) \otimes \varphi_t^*(dx^i)\\ &= \sigma_i^j J (F^{-T})_j^\alpha (F^{-1})_i^\beta (\partial_{X^\alpha} \otimes \hat{\mu}) \otimes dX^\beta\\ &= \Sigma_\beta^\alpha (\partial_{X^\alpha} \otimes \hat{\mu}) \otimes dX^\beta.\end{aligned}$$

Remark. The symmetry of σ comes from te symmetry of Σ.
Σ is also the pullback of P with respect to the second argument:

$$\Sigma := F^{-1} P.$$

It is the Lagrangian covector-valued 2-form in Lagrangian coordinate.

Chapter 9

Stress-Strain Relation for Elasticity

9.1 Constitutive Relation: Stress-Strain Relation

The stress is a surface force in response to material deformation. It can depend on the deformation gradient F, or higher order derivatives of the deformation, or even the history of F (i.e. $\{F(s)|s \le t\}$). We first give some definitions for commonly used materials.

- **Cauchy-elastic material** The *Cauchy-elastic materials* are those materials (also called rubber-like) whose stress tensor σ is only a function of the current deformation gradient F. That is,
$$\sigma(\mathbf{x}) = T(X,F)$$
Such a relation is called a constitutive relation, and T is called a *response function*. If T is independent of X, the material is called *homogeneous*.

- **Hyper-elastic materials** *The hyper-elastic materials are materials whose mechanical stresses are conservative.* This means that the work done by the stress through a closed-loop deformation is zero. This definition is equivalent to:
there exists a mechanical potential function $W(F)$ such that the Piola stress is $P = W'(F)$. Note that the hyper-elastic material is a special case of Cauchy-elastic material.

Below, we shall characterize the response functions of Cauchy-elastic materials and hyper-elastic materials. The basic assumption for the response function T is the frame-indifference assumption.

9.1.1 Frame Indifference

1. **Axiom of material frame-indifference for Cauchy-elastic materials** *The response function $T(F)$ for a Cauchy-elastic material should satisfy*

$$\boxed{T(OF) = OT(F)O^T \text{ for any rotation } O \in O(3).} \tag{9.1}$$

The reason is the follows. The stress should be independent of the frame of reference in the observer's space. Suppose we have two frames in the observer's space. Let $\mathbf{x}$ be the coordinate of the original frame, and $\mathbf{x}^*$ the coordinate in new frame, which is a rotation of the old frame. That is, $\mathbf{x}^* = O\mathbf{x}$, and O is a rotation. Then, we have $F^* := \partial \mathbf{x}^*/\partial X = OF$. Note that the normal and the tensile vector in the old and new frames are related by $\nu^* = O\nu$, $\mathbf{t}^* = O\mathbf{t}$. In terms of the response function, it reads

$$\begin{aligned} \mathbf{t}^* &= T(OF)\nu^* = T(OF)O\nu \\ O\mathbf{t} &= OT(F)\nu. \end{aligned}$$

Hence, $T(OF) = OT(F)O^T$.

The above frame-indifference can be expressed in terms of the Piola stress $P := J\sigma F^{-T}$. It reads

$$P(OF) = JT(OF)(OF)^{-T} = J(OT(F)O^T)O^{-T}F^{-T} = OJT(F)F^{-T} = OP(F).$$

That is,

$$\boxed{P(OF) = OP(F) \text{ for any rotation } O \in O(3).} \tag{9.2}$$

2. **Axiom of material frame-indifference for hyper-elastic materials** The potential energy W remains the same when we change to a new frame through rotation. That is

$$\boxed{W(OF) = W(F) \text{ for any rotation } O \in O(3).} \tag{9.3}$$

This definition is equivalent to the above definition. Indeed, we differentiate $P(F) = \frac{\partial W}{\partial P}(F)$ in F to get

$$P(F) = \frac{\partial}{\partial F}W(F) \stackrel{?}{=} \frac{\partial}{\partial F}W(OF) = O^T\frac{\partial W(OF)}{\partial (OF)} = O^T P(OF),$$

where

$$\frac{\partial W(OF)}{\partial F^i_\alpha} = \partial_{F^i_\alpha} W(O^j_k F^k_\beta) = W_{F^j_\beta}(OF)O^j_k\delta^{ik}\delta_{\alpha\beta} = O^j_i W_{F^j_\alpha}(OF) = O^j_i P(OF)^\alpha_j.$$

Thus, $P(OF) = OP(F)$ if and only if $\frac{\partial}{\partial F}(W(OF) - W(F)) = 0$.

9.1.2 Isotropic Materials

1. **Definition** *A material is called isotropic if its stress tensor is identical in all direction of the material.* More precisely, suppose we have two identical materials. One has material coordinate X, while the other is X^* with $X = OX^*$ and O being a rotation. The corresponding deformation gradient $F^* = \frac{\partial \mathbf{x}}{\partial X^*} = \frac{\partial \mathbf{x}}{\partial X}\frac{\partial X}{\partial X^*} = FO$. If these two materials deform in the same way and result in the same stresses, we call such material *isotropic*. Mathematically, this means

$$\boxed{T(FO) = T(F).} \tag{9.4}$$

This isotropic property can be expressed in terms of the Piola stress as the follows.

$$P(FO) = P(F)O \quad \text{for all rotation } O. \tag{9.5}$$

This follows from

$$P(FO) = JT(FO)(FO)^{-T} = JT(F)F^{-T}O = P(F)O.$$

2. **Isotropic property for hyper-elastic materials** A hyper-elastic material is isotropic if and only if

$$\boxed{W(FO) = W(F) \text{ for all } O \in O(3).} \tag{9.6}$$

This is because

$$P(F) = \frac{\partial}{\partial F}W(F) \stackrel{?}{=} \frac{\partial}{\partial F}W(FO) = \frac{\partial W(FO)}{\partial (FO)}O^T = P(FO)O^T.$$

where

$$\partial_{F^i_\alpha} W(F^j_\beta O^\beta_\gamma) = W_{F^j_\gamma}(FO)\frac{\partial F^j_\beta O^\beta_\gamma}{\partial F^i_\alpha} = \bar{P}^\gamma_j \delta^{ij}\delta_{\alpha\beta}O^\beta_\gamma = \bar{P}^\gamma_i O^\alpha_\gamma.$$

Here, $\bar{P}^\gamma_j := W_{F^j_\gamma}(FO) = P(FO)^\gamma_j$. Thus, $P(F)O = P(FO)$ is equivalent to $\frac{\partial}{\partial F}(W(FO) - W(F)) = 0$.

9.1.3 Representation of the Cauchy Stress

Some notations:

1. Let $\mathbb{M}^+(3)$, $\mathbb{S}^3$, $O(3)$ respectively be the set of all 3×3 matrices with positive determinants, symmetric positive definite matrices and rotation matrices.

2. Given a matrix $A \in \mathbb{M}_3$, its characteristic polynomial is defined as

$$p(\lambda) := \det(A - \lambda I) = -\lambda^3 + \iota_1 \lambda^2 - \iota_2 \lambda + \iota_3,$$

where the coefficients $\iota_1, \iota_2, \iota_3$ are called the *principal invariants of* A, which are given in terms of eigenvalues λ_1, λ_2, λ_3 of A as below:

$$\iota_1 = trA = \lambda_1 + \lambda_2 + \lambda_3 \tag{9.7}$$

$$\iota_2 = \frac{1}{2}\left((trA)^2 - tr(A^2)\right) = tr(\mathrm{Cof}A) = \lambda_1\lambda_2 + \lambda_2\lambda_3 + \lambda_3\lambda_1 \tag{9.8}$$

$$\iota_3 = \det A = \lambda_1\lambda_2\lambda_3. \tag{9.9}$$

The set of these principal invariants of A is denoted by ι_A.

Characterization of response functions

Proposition 9.6. *The response function $T(F)$ of an isotropic Cauchy material can be expressed as*

$$T(F) = \hat{T}(B), \quad B = FF^T$$

with $\hat{T}$ satisfying

$$\hat{T}(OBO^T) = O\hat{T}(B)O^T \text{ for any } B \in \mathbb{S}^3, \quad O \in O(3).$$

Proof. 1. For any $F \in \mathbb{M}^+(3)$, we can express it in polar form: $F = S_l O$ with $O \in O(3)$ and $S_l \in \mathbb{S}_3$. Then

$$B := FF^T = S_l O O^T S_l = S_l^2.$$

From (9.4), we have

$$T(F) = T(S_l O) \overset{(9.4)}{=} T(S_l) = \hat{T}(S_l^2) = \hat{T}(B) = \hat{T}(FF^T).$$

2. Suppose $B \in \mathbb{S}^3$. Then there exists S_l such that $B = S_l^2$. For any $O \in O(3)$, we have

$$\hat{T}(OBO^T) = \hat{T}(OS_l^2O^T) = \hat{T}(OS_l(OS_l)^T) = T(OS_l) \overset{(9.1)}{=} OT(S_l)O^T = O\hat{T}(B)O^T.$$

□

Representation of isotropic Cauchy stress

Theorem 9.8 (Rivlin-Ericksen representation Theorem for Cauchy stress)**.** *An isotropic Cauchy stress (i.e. frame-indifference + isotropicity) has the following representation*

$$\hat{T}(B) = \beta_0(\iota_B)I + \beta_1(\iota_B)B + \beta_2(\iota_B)B^2,$$

for some smooth functions β_i, $i = 0,1,2$.

This theorem is a corollary of the following representation theorem.

Theorem 9.9 (Rivlin-Ericksen Representation Theorem)**.** *Suppose a function $\hat{T} : \mathbb{S}^3 \to \mathbb{S}^3$ satisfying*

$$\hat{T}(OQO^T) = O\hat{T}(Q)O^T \quad \textit{for all } O \in O(3),$$

then it has the representation:

$$\hat{T}(Q) = \beta_0(Q)I + \beta_1(Q)Q + \beta_2(Q)Q^2$$

for some smooth scalar functions $\beta_i(Q)$, $i = 0,1,2$.

Proof.

1. Let λ_i and p_i, $i = 1,2,3$ be the eigenvalues and eigenvectors of Q. The proof of this theorem is divided into three cases: (i) λ_i are distinct, (ii) $\lambda_1 \neq \lambda_2 = \lambda_3$, (iii) all eigenvalues are equal.

2. Case 1, λ_i are distinct: We have

$$\begin{cases} I = p_1p_1^T + p_2p_2^T + p_3p_3^T \\ Q = \lambda_1 p_1p_1^T + \lambda_2 p_2p_2^T + \lambda_3 p_3p_3^T \\ Q^2 = \lambda_1^2 p_1p_1^T + \lambda_2^2 p_2p_2^T + \lambda_3^2 p_3p_3^T. \end{cases}$$

The condition λ_i being distinct leads to an inversion from $(p_1p_1^T, p_2p_2^T, p_3p_3^T)$ to I, Q, Q^2. Next, from $\hat{T}(O^TQO) = O^T\hat{T}(Q)O$, we see that $\hat{T}(Q)$ can be diagonalized by $O = [p_1, p_2, p_3]$. That is

$$O^TQO = \mathrm{diag}(\lambda_1, \lambda_2, \lambda_3) = \Lambda,$$

$$\begin{aligned} \hat{T}(Q) &= O\hat{T}(O^TQO)O^T = O\hat{T}(\Lambda)O^T \\ &= \mu_1 p_1p_1^T + \mu_2 p_2p_2^T + \mu_3 p_3p_3^T. \end{aligned}$$

with μ_i are functions of λ_i only. By inverting $(p_1p_1^T, p_2p_2^T, p_3p_3^T)$ to I, Q, Q^2, we get that $\hat{T}(Q)$ can be expressed in terms of I, Q, Q^2 with coefficients depending on Q.

3. Case 2, $\lambda_1 \neq \lambda_2 = \lambda_3$: We have

$$I = p_1 p_1^T + (p_2 p_2^T + p_3 p_3^T)$$
$$Q = \lambda_1 p_1 p_1^T + \lambda_2 (p_2 p_2^T + p_3 p_3^T)$$

   Since $\lambda_1 \neq \lambda_2$, we can invert $(p_1 p_1^T, p_2 p_2^T + p_3 p_3^T)$ to I, Q. Next, the spectral mapping theorem gives
$$\hat{T}(Q) = \mu_1 p_1 p_1^T + \mu_2 p_2 p_2^T + \mu_3 p_3 p_3^T.$$
   We claim that $\mu_2 = \mu_3$. From $\hat{T}(O^T Q O) = O^T \hat{T}(Q) O$ and taking $O = [p_1, p_2, p_3]$, wee see that O can diagonalize Q as well as $\hat{T}(Q)$. Since in the subspace spanned by p_2 and p_3, the matrix Q representation under the basis $\{p_2, p_3\}$ is $\lambda_2 I$. Thus, the same matrix representation for $\hat{T}(Q)$ also has the form μI. This shows $\mu_2 = \mu_3$. This leads to
$$\hat{T}(Q) = \beta_0(Q) I + \beta_1(Q) Q.$$

4. Case 3, $\lambda_1 = \lambda_2 = \lambda_3$: In this case, we have $\hat{T}(Q) = \beta_0(Q) I$.

5. It remains to show that $\beta_i(Q)$ are indeed functions of the invariants of Q. For case 1, from the independence of I, Q, Q^2 and $\hat{T}(OQO^T) = O\hat{T}(Q)O^T$, we can choose O to diagonalize Q, then $\beta_i(Q) = \beta_i(OQO^T) = \beta_i(\text{diag}(Q))$. This leads to β_i are only functions of the three principal invariants. The proofs for the other two cases are similar.

□

Homework Show that the second Piola stress $\Sigma := F^{-1}P$ has the following representation:
$$\Sigma(C) = \gamma_0(\iota_C) I + \gamma_1(\iota_C) C + \gamma_2(\iota_C) C^2$$
where $C = F^T F$, the right Cauchy-Green deformation tensor.

9.1.4 Representation of Isotropic Hyper-elastic Stress

The goal of this subsection is to have representation of Cauchy stress in terms of invariants of F. Firs, we have an important property of the hyper-elastic materials.

Proposition 9.7. *The Cauchy stress σ of hyper-elastic material is symmetric.*

Proof. 1. The potential energy function W for a hyper-elastic material satisfies the frame-indifference hypothesis: $W(OF) = W(F)$ for all $O \in O(3)$. This implies the potential W can be expressed in terms of $F^T F$:

$$W(F) = W(OS_r) = W(S_r) := \check{W}(C), \quad C = F^T F = S_r^2.$$

2. The Cauchy stress can be expressed as

$$
\begin{aligned}
\sigma_{ij} &= J^{-1} P^i_\alpha F^j_\alpha = J^{-1} \frac{\partial W}{\partial F^i_\alpha} F^j_\alpha \\
&= J^{-1} \frac{\partial \check{W}}{\partial C_{\beta\gamma}} \frac{\partial C_{\beta\gamma}}{\partial F^i_\alpha} F^j_\alpha = J^{-1} \frac{\partial \check{W}}{\partial C_{\beta\gamma}} \frac{\partial (F^k_\beta F^k_\gamma)}{\partial F^i_\alpha} F^j_\alpha \\
&= J^{-1} \frac{\partial \check{W}}{\partial C_{\beta\gamma}} \left(\delta^{ik} \delta_{\beta\alpha} F^k_\gamma + \delta^{ik} \delta_{\gamma\alpha} F^k_\beta \right) F^j_\alpha \\
&= J^{-1} \frac{\partial \check{W}}{\partial C_{\beta\gamma}} \left(F^i_\gamma F^j_\beta + F^i_\beta F^j_\gamma \right) \\
&= 2J^{-1} \frac{\partial \check{W}}{\partial C_{\beta\gamma}} F^i_\gamma F^j_\beta \\
&= 2J^{-1} \frac{\partial \check{W}}{\partial C_{\gamma\beta}} F^j_\beta F^i_\gamma = \sigma_{ji}
\end{aligned}
$$

Here, we have used symmetry of $C = F^T F$.

□

Remark The symmetry of the Cauchy stress for hyper-elastic materials is a consequence of hyper-elasticity and frame-indifference. The is to compare with the symmetry property derived from the principle of conservation of angular momentum.

Proposition 9.8. *For isotropic hyper-elastic material, σ can also be represented in terms of B:*

$$\boxed{\sigma = 2J^{-1} \hat{W}_B B.} \tag{9.10}$$

Proof. Recall $B^{k\ell} = F^k_\beta F^\ell_\beta$. We have

$$
\begin{aligned}
P^i_\alpha = W_{F^i_\alpha} = \frac{\partial \hat{W}(FF^T)}{\partial F^i_\alpha} &= \hat{W}_{B^{k\ell}} \frac{\partial B^{k\ell}}{\partial F^i_\alpha} = \hat{W}_{B^{k\ell}} \frac{\partial F^k_\beta F^\ell_\beta}{\partial F^i_\alpha} \\
&= \hat{W}_{B^{k\ell}} \left(\delta^{ik} \delta_{\alpha\beta} F^\ell_\beta + F^k_\beta \delta^{i\ell} \delta_{\alpha\beta} \right) = \hat{W}_{B^{i\ell}} F^\ell_\alpha + \hat{W}_{B^{ki}} F^k_\alpha \\
&= 2\hat{W}_{B^{ik}} F^k_\alpha
\end{aligned}
$$

Here, we have used symmetries of $B = FF^T$ and $\hat{W}_B$. Thus,

$$\sigma^{ij} = J^{-1} P^i_\alpha F^j_\alpha = 2J^{-1} \hat{W}_{B^{ik}} F^k_\alpha F^j_\alpha = 2J^{-1} \hat{W}_{B^{ik}} B^{kj}.$$

□

Proposition 9.9. *The stored energy $W(F)$ of an isotropic hyper-elastic material satisfies*

$$W(F) = \overline{W}(\imath(FF^T)).$$

Proof. 1. Recall isotropicity: $W(FO) = W(F)$ for all $O \in O(3)$.

2. Let $F = O_{\mathbf{n}}\Lambda O_{\mathbf{N}}^T$ be the singular value decomposition of F, then

$$W(F) = W(O_{\mathbf{n}}\Lambda O_{\mathbf{N}}^T) = W(\Lambda).$$

There is a 1-1 correspondence between $\{\imath(F)\}$ and $\{\imath(FF^T)\}$, thus we can express

$$W(F) = \overline{W}(\imath_1(B), \imath_2(B), \imath_3(B)),$$

where $B = FF^T$.

□

Homework Check (11.7).

Theorem 9.10 (Representation of stress)**.** *Let us denote the invariants $\imath_k(B)$ by I_k. The Cauchy stress for an isotropic hyper-elastic material with restoration energy function $\overline{W}(I_1, I_2, I_3)$ is given by*

$$\sigma = \frac{2}{\sqrt{I_3}}\left(I_3\overline{W}_{I_3}I + (\overline{W}_{I_1} + I_1\overline{W}_{I_2})B - \overline{W}_{I_2}B^2\right) \tag{9.11}$$

Another Finger's formula is

$$\sigma = \frac{2}{\sqrt{I_3}}\left((I_2\overline{W}_{I_2} + I_3\overline{W}_{I_3})I + \overline{W}_{I_1}B - I_3\overline{W}_{I_2}B^{-1}\right). \tag{9.12}$$

Proof. 1. We use $\sigma = 2J^{-1}\hat{W}_B B$.

2. The formula $\hat{W}_B$ in terms of I_1, I_2, I_3 is given by the second Finger's formula below with Q replaced by B.

$$\begin{aligned}
\sigma &= 2J^{-1}\hat{W}_B B \\
&= 2J^{-1}[(\overline{W}_{I_1} + I_1\overline{W}_{I_2})I - \overline{W}_{I_2}B + I_3\overline{W}_{I_3}B^{-1}]B \\
&= 2J^{-1}[I_3\overline{W}_{I_3}I + (\overline{W}_{I_1} + I_1\overline{W}_{I_2})B - \overline{W}_{I_2}B^2]
\end{aligned}$$

3. $J = \sqrt{I_3}$ because $I_3 = \det(FF^T) = J^2$.

4. The first Finger's formula can be obtained from the second Finger's formula and the Caley-Hamilton formula
$$\iota_3 B^{-1} = B^2 - \iota_1 B + \iota_2 I.$$

□

Proposition 9.10 (Finger's formula)**.** *Let W be a smooth function of $\iota_1(Q), \iota_2(Q)$ and $\iota_3(Q)$, where Q is a 3×3 matrix. Then*

$$\begin{aligned} W_Q = &[W_{\iota_1} + \iota_1(Q) W_{\iota_2} + \iota_2(Q) W_{\iota_3}] I \\ &- [W_{\iota_2} + \iota_1(Q) W_{\iota_3}] Q^T + W_{\iota_3} (Q^T)^2. \end{aligned} \tag{9.13}$$

It can also be expressed as

$$W_Q = [W_{\iota_1} + \iota_1(Q) W_{\iota_2}] I - W_{\iota_2} Q^T + \iota_3(Q) W_{\iota_3} Q^{-T}. \tag{9.14}$$

Proof. 1. $W(\iota_1(Q), \iota_2(Q), \iota_3(Q))_Q = \sum_{k=1}^3 W_{\iota_k} [\iota_k(Q)]_Q$

2. $[\iota_1(Q)]_Q = I$. This is because $\iota_1(Q) = I : Q$, where $A : B := \sum_{i,j} a_{ij} b_{ij}$.

3. In general, we can show that $[\iota_1(Q^n)]_Q = n(Q^T)^{n-1}$. To show this, let us check the case of $n = 2$.
$$\delta \iota_1(Q^2) = \delta\left(I : Q^2\right) = 2I : (Q \cdot \delta Q) = 2Q : \delta Q = 2Q^T : \delta Q^T.$$

4. By direct computation, we get
$$\begin{aligned} \iota_2(Q) &= \frac{1}{2}\left(\iota_1^2(Q) - \iota_1(Q^2)\right) \\ \iota_3(Q) &= \frac{1}{3}\left(\iota_1(Q^3) - \iota_1^3(Q) + 3\iota_1(Q)\iota_2(Q)\right) \end{aligned}$$

5. From above two steps, we get
$$\begin{aligned} [\iota_2(Q)]_Q &= \iota_1(Q) I - Q^T \\ [\iota_3(Q)]_Q &= \iota_2(Q) I - \iota_1(Q) Q^T + (Q^T)^2 \end{aligned}$$

6. We arrive
$$\begin{aligned} W_Q &= W_{\iota_1} [\iota_1(Q)]_Q + W_{\iota_2} [\iota_2(Q)]_Q + W_{\iota_3} [\iota_3(Q)]_Q \\ &= W_{\iota_1} I + W_{\iota_2} [\iota_1(Q) I - Q^T] + W_{\iota_3} [\iota_2(Q) I - \iota_1(Q) Q^T + (Q^T)^2] \\ &= [W_{\iota_1} + \iota_1(Q) W_{\iota_2} + \iota_2(Q) W_{\iota_3}] I - [W_{\iota_2} + \iota_1(Q) W_{\iota_3}] Q^T + W_{\iota_3} (Q^T)^2 \end{aligned}$$

7. The second Finger's formula can be obtained by

$$\begin{aligned}[\iota_3(Q)]_Q &= \iota_2(Q)I - \iota_1(Q)Q^T + (Q^T)^2 \\ &= \left(\iota_2(Q)Q^T - \iota_1(Q)(Q^T)^2 + (Q^T)^3\right)(Q^T)^{-1} \\ &= \iota_3(Q)(Q^T)^{-1}\end{aligned}$$

In the last step, we have used the Caley-Hamilton formula:

$$-Q^3 + \iota_1 Q^2 - \iota_2 Q + \iota_3 I = 0.$$

$\square$

Representation of the second Piola stress We can also have the representation of the second Piola stress as the follows. Recall that the second Piola stress is defined as

$$\Sigma = JF^{-1}\sigma F^{-T}.$$

With the representation of σ, we get

$$\Sigma = 2\left(\psi_0(C)C^{-1} + \psi_1(C)I + \psi_2(C)C\right). \tag{9.15}$$

where

$$\psi_0 = I_3\overline{W}_{I_3}, \quad \psi_1 = \overline{W}_{I_1} + I_1\overline{W}_{I_2}, \quad \psi_2 = -\overline{W}_{I_2}. \tag{9.16}$$

Note that $\iota(C) = \iota(B)$. Using the Caley-Hamilton theorem, we have

$$\iota_3(C)C^{-1} = C^2 - \iota_1(C)C + \iota_2(C)I.$$

Plug this into the above representation formula and abbreviate $\iota_k(C)$ by I_k, we get

$$\begin{aligned}\Sigma &= 2\left(\frac{\psi_0}{I^3}(C^2 - I_1C + I_2I) + \psi_1 I + \psi_2 C\right) \\ &= 2\left(\psi_1 + \frac{\psi_0 I_2}{I_3}\right)I + 2\left(\psi_2 - \frac{\psi_0 I_1}{I_3}\right)C + 2\frac{\psi_0}{I_3}C^2 \\ &= 2\left(\gamma_0 I + \gamma_1 C + \gamma_2 C^2\right). \end{aligned} \tag{9.17}$$

The first Piola stress is represented as

$$P = F\Sigma \tag{9.18}$$

with Σ represented by (9.15) or (9.17).

9.1.5 Small Strain Limits

From frame-indifference and isotropic properties, we can treat the second Piola stress as a function of $C = F^T F$. That is $\Sigma = \check{\Sigma}(C)$. The small strain is to study $\check{\Sigma}(C)$ for $C \sim I$. [1] Recall we have defined the following infinitesimal strains:

- $E = \frac{1}{2}(C - I)$,
- $F = I + \mathbf{u}_X$
- $\mathbf{e} = \frac{1}{2}\left(\mathbf{u}_X + \mathbf{u}_X^T\right)$.

We want to expand the stress $\check{\Sigma}(C)$ and the stored energy function in E for $E \sim 0$.

Theorem 9.11. *For an isotropic elastic material, by normalizing $\check{\Sigma}(I) = 0$, the second Piola stress tensor has the following representation:*

$$\check{\Sigma}(C) = \lambda(trE)I + 2\mu E + o(E). \tag{9.19}$$

Here, λ and μ are called the Lamé moduli, $E = \frac{1}{2}(C - I)$. The potential W has the following representation:

$$W(E) = \frac{\lambda}{2}(trE)^2 + \mu tr(E^2) + o(E^2), \tag{9.20}$$

or

$$W(E) = \overline{W}(I_1, I_2, I_3) = \mu(I_1 - 3) + \frac{\lambda + 2\mu}{8}(I_1 - 3)^2 - \frac{\mu}{3}(I_2 - 3) + o(E^2). \tag{9.21}$$

where I_k are invariants of C.

Proof. 1. We want to expand Σ in terms of E. Recall that

$$\Sigma = 2\left(\psi_0 C^{-1} + \psi_1 I + \psi_2 C\right).$$

The terms C and C^{-1} are expanded in E as

$$C = I + 2E + o(E), \quad C^{-1} = I - 2E.$$

2. The coefficients ψ_0, ψ_1, ψ_2 can be expanded in E as

$$\begin{aligned}
\psi_0 &= I_3 \overline{W}_{I_3} = (1 + 2tr(E))\overline{W}_{I_3} + o(E) \\
\psi_1 &= \overline{W}_{I_1} + I_1 \overline{W}_{I_2} = \overline{W}_{I_1} + \overline{W}_{I_2}(3 + 2tr(E)) + o(E) \\
\psi_2 &= -\overline{W}_{I_2}.
\end{aligned}$$

Here, we have used the expansion of invariants I_1, I_2, I_3 in terms of E, which is shown below.

[1] Cialet vol. I, pp. 155

3. Expand the invariants:

$$
\begin{aligned}
I_1(C) &= trC = 3 + 2tr(E) \\
I_2(C) &= \frac{1}{2}\left((trC)^2 - trC^2\right) = 3 + 4tr(E) + o(E) \\
I_3(C) &= \frac{1}{6}(trC)^3 - \frac{1}{2}trC\,trC^2 + \frac{1}{3}trC^3 \\
&= 1 + 2tr(E) + o(E).
\end{aligned}
$$

Here, we have used

$$
\begin{aligned}
trC &= 3 + 2tr(E) \\
trC^2 &= 3 + 4tr(E) + o(E) \\
trC^3 &= 3 + 6tr(E) + o(E).
\end{aligned}
$$

4. Thus,

$$
\begin{aligned}
\Sigma &= 2\left((1+2tr(E))\overline{W}_{I_3}(I-2E) + (\overline{W}_{I_1} + \overline{W}_{I_2}(3+2tr(E)))I - \overline{W}_{I_2}(I+2E)\right) \\
&= 2\left[\left(\overline{W}_{I_1} + 2\overline{W}_{I_2} + \overline{W}_{I_3}\right) + \left(\overline{W}_{I_2} + 2\overline{W}_{I_3}\right)tr(E)\right]I - 4(\overline{W}_{I_2} + \overline{W}_{I_3})E + o(E)
\end{aligned}
$$

Since $\Sigma(0) = 0$ when there is no strain (i.e. $E = 0$), we get

$$
\overline{W}_{I_1} + 2\overline{W}_{I_2} + \overline{W}_{I_3} = 0, \tag{9.22}
$$

and

$$
\Sigma = \left[2\left(\overline{W}_{I_2} + 2\overline{W}_{I_3}\right)tr(E)\right]I - 4(\overline{W}_{I_2} + \overline{W}_{I_3})E + o(E).
$$

5. Let us call

$$
2\left(\overline{W}_{I_2} + 2\overline{W}_{I_3}\right) = \lambda, \quad -2\left(\overline{W}_{I_2} + \overline{W}_{I_3}\right) = \mu
$$

or

$$
\overline{W}_{I_2} = -\frac{\lambda}{2} - \mu, \quad \overline{W}_{I_3} = \frac{\lambda}{2} + \frac{\mu}{2},
$$

we then get

$$
\Sigma = \lambda(trE)I + 2\mu E + o(E).
$$

6. Formula (9.20) is obtained by integrating (9.19) in E.

Remark In the linear elasticity theory, we use the infinitesimal strain

$$\mathbf{e} := \frac{1}{2}\left(\mathbf{u}_X + \mathbf{u}_X^T\right),$$

which satisfies

$$\mathbf{e} = E + o(E).$$

In the above stress-strain relation for infinitesimal strain, we can replace E by $\mathbf{e}$.

□

9.2 Hyperelastic Models

To establish mathematical models for hyperelastic materials, there are two requirements that the stored energy W should satisfy:

- $W \to \infty$ as $J \to 0$,
- W_{FF} satisfies strong ellipticity condition.

These are the theme of this subsection. We start from the ellipticity condition, which is equivalent to the hyperbolicity condition for the time-dependent elasticity equation.

9.2.1 Hyperbolicity for isotropic materials

Below, we want to find the condition on $\overline{W}(I_1, I_2, I_3)$ which is equivalent to the hyperbolicity of $W(F)$. let $I_p = \iota(F^T F)$, $p = 1,2,3$ be the three invariants of $F^T F$. The restored energy W is a function of I_1, I_2, I_3. We have

$$\frac{\partial^2 \overline{W}}{\partial F \partial F}(I_1, I_2, I_3) = \sum_{p=1}^{3}\left(\overline{W}_{I_p}\frac{\partial^2 I_p}{\partial F \partial F} + \sum_{q=1}^{3}\overline{W}_{I_p I_q}\left(\frac{\partial I_p}{\partial F}\right)\left(\frac{\partial I_q}{\partial F}\right)\right). \tag{9.23}$$

Recall I_p has the following expression: let $C = F^T F$,

- $I_1(C) = Tr(C)$,
- $I_2(C) = \frac{1}{2}\left(Tr(C)^2 - Tr(C^2)\right)$,
- $I_3(C) = \det(C) = J^2 = \frac{1}{6}(TrC)^3 - \frac{1}{2}(TrC)(TrC^2) + \frac{1}{3}(TrC^3)$.
- $J = \det(F)$,

Lemma 9.7. *We have the following formulae for I_p:*

$$\frac{\partial I_1}{\partial F} = 2F, \tag{9.24}$$
$$\frac{\partial I_2}{\partial F^i_\alpha} = 2I_1 F^i_\alpha - 2F^i_\beta F^k_\beta F^k_\alpha, \tag{9.25}$$
$$\frac{\partial I_3}{\partial F^i_\alpha} = 2J^2 \left(F^{-1}\right)^\alpha_i \tag{9.26}$$
$$\frac{\partial^2 I_1}{\partial F^i_\alpha \partial F^j_\beta} = 2\delta^{ij}\delta_{\alpha\beta}, \tag{9.27}$$
$$\frac{\partial^2 I_2}{\partial F^j_\beta \partial F^i_\alpha} = 2I_1\delta^{ij}\delta_{\alpha\beta} + 4F^i_\alpha F^j_\beta - 2\left(\delta^{ij}F^k_\alpha F^k_\beta + \delta_{\alpha\beta}F^i_\gamma F^j_\gamma + F^i_\beta F^j_\alpha\right) \tag{9.28}$$
$$\frac{\partial^2 I_3}{\partial F^i_\alpha \partial F^j_\beta} = 4J^2 \left(F^{-1}\right)^\alpha_i \left(F^{-1}\right)^\beta_j - 2J^2 \left(F^{-1}\right)^\alpha_j \left(F^{-1}\right)^\beta_i \tag{9.29}$$

Proof. 1. From $I_1(C) = F^i_\alpha F^i_\alpha$, we get $I_{1,F} = 2F$.

2. From $\frac{\partial I_1}{\partial F} = 2F$, we get $\frac{\partial^2 I_1}{\partial F^i_\alpha \partial F^j_\beta} = 2\delta^{ij}\delta_{\alpha\beta}$.

3. $I_{2,F} = I_1 I_{1,F} - \frac{1}{2}\frac{\partial Tr(C^2)}{\partial C}\frac{\partial C}{\partial F} = 2I_1F - C(F+F^T) = 2I_1F - 2CF$.

4. From $I_3 = J^2$, we get $\frac{\partial I_3}{\partial F^i_\alpha} = 2J\frac{\partial J}{\partial F^i_\alpha} = 2J\left(F^{-1}\right)^\alpha_i$. Here, we have used

$$\frac{\partial J}{\partial F^i_\alpha} = J\left(F^{-T}\right)^i_\alpha = J\left(F^{-1}\right)^\alpha_i.$$

We also have

$$\begin{aligned}
\frac{\partial^2 I_3}{\partial F^j_\beta \partial F^i_\alpha} &= 4J\cdot J\left(F^{-1}\right)^\beta_j \left(F^{-1}\right)^\alpha_i + 2J^2\frac{\partial \left(F^{-1}\right)^\alpha_i}{\partial F^j_\beta} \\
&= 4J^2\left(F^{-1}\right)^\beta_j \left(F^{-1}\right)^\alpha_i - 2J^2\left(F^{-1}\right)^\alpha_k \frac{\partial F^k_\gamma}{\partial F^j_\beta}\left(F^{-1}\right)^\gamma_i \\
&= 4J\cdot J\left(F^{-1}\right)^\beta_j \left(F^{-1}\right)^\alpha_i - 2J^2\left(F^{-1}\right)^\alpha_j \left(F^{-1}\right)^\beta_i.
\end{aligned}$$

□

Separable case Let us assume $\overline{W}$ is separable. This means that

$$\frac{\partial^2 \overline{W}}{\partial I_p \partial I_q} = 0, \text{ when } p \neq q.$$

Effect of I_1 Suppose $\overline{W}$ is only a function of I_1. Let us call $\overline{W}$ by $\overline{W}_1$. We have

$$\frac{\partial^2 \overline{W}_1(I_1)}{\partial F^j_\beta \partial F^i_\alpha} = 2\overline{W}_{1,I_1}\delta^{ij}\delta_{\alpha\beta} + 4\overline{W}_{1,I_1 I_1} F^i_\alpha F^j_\beta. \tag{9.30}$$

The hyperbolicity condition for $\overline{W}_1$ reads

$$\sum_{i,j,\alpha,\beta} \frac{\partial^2 \overline{W}_1(I_1)}{\partial F^j_\beta \partial F^i_\alpha} \xi^i \xi^j \eta^\alpha \eta^\beta > 0.$$

Using (9.30), this condition is

$$2\overline{W}'_1 |\xi|^2 |\eta|^2 + 4\overline{W}''_1 \left(\xi^1 + \xi^2 + \xi^3\right)^2 \left(\eta^1 + \eta^2 + \eta^3\right)^2 > 0. \tag{9.31}$$

By choosing $\xi \neq 0$ but $\xi^1 + \xi^2 + \xi^3 = 0$, then the second term is zero. Thus, a necessary condition for (9.31) is

$$\overline{W}'_1 > 0. \tag{9.32}$$

We note that

$$\left(\xi^1 + \xi^2 + \xi^3\right)^2 \leq 3|\xi|^2, \quad \left(\eta^1 + \eta^2 + \eta^3\right)^2 \leq 3|\eta|^2.$$

Then a necessary and sufficient condition for hyperbolicity (9.31) is

$$\overline{W}'_1 > 0 \quad \text{ and } \quad \overline{W}'_1 - 18|\overline{W}''_1| > 0. \tag{9.33}$$

Examples of $\overline{W}_1$:

- $\overline{W}_1 = \frac{H}{2} I_1$. $\overline{W}_{I_1} = \frac{H}{2} > 0$. Thus, this model is hyperbolic.
- $\overline{W}_1 = \frac{\lambda}{2} I_1^2 + \mu I_1$. In this model, $\overline{W}'_1 = \lambda I_1 + \mu$; $\overline{W}''_1 = \lambda$. The hyperbolicity $\overline{W}'_1 - 18|\overline{W}''_1|$ is equivalent to $\lambda I_1 + \mu - 18\lambda > 0$. Need Double Check.

Effect of I_2 TO BE CONTINUED

Effect of I_3 Physically, we are not allowed to have $\rho \to \infty$. This is equivalent to the specific volume $V \to 0$, or equivalently, $J \to 0$, or $I_3 \to 0$. This means that the stored energy should satisfy

$$\overline{W} \to \infty \text{ as } I_3 \to 0.$$

One example is the γ-law:

$$\overline{W}_3(I_3) = \frac{\mu}{\gamma - 1} I_3^{(1-\gamma)/2}, \quad \gamma > 1,$$

Another is the Log law:

$$\overline{W}_3(I_3) = cI_3 - \frac{d}{2}\log(I_3).$$

TO BE Continued for hyperbolicity in terms of I_k.

9.2.2 Linear materials

When $F^T F = I$, then F is a rotation. In this situation, there is no elastic deformation (stretching or shrinking). When $F^T F \sim I$, then the material has small deformation, or equivalently, the strain is small. Recall

$$F = \mathbf{u}_X + I,$$

$$E := \frac{1}{2}(C - I) = \frac{1}{2}\left((\mathbf{u}_X + I)^T(\mathbf{u}_X + I) - I\right) = \frac{1}{2}\left(\mathbf{u}_X + \mathbf{u}_X^T + \mathbf{u}_X^T \mathbf{u}_X\right).$$

The infinitesimal strain theory is to study elastic motions when $|u_X|$ is small. The infinitesimal strain is defined to be

$$\mathbf{e} := \frac{1}{2}\left(\mathbf{u}_X + \mathbf{u}_X^T\right). \tag{9.34}$$

The linear model has the Piola stress being linear in $\mathbf{e}$.

$$P_{ik} = \frac{\partial W}{\partial F_k^i} = (A\mathbf{e})_{ik} = a_{ijkl} e_{jl},$$

where

$$a_{ijkl} := \frac{\partial^2 W}{\partial F_j^i \partial F_l^k}(I).$$

The equation of motion is

$$\rho_0 \ddot{u}^i = \sum_{j,k,l=1}^{3} a_{ijkl} \frac{\partial^2 u^k}{\partial X^j \partial X^l}.$$

Property of a_{ijkl}

Proposition 9.11. *The coefficients $a_{ijkl} := \frac{\partial^2 W}{\partial F^i_j \partial F^k_l}(I)$ has the following symmetries:*

$$a_{ijkl} = a_{klij}, \quad a_{ijkl} = a_{ijlk}, \quad a_{ijkl} = a_{jikl}, \quad P_{ij} = P_{ji}.$$

Proof.

1. $a_{ijkl} = a_{klij}$ is due to $\frac{\partial^2 W}{\partial F^i_j \partial F^k_l} = \frac{\partial^2 W}{\partial F^k_l \partial F^i_j}$.

2. We note that $\Sigma = FP = P + o(\mathbf{e})$. Further, $P(I) = 0$,

$$P(C) = \frac{1}{2}A(C-I) + o(\mathbf{e}) = A\mathbf{e} + o(\mathbf{e}).$$

   Here, $C = F^T F$, $\mathbf{e} = \frac{1}{2}\left(F + F^T\right) - I$. Thus,

$$a_{ijkl} = 2\left(\frac{\partial P_{ij}}{\partial C_{kl}}\right)_{C=I}$$

   Since C is symmetric, this shows $a_{ijkl} = a_{ijlk}$.

3. We have

$$a_{ijkl} = a_{klij} = a_{klji} = a_{jikl}.$$

   This shows the third equality.

4. The last equality is due to the fact that $P_{ij}(C) = \Sigma_{ij}(C) + o(\mathbf{e})$ and Σ is symmetric.

$\square$

Thus, the constitutive law for the linear elastic model is

$$W(\mathbf{e}) = \frac{1}{2}\langle A\mathbf{e}, \mathbf{e}\rangle, \quad P = A\mathbf{e}.$$

The total number of coefficients of a_{ijkl} are $(6+1)\cdot 3 = 21$. [2]

[2]From $a_{ijkl} = a_{jikl}$, we get number of independent (ij)'s is 6 (i.e. $(ij) = (11),(21),(22),(31),(32),(33)$). Similarly, from $a_{ijkl} = a_{ijlk}$, we see possible independent (kl)'s are also $(11),(21),(22),(31),(32),(33)$. From $a_{ijkl} = a_{klij}$, we get independent (ij,kl) are

$$(11,11),(11,21),(11,22),(11,31),(11,32),(11,33),(21,21),(21,22),...,(33,33).$$

The total number of these list is $6+5+\cdots+1 = 21$.

Linear isotropic material When a linear elastic material is also isotropic, that is $F^T F \sim I$, then W has the expansion: (Theorem 9.11)

$$W(E) = \frac{\lambda}{2}(TrE)^2 + \mu Tr(E^2) + o(E^2).$$

Note that

$$E = \frac{1}{2}(C-I) = \frac{1}{2}\left(\mathbf{u}_X + (\mathbf{u}_X)^T\right) + (\mathbf{u}_X)^T(\mathbf{u}_X) = \mathbf{e} + o(\mathbf{e})$$

and

$$P = F\Sigma = \Sigma + o(\mathbf{e}).$$

Thus, from Theorem 9.11, we have

$$W = \frac{\lambda}{2}(Tr(\mathbf{e}))^2 + \mu Tr(\mathbf{e}^2), \tag{9.35}$$

$$P = \lambda Tr(\mathbf{e})I + 2\mu\mathbf{e}, \quad P_{ij} = \lambda(e_{11}+e_{22}+e_{33})\delta_{ij} + 2\mu e_{ij}. \tag{9.36}$$

That is,

$$a_{ijkl} = \lambda\delta_{ij}\delta_{kl} + \mu\left(\delta_{ik}\delta_{jl} + \delta_{il}\delta_{jk}\right). \tag{9.37}$$

There are only two physical parameters μ and λ in this expression. Let us study their physical meaning. Consider a simple deformation: we stretch the material in X_1 direction, it results in elongation in X_1 direction and shrinking in X_2 and X_3 directions. The strain in X_1 direction is e_{11}. The ratio

$$E := \frac{P_{11}}{e_{11}} \tag{9.38}$$

is called the *Young modulus*. (Modulus means a ratio between stress and strain.) The shrinking of the material can be measured by

$$\nu := -\frac{e_{22}}{e_{11}} = -\frac{e_{33}}{e_{11}}. \tag{9.39}$$

This parameter is called the *Poisson ratio*. From (9.36), we get

$$\begin{aligned} P_{11} &= Ee_{11} = \lambda\left(e_{11} - 2\nu e_{11}\right) + 2\mu e_{11} \\ P_{22} &= 0 = \lambda\left(e_{11} - 2\nu e_{11}\right) - 2\mu\nu e_{11}. \end{aligned}$$

We can express λ and μ in terms of E and ν, and vice versa:

$$\lambda = \frac{E\nu}{(1+\nu)(1-2\nu)}, \quad \mu = \frac{E}{2(1+\nu)}, \tag{9.40}$$

$$E = \frac{\mu(3\lambda+2\mu)}{\lambda+\mu}, \quad \nu = \frac{\lambda}{2(\lambda+\mu)}. \tag{9.41}$$

We can express strain in terms of stress. The inversion of (9.36) reads

$$e_{ij} = \frac{1}{2\mu}P_{ij} - \frac{\lambda}{2\mu(3\lambda+2\mu)}Tr(P)\delta_{ij}. \tag{9.42}$$

In terms of E and ν, it reads

$$\begin{aligned} e_{11} &= \frac{1}{E}\left(P_{11} - \nu(P_{22}+P_{33})\right) \\ e_{22} &= \frac{1}{E}\left(P_{22} - \nu(P_{33}+P_{11})\right) \\ e_{33} &= \frac{1}{E}\left(P_{33} - \nu(P_{11}+P_{22})\right) \\ e_{ij} &= \frac{1}{2\mu}P_{ij}, \quad i \neq j. \end{aligned}$$

Another parameters are the shear modulus and bulk modulus. Let us decompose $\mathbf{e}$ into

$$\mathbf{e} = (\mathbf{e} - \frac{1}{3}Tr(\mathbf{e})I) + \frac{1}{3}Tr(\mathbf{e})I := \mathbf{e}^D + \mathbf{e}^S,$$

Then P can be expressed as

$$P = 2\mu\mathbf{e}^D + (3\lambda+2\mu)\mathbf{e}^S.$$

$$\begin{aligned} P^D &= 2\mu\mathbf{e}^D \\ P^S &= (3\lambda+2\mu)\mathbf{e}^S \end{aligned}$$

We call μ the *shear modulus* and $K := \lambda + \frac{2}{3}\mu$ the *bulk modulus*.

A Table of average values of these physical parameters for common materials can be fund in [Cialet pp. 129].

Hookean model The Hookean law is

$$W(F) = \frac{H}{2}\sum_{i,\alpha}|F^i_\alpha|^2 = \frac{H}{2}tr(F^TF), \quad H > 0.$$

This gives $P^i_\alpha = HF^i_\alpha$. The equation of motion is

$$\rho_0(X)\ddot{\mathbf{x}} = \nabla_X \cdot P, \quad \text{or} \quad \rho_0\ddot{x}^i = \partial_{X^\alpha}P^i_\alpha = \partial_{X^\alpha}H\partial_{X^\alpha}x^i = H\sum_\alpha \partial^2_{X^\alpha}x^i.$$

This is the standard wave equation. This is equivalent to the above linear isotropic model with $\mu = H$ and $\lambda = -H$.

9.2.3 St. Venant-Kirchhoff Model

The model is express as

$$\Sigma = \lambda(TrE)I + 2\mu E, \quad E = \frac{1}{2}(C - I).$$

or

$$W = \frac{\lambda}{2}(TrE)^2 + \mu Tr(E^2).$$

It is the simplest nonlinear elastic model. Its linearization, which replaces

$$E = \frac{1}{2}(F^T F - I) = \frac{1}{2}\left(\nabla_X \mathbf{u} + (\nabla_X \mathbf{u})^T + \nabla_X \mathbf{u}^T \nabla_X \mathbf{u}\right) \quad \text{by} \quad \mathbf{e} = \frac{1}{2}\left(\nabla_X \mathbf{u} + (\nabla_X \mathbf{u})^T\right),$$

is the linear isotropic model we have seen earlier. Note that the St. Venant-Kirchhoff model is not polyconvex, which is a sufficient condition for existence and uniqueness for steady state problems.

St. Venant-Kirchhoff model can be expressed in terms of the invariants $I_k = \iota_k(C)$ as

$$\overline{W}(I_1, I_2) = \frac{\lambda}{8} I_1^2 + \frac{\mu}{4}\left(I_1^2 - 2I_1 + 2I_2\right) - 9\left(\frac{\lambda}{8} + \frac{\mu}{4}\right).$$

9.2.4 Fluid-solid model

When $W = \overline{W}_3(I_3)$, this is a simple compressible fluid model. Recall $I_3 = det(F^T F) = J^2$. Given ρ_0, we define ρ such that $\rho J = \rho_0$. Thus, we can view I_3 as a function of ρ:

$$I_3 = \left(\frac{\rho_0}{\rho}\right)^2.$$

The Cauchy stress is (11.11)

$$\sigma = \frac{2}{\sqrt{I_3}} I_3 \overline{W}_{I_3} I = -p(\rho) I.$$

A particular example is the γ-law simple gas, where

$$\overline{W}_3(I_3) = \frac{\mu}{\gamma - 1} I_3^{(1-\gamma)/2}, \quad \gamma > 1,$$

$$p = -2\sqrt{I_3}\overline{W}_{I_3} = \mu I_3^{-\gamma/2} = \mu\left(\frac{\rho}{\rho_0}\right)^{\gamma}.$$

9.2.5 Ogden hyperelastic models

Ogden proposed a class of models which are *polyconvex* and satisfies growth conditions. Let μ_i are singular values of F, the Ogden model reads:

$$\begin{aligned}
W &:= \overline{W}_1 + \overline{W}_2 + \overline{W}_3, \\
\overline{W}_1 &:= \sum_{i=1}^{M} a_i \left(\mu_1^{\alpha_i} + \mu_2^{\alpha_i} + \mu_3^{\alpha_i} - 3\right) \\
\overline{W}_2 &:= \sum_{i=1}^{N} b_i \Big((\mu_2\mu_3)^{\beta_i} + (\mu_3\mu_1)^{\beta_i} + (\mu_1\mu_2)^{\beta_i} - 3\Big) \\
\overline{W}_3 &:= \overline{W}_3(\mu_1\mu_2\mu_3), \quad \overline{W}_3(I_3) \to \infty \text{ as } I_3 \to 0+.
\end{aligned}$$

Examples of $\overline{W}_3$ are

$$\begin{aligned}
\overline{W}_3(I_3) &= \frac{\mu}{\gamma-1} I_3^{(1-\gamma)/2}, \quad \gamma > 1, \\
\overline{W}_3(I_3) &= cI_3 - \frac{d}{2}\ln I_3
\end{aligned}$$

Special cases are

- **neo-Hookean model**:

$$\overline{W} = \frac{\mu}{2}(I_1 - 3) + \overline{W}_3(I_3) = \frac{\mu}{2}\left[(I_1 - 3) + \frac{1}{k}(I_3^{-k} - 1)\right], \quad k = \frac{\gamma - 1}{2}.$$

  Here, we normalize $\overline{W}$ so that $\overline{W}(3,3,1) = 0$. The term I_1 gives the Hookean elastic model, whereas $\overline{W}_3(I_3)$ gives the compressible fluid model.

- **Mooney-Rivlin compressible solid**

$$\overline{W} = c_1(I_1 - 3) + c_2(I_2 - 3) + \overline{W}_3(I_3).$$

- **Knowles solid**

$$\overline{W} = \frac{\mu}{2}[(I_1 - 3)\overline{W}_1(I_3) + (I_2 - 3)\overline{W}_2(I_3) + \overline{W}_3(I_3)]$$

For more models, see Drozdov (pp. 103-118).

9.3 Appendix

Here, we review some notations in matrix theory. Let $\mathbf{A} = (a_{ij})$ be an $n \times n$ matrix in $\mathbb{C}^n$. We recall the following notations.

- Minor: the minor of $\mathbf{A}$ is defined to be (A_{ij}), where A_{ij} is the determinant of the matrix which eliminate row i and column j from A;
- Cofactor: $\mathrm{Cof}(\mathbf{A}) := ((-1)^{i+j}A_{ij})$ is called the cofactor of $\mathbf{A}$,
- Adjugate of A is defined to be $\mathrm{adj}(\mathbf{A}) := (\mathrm{Cof}A)^T$,
- An important property of adjugate of $\mathbf{A}$ is
$$\mathbf{A}\,\mathrm{adj}(\mathbf{A}) = \mathrm{adj}(\mathbf{A})A = \det(A)I.$$
Thus,
$$\mathrm{adj}(A) = \det(A)A^{-1}, \quad \mathrm{Cof}(\mathbf{A}) = \det(A)A^{-T}$$

Theorem 9.12 (Caley-Hamilton). *Let $p_A(\lambda) := \det(\lambda\mathbf{I} - \mathbf{A})$ be the characteristic polynomial of $\mathbf{A}$. Then $p_A(\mathbf{A}) = \mathbf{0}$.*

Proof.

1. We use the adjugate matrix property. The adjugate matrix $\mathrm{adj}(M)$ of a matrix M is defined to be the transpose of the cofactor matrix of M. The i-j entry of the cofactor matrix M_{ij} is the determinant of the $(n-1)\times(n-1)$ matrix which eliminate the ith row and jth column of the matrix M. The adjugate matrix has the following property:
$$\mathrm{adj}(\mathbf{M})\cdot\mathbf{M} = \mathbf{M}\cdot\mathrm{adj}(\mathbf{M}) = det(\mathbf{M})\mathbf{I}_n.$$
Applying this property to $\mathbf{M} = \lambda\mathbf{I}_n - \mathbf{A}$, we get
$$(\lambda\mathbf{I}_n - \mathbf{A})\cdot\mathrm{adj}(\lambda\mathbf{I} - \mathbf{A}) = det(\lambda\mathbf{I}_n - \mathbf{A})\mathbf{I}_n.$$
2. The right-hand side is
$$det(\lambda\mathbf{I}_n - \mathbf{A})\mathbf{I}_n = \sum_{i=0}^{n}\lambda^i c_i\mathbf{I}_n.$$
3. Notice that the adjugate matrix $\mathrm{adj}(\lambda\mathbf{I} - \mathbf{A})$ can be expressed as polynomial in λ of degree $(n-1)$:
$$\mathrm{adj}(\lambda\mathbf{I} - \mathbf{A}) = \sum_{i=0}^{n-1}\mathbf{B}_i\lambda^i.$$

Thus, the left-hand side is

$$
\begin{aligned}
(\lambda \mathbf{I}_n - \mathbf{A}) \cdot \mathrm{adj}(\lambda \mathbf{I} - \mathbf{A}) &= \sum_{i=0}^{n-1} (\lambda \mathbf{I} - \mathbf{A}) \cdot \mathbf{B}_i \lambda^i \\
&= \lambda^n \mathbf{B}_{n-1} + \sum_{i=1}^{n-1} \lambda^i (\mathbf{B}_{i-1} - \mathbf{A}\mathbf{B}_i) - \mathbf{A}\mathbf{B}_0.
\end{aligned}
$$

4. By comparing both polynomials, we obtain

$$
\mathbf{I}_n = \mathbf{B}_{n-1}, \quad c_i \mathbf{I}_n = \mathbf{B}_{i-1} - \mathbf{A}\mathbf{B}_i, 1 \le i \le n-1, \quad c_0 \mathbf{I}_n = -\mathbf{A}\mathbf{B}_0.
$$

5. Multiply the above ith equation by $\mathbf{A}^i$ them sum over i from 0 to n, we obtain

$$
\sum_{i=0}^{n} c_i \mathbf{A}^i = \mathbf{A}^n \mathbf{B}_{n-1} + \sum_{i=1}^{n-1} \mathbf{A}^i (\mathbf{B}_{i-1} - \mathbf{A}\mathbf{B}_i) - \mathbf{A}\mathbf{B}_0 = 0.
$$

□

Spectral properties of a matrix In order to characterize the response function of an isotropic material, we review some spectral properties of 3×3 matrices Let us denote the set of all 3×3 matrices by $\mathbb{M}_3$.

- Given a matrix $A \in \mathbb{M}_3$, its characteristic polynomial is defined as

  $$
  p(\lambda) := \det(A - \lambda I) = -\lambda^3 + \iota_1 \lambda^2 - \iota_2 \lambda + \iota_3,
  $$

  where the coefficients $\iota_1, \iota_2, \iota_3$ are called the principal invariants of A, which are given in terms of eigenvalues λ_1, λ_2, λ_3 of A as below:

  $$
  \iota_1 = trA = \lambda_1 + \lambda_2 + \lambda_3 \tag{9.43}
  $$

  $$
  \iota_2 = \frac{1}{2}\left((trA)^2 - tr(A^2)\right) = tr(\mathrm{Cof}A) = \lambda_1\lambda_2 + \lambda_2\lambda_3 + \lambda_3\lambda_1 \tag{9.44}
  $$

  $$
  \iota_3 = \det A = \lambda_1 \lambda_2 \lambda_3. \tag{9.45}
  $$

  We denote the set of these principal invariants of A by ι_A.

- An important matrix theorem is the Caley-Hamilton Theorem, which states $p(A) = 0$. That is,

  $$
  -A^3 + \iota_1 A^2 - \iota_2 A + \iota_3 I = 0.
  $$

- Consequently, the matrix power A^p, with $p \in \mathbb{Z}$ and $p \geq 0$, or with $p \in \mathbb{Z}$ and $p \leq -1$ if A is invertible, has the following representation:

$$A^p = \alpha_{0,p}(\iota_A)I + \alpha_{1,p}(\iota_A)A + \alpha_{2,p}(\iota_A)A^2,$$

  where $\alpha_{k,p}$ are functions of principal invariants.

- Spectral mapping theorem: If B is a self-adjoint operator with eigenvalues/eigenvectors λ_i and p_i, $i = 1,2,3$. Let $\beta(\lambda)$ be a smooth function, then

$$\beta(B) = \sum_{i=1}^{3} \beta(\lambda_i) p_i p_i^T.$$

Chapter 10

Dynamics of Simple Elasticity

Theory of simple elasticity studies mechanical dynamics of elastic materials, no heat transfer is considered. The dynamics involving both mechanical energy and heat will be investigated in theory of thermo-elasticity in later Chapter.

10.1 Lagrangian Formulation for Simple Elasticity

10.1.1 Variational Approach for Compressible Simple Elasticity

Assumption We will derive equation of motion of simple elasticity without body forces in Lagrange coordinate. Suppose we are given a material domain Ω_0 and a density function ρ_0 on Ω_0. The material is called hyper-elastic if there exists a stored energy function $W(F)$ such that the internal energy density of the material is given by $U = W(F)$.

Action Given a flow map $\mathbf{x}(\cdot,\cdot)$, we define its action in the Lagrange coordinate as

$$\mathcal{S}[\mathbf{x}] = \int_{t_0}^{t_1} \int_{\Omega_0} \left(\frac{1}{2} \rho_0(X) |\dot{\mathbf{x}}(t,X)|^2 - W\left(\frac{\partial \mathbf{x}(t,X)}{\partial X} \right) \right) dX\, dt$$

where the first term is the kinetic energy, the second term is the internal energy.

Admissible class We will look for extremal of $\mathcal{S}[\mathbf{x}]$ for flow maps in an admissible class. For different boundary conditions, there are different admissible class. Let us introduce the simplest admissible class:

$$\mathcal{X} := \{\mathbf{x} : \Omega_0 \to \mathbb{R}^3 | \mathbf{x} \text{ is Lipschitz continuous}, \mathbf{x}(X) = \mathbf{x}_0(X), X \in \partial\Omega_0\} \tag{10.1}$$

Here, $\mathbf{x}_0$ is a given function on the boundary.

D'Alembert least action principle *The dynamics of a physical flow map $\mathbf{x}(t,\cdot)$ is the extremal of the action functional $\mathcal{S}[\mathbf{x}]$ among all admissible flow maps.* Thus, we look for

$$\mathbf{x} = \arg\min\{\mathcal{S}[\mathbf{x}] | \mathbf{x} \in \mathcal{X}\}. \tag{10.2}$$

Variation w.r.t. flow maps We shall study the variation of the action with respect to the flow map $\mathbf{x}(\cdot,\cdot)$. Let us perturb the flow map by $\mathbf{x}_\varepsilon(t,X)$ with $\mathbf{x}_0(t,X) = \mathbf{x}(t,X)$, the original unperturbed one. We call

$$\delta\mathbf{x}(t,X) := \frac{\partial}{\partial\varepsilon}|_{\varepsilon=0}\mathbf{x}_\varepsilon(t,X),$$

the variation of the flow map $\mathbf{x}(\cdot,\cdot)$. We write the variation of $\mathbf{x}$ by $\delta\mathbf{x}$ (or $\mathring{\mathbf{x}}$). Since, for small ε, $\mathbf{x}_\varepsilon(t,\cdot)$ are flow maps, its variation

$$\delta\mathbf{x}(t,X) = \lim_{\varepsilon\to 0}\frac{\mathbf{x}_\varepsilon - \mathbf{x}_0}{\varepsilon}$$

is an infinitesimal variation of position, thus, is also called a pseudo-velocity. The derivative

$$\frac{d}{d\varepsilon}|_{\varepsilon=0}\mathcal{S}[\mathbf{x}_\varepsilon]$$

is called the variation of the functional $\mathcal{S}[\mathbf{x}]$ in direction $\delta\mathbf{x}$. We denote it by

$$\delta\mathcal{S}[\mathbf{x}]\cdot\delta\mathbf{x} := \frac{d}{d\varepsilon}|_{\varepsilon=0}\mathcal{S}[\mathbf{x}_\varepsilon].$$

This means that the physical solution $\mathbf{x}(t,X)$ satisfies

$$\delta\mathcal{S}[\mathbf{x}]\cdot\delta\mathbf{x} = 0$$

for all possible variations $\delta\mathbf{x}$.

Euler-Lagrange equation Let us compute $\delta\mathcal{S}$:

$$
\begin{aligned}
\delta\mathcal{S}[x]\cdot\delta\mathbf{x} &= \frac{d}{d\varepsilon}\bigg|_{\varepsilon=0}\int_{t_0}^{t_1}\int_{\Omega_0}\left(\frac{1}{2}\rho_0(X)|\dot{\mathbf{x}}_\varepsilon(t,X)|^2 - W\left(\frac{\partial\mathbf{x}_\varepsilon(t,X)}{\partial X}\right)\right)dX\,dt\\
&= \int_{t_0}^{t_1}\int_{\Omega_0}\big(\rho_0(X)\dot{\mathbf{x}}(t,X)\cdot\delta\dot{\mathbf{x}} - W'(F)\delta F\big)\,dX\,dt\\
&= \int_{t_0}^{t_1}\int_{\Omega_0}\left(-\frac{d}{dt}\left(\rho_0(X)\dot{\mathbf{x}}(t,X)\right)\cdot\delta\mathbf{x} - W'(F)\frac{\delta\partial\mathbf{x}}{\partial X}\right)dX\,dt\\
&= \int_{t_0}^{t_1}\int_{\Omega_0}\left(-\rho_0(X)\ddot{\mathbf{x}}(t,X)\cdot\delta\mathbf{x} - W'(F)\frac{\partial\delta\mathbf{x}}{\partial X}\right)dX\,dt\\
&= \int_{t_0}^{t_1}\int_{\Omega_0}\left(-\rho_0(X)\ddot{\mathbf{x}}(t,X)\cdot\delta\mathbf{x} + \left(\frac{\partial}{\partial X}W'(F)\right)\cdot\delta\mathbf{x}\right)dX\,dt - B.C.\\
&= \int_{t_0}^{t_1}\int_{\Omega_0}\left[-\rho_0(X)\ddot{\mathbf{x}}(t,X) + \frac{\partial}{\partial X}W'\left(\frac{\partial\mathbf{x}}{\partial X}\right)\right]\cdot\delta\mathbf{x}\,dX\,dt - B.C.
\end{aligned}
$$

Here,

$$
\begin{aligned}
B.C. &= \int_{t_0}^{t_1}\int_{\Omega_0}\nabla_X\cdot\left(W'(F)\delta\mathbf{x}\right)dX\,dt\\
&= \int_{t_0}^{t_1}\int_{\partial\Omega_0}W'(F)_i^\alpha N_\alpha\delta x^i\,dX\,dt, \quad \mathbf{N}\text{ is the outer normal of }\partial\Omega_0
\end{aligned}
$$

is the term coming from integration by part. From boundary condition of the admissible class, we have $\delta\mathbf{x}(t,X)=0$ on the boundary $\partial\Omega_0$. Thus, $B.C.=0$. The D'Alembert least action principle gives

$$
\delta\mathcal{S}[\mathbf{x}]\cdot\delta\mathbf{x} = \int_{t_0}^{t_1}\int_{\Omega_0}\left[-\rho_0(X)\ddot{\mathbf{x}}(t,X) + \frac{\partial}{\partial X}W'\left(\frac{\partial\mathbf{x}}{\partial X}\right)\right]\cdot\delta\mathbf{x}\,dX\,dt = 0,
$$

for all $\delta\mathbf{x}$ in the tangent space of $\mathcal{X}$. This leads to the following Euler-Lagrange equation

$$
\boxed{\rho_0(X)\ddot{\mathbf{x}}(t,X) = \nabla_X\cdot P\left(\frac{\partial\mathbf{x}}{\partial X}\right)\qquad\text{for } X\in\Omega_0,} \tag{10.3}
$$

Here, $P := W'(F)$ is called the first Piola-Kirchhoff stress tensor, or just the Piola stress. Its component form is

$$
P_i^\alpha = \frac{\partial W}{\partial F_\alpha^i},\quad F_\alpha^i := \frac{\partial x^i}{\partial X^\alpha}.
$$

This first Piola stress is the potential difference due to the small variation of $\frac{\partial \mathbf{x}}{\partial X}$. Because the variation of the deformation has the form $\frac{\partial \delta \mathbf{x}}{\partial X}$, the corresponding force (potential difference) is a surface force $\frac{\partial W_F}{\partial X}$. [1]

The above Euler-Lagrange equation (10.3) is a second-order PDE for $\mathbf{x}(t,X)$. We need to impose initial condition and boundary condition.

- **Initial condition** For the second-order equation (10.8), we need to impose two initial conditions:
$$\mathbf{x}(0,X) = \mathbf{x}_0(X) \quad \text{and} \quad \dot{\mathbf{x}}(0,X) = \mathbf{v}_0(X), \quad X \in \Omega_0.$$
- **Boundary conditions** The boundary $\partial\Omega_0$ is a disjoint union of $\partial\Omega_0 = \Gamma_0^d \cup \Gamma_0^n$. The boundary conditions on each are
  - Dirichlet boundary condition
$$\mathbf{x}(t,X) = \mathbf{x}_0(X) \text{ for } X \in \Gamma_0^d. \tag{10.4}$$
  - Neumann boundary condition:
$$W'(F)_i^\alpha N_\alpha = g_i \text{ for } X \in \Gamma_0^n. \tag{10.5}$$
  The function $\mathbf{g} = g_i dx^i$ is an applied traction. [2]

External forces There are two kinds of external forces:

- body force: we assume it is conservative. $\mathbf{f}(\mathbf{x}) = -\nabla_{\mathbf{x}} V(\mathbf{x})$ for some potential function V;

We define the admissible class to be
$$\mathcal{X} = \{\mathbf{x} | \mathbf{x}(t,X) = \mathbf{x}_0(X) \text{ for } X \in \Gamma_0^d\}$$
We also need to add the energies contributed from these two forces to our action functional: [3]
$$\begin{aligned} \mathcal{S}[\mathbf{x}] := & \int_{t_0}^{t_1} \int_{\Omega_0} \left(\frac{1}{2} \rho_0(X) |\dot{\mathbf{x}}(t,X)|^2 - W\left(\frac{\partial \mathbf{x}(t,X)}{\partial X} \right) \right) dX\, dt \\ & - \int_{t_0}^{t_1} \int_{\Omega_0} V(\mathbf{x}(t,X))\, J\, dX\, dt + \int_{t_0}^{t_1} \int_{\Gamma_0^n} \mathbf{g}(X) \cdot \mathbf{x}(t,X)\, dS_0. \end{aligned} \tag{10.6}$$

[1] If the potential W also depends on $K := \frac{\partial^2 \mathbf{x}}{\partial X^2}$, say $W(F,K)$, then the corresponding Euler-Lagrange equation has an additional force of the form $-\frac{\partial^2 W_K}{\partial X^2}$. More boundary conditions are also needed.

[2] The tensor type of force is an 1-form, because this tensor type is consistent to that of a conservative force $f = dV$.

[3] The work is minus of force times displacement

Here, $J\,dX = d\mathbf{x}$. The last two terms are the potentials due to the body force and the traction.

We take variation of $\mathcal{S}$ with respective to $\mathbf{x} \in \mathcal{X}$. This gives

$$\delta\mathcal{S}[\mathbf{x}]\cdot\delta\mathbf{x} = \int_{t_0}^{t_1}\int_{\Omega_0}\left[-\rho_0(X)\ddot{\mathbf{x}}(t,X) + \frac{\partial}{\partial X}W'\left(\frac{\partial \mathbf{x}}{\partial X}\right) - \nabla_{\mathbf{x}}V(\mathbf{x})J\right]\cdot\delta\mathbf{x}\,dX\,dt$$
$$-\int_{t_0}^{t_1}\int_{\Gamma_0^n}\left(W'\cdot\mathbf{N}-\mathbf{g}\right)\cdot\delta\mathbf{x}\,dS_0\,dt = 0, \tag{10.7}$$

The boundary term $\int_{\Gamma_0^d} W'\cdot\mathbf{N}\cdot\delta\mathbf{x} = 0$ because $\delta\mathbf{x} = 0$ on Γ_0^d for $\delta\mathbf{x}$ in the tangent space of $\mathcal{X}$. Thus, the corresponding Euler-Lagrange becomes

$$\boxed{\rho_0(X)\ddot{\mathbf{x}}(t,X) = \nabla_X\cdot P\left(\frac{\partial \mathbf{x}}{\partial X}\right) + \mathbf{f}(t,\mathbf{x}(t,X))\det\left(\frac{\partial \mathbf{x}}{\partial X}\right) \text{ in } \Omega_0.} \tag{10.8}$$

where $\mathbf{f} = -\nabla_{\mathbf{x}}V(\mathbf{x})$ is the body force. The initial condition is the same. The boundary conditions on $\partial\Omega_0 = \Gamma_0^d \cup \Gamma_0^n$ are casted as

- Dirichlet boundary condition on Γ_0^d:

$$\mathbf{x}(t,X) = \mathbf{x}_0(X) \text{ for } X \in \Gamma_0^d. \tag{10.9}$$

- Neumann boundary condition on Γ_0^n:

$$P_i^\alpha(F(t,X))N_\alpha(X) = \mathbf{g}_i(X) \text{ for } X \in \Gamma_0^n. \tag{10.10}$$

Remark The component form acceleration term $\rho_0\ddot{\mathbf{x}}$ should be

$$\frac{d}{dt}\flat(\rho\dot{\mathbf{x}}) = \frac{d}{dt}\flat\left(\rho_0\dot{x}^i\partial_{x^i}\right) = \frac{d}{dt}\rho_0\dot{x}_i dx^i.$$

The index has been moved down!

10.1.2 Equation of Motion as a First-order System

Let us introduce $\mathbf{v}(t,X) := \dot{\mathbf{x}}(t,X)$ and $F(t,X) = \frac{\partial \mathbf{x}}{\partial X}(t,X)$ and express the above second-order equation as the following first order system:

$$\boxed{\begin{array}{l} \dot{F} = \frac{\partial \mathbf{v}}{\partial X} \\ \rho_0\dot{\mathbf{v}} = \nabla_X P(F) \end{array}} \tag{10.11}$$

The unknowns are $(F,\mathbf{v})$. There are $9+3 = 12$ of them. The Piola stress $P(F)$ is given as a constitutive relation $P(F) = W'(F)$.

Compatibility condition Since F is the gradient of the flow map $\mathbf{x}(t,X)$, it has to satisfy the following condition:

$$\partial_{X^i}\partial_{X^j}\mathbf{x} = \partial_{X^j}\partial_{X^i}\mathbf{x}$$

In terms of F, it reads

$$\boxed{\nabla_X \times F^T = 0.} \tag{10.12}$$

This is called the *compatibility condition* for F. From $\dot{F} = \frac{\partial \mathbf{v}}{\partial X}$, we get

$$\frac{d}{dt}\nabla_X \times F^T = \nabla_X \times (\nabla_X \mathbf{v})^T = 0.$$

Thus, if $\nabla_X \times F^T = 0$ initially, then it is zero for all later time.

We have seen that if $\mathbf{x}(t,\mathbf{x})$ is a solution of (10.8), then $\dot{\mathbf{x}} = \mathbf{v}$ and $\frac{\partial \mathbf{x}}{\partial X}$ satisfy (10.11) and the compatibility condition. Conversely, if $\mathbf{v}$ and F satisfy (10.11) and the compatibility condition, then there exists a function $\mathbf{x}(t,X)$ such that $\dot{\mathbf{x}} = \mathbf{v}$ and $\frac{\partial \mathbf{x}}{\partial X} = F$. The function $\mathbf{x}$ is obtained by a line integral

$$x^i(t,X) = \int^{(t,X)} \left(\mathbf{v}^i\,dt + \sum_{\alpha=1}^{3} F^i_\alpha\,dX^\alpha \right)$$

The line integral is independent path because the compatibility condition.

If there is a body force which depends on $\mathbf{x}(t,X)$, then we should add the equation for $\mathbf{x}$. The equation of motion becomes

$$\boxed{\begin{array}{l} \dot{\mathbf{x}} = \mathbf{v} \\ \dot{F} = \frac{\partial \mathbf{v}}{\partial X} \\ \rho_0 \dot{\mathbf{v}} = \nabla_X \cdot P(F) + \mathbf{f}(t,\mathbf{x})\det(F). \end{array}} \tag{10.13}$$

The unknowns are $\mathbf{x}, F, \mathbf{v}$. There are $3+9+3 = 15$ unknowns and equations.

Initial condition For the first order system (10.13), we impose

$$\mathbf{v}(0,X) = \mathbf{v}_0(X), \quad F(0,X) = I, \quad X \in \Omega_0.$$

Boundary condition for the first-order system We need to translate the boundary conditions (10.9) and (10.10) in terms of $(\mathbf{v}, F)$. We differentiate these boundary conditions in t and in X in the tangential direction of $\partial\Omega_0$ to get

- Dirichlet: $\mathbf{v}(t,X) = 0$ on Γ_0^d.
- Neumann: [4]

$$P_i^\alpha(F(t,X))N_\alpha(X) = \mathbf{g}_i(X) \text{ for } X \in \Gamma_0^n.$$

[4] References:

Two examples:

1. One dimension: In one dimension, the deformation gradient is $F^1_1 = \frac{\partial x}{\partial X}$. Let $u := F^1_1 - 1$ the strain, $v := \frac{\partial x}{\partial t}$ the velocity. The Piola stress is a given function $P(u)$ satisfying $P'(u) > 0$. We assume $\rho_0(X) \equiv 1$. The equation of motion is
$$\partial_t v = \partial_X P(u) \tag{10.14}$$
$$\partial_t u = \partial_X v. \tag{10.15}$$
Here, ∂_t means $\frac{\partial}{\partial t}|_X$. Such an equation is a 2×2 hyperbolic system. Namely, the eigenvalues of
$$\begin{bmatrix} 0 & P'(u) \\ 1 & 0 \end{bmatrix}$$
are $\pm\sqrt{P'}$, which are real and the characteristic speeds of the system. Note that the stress function P is in general non-convex. This leads to a special type of shock wave, called contact shock, where a rarefaction wave is attached to a shock wave. A simple model is $P(u) = \tanh(u)$, which gives so-called soft springs. The stress changes small as the strain increases big.

2. Linear elasticity: In the Hookean case where $W(F) = \frac{k}{2}|F|^2$, the stress is $P(F) = kF$, where k is a constant called the stiffness. The equation of motion becomes
$$\rho_0(X)\partial_t \mathbf{v} = k\nabla_X \cdot F \tag{10.16}$$
$$\partial_t F = \nabla_X \mathbf{v} \tag{10.17}$$
Eliminating F, we get
$$\rho_0(X)\partial_t^2 \mathbf{v} = k\nabla_X^2 \mathbf{v}.$$
This is the wave equation.

10.1.3 Variational Approach for Incompressible Simple Elasticity

A flow map $\mathbf{x}(t,X)$ is called incompressible if
$$J(t,X) := \det\left(\frac{\partial \mathbf{x}}{\partial X}(t,X)\right) = \det F = 1.$$

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1. Antman, Nonlinear Problems in Elasticity, pp. 424-426.
2. Cialet and Mardare, Boundary conditions in intrinsic nonlinear elasticity, J. Math Pure Appl. 2014.

This means its volume is unchanged. Thus, in the above variation of action, we should add a constraint term with a Lagrange multiplier:

$$\delta \mathcal{S}[\mathbf{x}] + \delta \int_{t_0}^{t_1} \int p(t,X)(\det F - 1)\, dX\, dt = 0.$$

Here, p is the Lagrange multiplier. The variation

$$\delta(\det F) = tr(F^{-T}(\delta F)) \det F = tr(F^{-T}(\delta F)),$$

where

$$tr(F^{-T}(\delta F)) = \sum_{i,\alpha} (F^{-T})_i^\alpha (\delta F)^i_\alpha = \sum_{i,\alpha} (F^{-T})_i^\alpha \frac{\partial \delta x^i}{\partial X^\alpha}.$$

We take integration-by-part in the variation form below to get

$$\begin{aligned}
&\delta \int_{t_0}^{t_1} \int_{\Omega_0} p(t,X)(\det F - 1)\, dX\, dt = \int_{t_0}^{t_1} \int p(t,X) \delta(\det F - 1)\, dX\, dt \\
&= \int_{t_0}^{t_1} \int p \sum_{i,\alpha} (F^{-T})_i^\alpha \frac{\partial \delta x^i}{\partial X^k}\, dX\, dt = \int_{t_0}^{t_1} \int \sum_{i,\alpha} \left[\frac{\partial}{\partial X^\alpha} \left((pF^{-T})_i^\alpha \delta x^i \right) - \left(\frac{\partial}{\partial X^\alpha} (pF^{-T})_i^\alpha \right) \delta x^i \right] dX\, dt \\
&= -\int_{t_0}^{t_1} \int_{\Omega_0} [\nabla_X \cdot \left(p(F^{-T})\right)] \cdot \delta \mathbf{x}\, dX\, dt + \int_{t_0}^{t_1} \int_{\partial\Omega_0} (pF^{-T})_i^\alpha \delta x^i N_\alpha\, dS dt.
\end{aligned}$$

We recall the variation of the action is (10.7):

$$\begin{aligned}
\delta \mathcal{S}[\mathbf{x}] \cdot \delta \mathbf{x} = &\int_{t_0}^{t_1} \int_{\Omega_0} \left[-\rho_0(X) \ddot{\mathbf{x}}(t,X) + \frac{\partial}{\partial X} W' \left(\frac{\partial \mathbf{x}}{\partial X} \right) - \nabla_{\mathbf{x}} V(\mathbf{x}) J \right] \cdot \delta \mathbf{x}\, dX\, dt \\
&- \int_{t_0}^{t_1} \int_{\Gamma_0^n} \left(W' \cdot \mathbf{N} - \mathbf{g} \right) \cdot \delta \mathbf{x}\, dS_0\, dt = 0,
\end{aligned}$$

Combining these two, we obtain the constraint flow equation:

$$\rho_0 \ddot{\mathbf{x}} = \nabla_X \cdot (P - pF^{-T}) + \mathbf{f} J.$$

with the natural boundary condition:

$$\left[\left(P - pF^{-T}\right) \cdot \mathbf{N} - \mathbf{g} \right] \cdot \delta \mathbf{x} = 0. \tag{10.18}$$

where $\mathbf{N}$ is the outer normal of $\partial\Omega_0$. We should impose a boundary condition to make this term zero. The full set of equations are

$$\left\{ \begin{array}{rcl} \rho_0 \dot{\mathbf{v}} & = & \nabla_X \cdot (P(F) - pF^{-T}) + \mathbf{f} J \\ \dot{F} & = & \nabla_X \mathbf{v} \\ \det F & = & 1 \end{array} \right.$$

The unknowns are $(\mathbf{v}, F, p)$.

Boundary conditions for incompressible elasticity From (10.18), we should decompose $\partial\Omega_0$ into disjoint two subsets Γ_0^d and Γ_0^n. We impose

- $\mathbf{v} = 0$ for $X \in \Gamma_0^d$ (This leads to $\delta\mathbf{x} = 0$.)
- $(P - pF^{-1}) \cdot \mathbf{N} = \mathbf{g}$, for $X \in \Gamma_0^n$.

10.2 Eulerian Formulation for Simple Elasticity

10.2.1 Formulation of Compressible Simple Elasticity in terms of F

We recall the transformation formulae of conservation laws between Lagrange and Euler coordinate systems (2.12), (2.6) and (2.13):

$$\partial_t \mathcal{U} + \nabla_{\mathbf{x}} \cdot \mathcal{F} = \mathcal{R} \tag{10.19}$$

$$\frac{d}{dt}\mathcal{W} + \nabla_X \cdot \mathcal{G} = \mathcal{R}J. \tag{10.20}$$

where

$$\mathcal{U} = \begin{bmatrix} \rho \\ \rho\mathbf{v} \end{bmatrix}, \quad \mathcal{F} = \begin{bmatrix} \rho\mathbf{v} \\ \rho\mathbf{v}\mathbf{v} - \sigma \end{bmatrix}, \quad \mathcal{R} = \begin{bmatrix} 0 \\ \mathbf{f} \end{bmatrix}$$

$$\mathcal{W} = \mathcal{U}J, \quad \mathcal{G} := (\mathcal{F} - \mathcal{U}\mathbf{v}) \cdot JF^{-T}. \tag{10.21}$$

Here, the Cauchy stress

$$\sigma(F) = J^{-1}\frac{\partial W}{\partial F} \cdot F^T,$$

where W is the material potential energy, F is the deformation gradient, and $J = \det(F)$.

We still need an equation for F. By differentiating the equality

$$\dot{\mathbf{x}}(t,X) = \mathbf{v}(t,\mathbf{x}(t,X)),$$

in X, we get the equation for F in Lagrangian coordinate:

$$\dot{F}^i_\alpha(t,X) = \frac{\partial v^i}{\partial X^\alpha}.$$

By changing variable from X to $\mathbf{x}$, and treat $\bar{F}(t,\mathbf{x})$ to be $F(t,X(t,\mathbf{x}))$, we get the above equation in Eulerian coordinate:

$$\partial_t \bar{F} + \mathbf{v} \cdot \nabla_{\mathbf{x}} \bar{F} = (\nabla_{\mathbf{x}}\mathbf{v})\bar{F} \quad \text{in } \Omega_t.$$

Note that the matrix $\bar{F}$ is a function of $(t,\mathbf{x})$, but it has the same value of $F(t,X)$. Thus, we shall use the notation F instead of $\bar{F}$ in this note. Thus, we write

$$\boxed{\partial_t F + \mathbf{v}\cdot\nabla_{\mathbf{x}} F = (\nabla_{\mathbf{x}}\mathbf{v})F \quad \text{for } \mathbf{x}\in\Omega_t} \tag{10.22}$$

with an understanding that $F(t,\mathbf{x})$ is $\left(\frac{\partial \mathbf{x}}{\partial X}\right)(t,X(t,\mathbf{x}))$. We list the equations for simple elasticity as

$$\begin{array}{rcl} & \partial_t\rho + \nabla\cdot(\rho\mathbf{v}) = 0 & \\ \rho\left(\partial_t\mathbf{v} + \mathbf{v}\cdot\nabla\mathbf{v}\right) & = & \nabla\cdot\sigma + \mathbf{f} \\ \partial_t F + \mathbf{v}\cdot\nabla F & = & (\nabla\mathbf{v})F \end{array} \qquad \text{in } \Omega_t. \tag{10.23}$$

The unknowns for this system are $\rho,\mathbf{v},F$. The Cauchy stress is given by a constitutive relation

$$\sigma = T(F).$$

The function $\mathbf{f}$ is an external force. We also need the density constraint $\rho\det(F) = \rho_0$ as a compatibility condition.

Remarks

1. The continuity equation for ρ is indeed redundant. In the Lagrange formulation, it is equivalent to $\frac{d}{dt}\rho_0(X) = 0$. In the Eulerian formulation, we define $\rho = \rho_0/J$. Or equivalently, we define the specific volume $V := J/\rho_0$ and define the density $\rho = 1/V$. With this definition, ρ satisfies the continuity equation. Thus, the continuity equation is equivalent to

$$\dot{J} = (\nabla\cdot\mathbf{v})J.$$

   But this equation is inherited in the equation

$$\dot{F} = (\nabla\mathbf{v})F,$$

   because $J = \det(F)$ and $\frac{d}{dt}(\det(F)) = (\nabla\cdot\mathbf{v})\det(F)$. Therefore, we call the algebraic equation

$$\rho(t,\mathbf{x}(t,X))J(t,X) = \rho_0(X) \tag{10.24}$$

   the density constraint for the Euler equation of elasticity.

2. We need a *compatibility condition* in Eulerian coordinate for F, which is parallel to the compatibility condition $\nabla_X \times F^T = 0$ in the Lagrangian coordinate. It is easier to express such condition in terms of F^{-1}, which will be discussed in the next section.

Boundary conditions in Euler coordinate Let $\Gamma_t^d = \mathbf{x}(t, \Gamma_0^d)$ and $\Gamma_t^n = \mathbf{x}(t, \Gamma_0^n)$ be the Dirichlet and Neumann boundaries at time t. In the Eulerian coordinate, the above boundary conditions read

- Dirichlet: $\mathbf{v}(t,\mathbf{x}) = 0$ for $\mathbf{x} \in \Gamma_t^d$;
- Neumann: $\sigma(\mathbf{x}) \cdot \nu = \mathbf{g}(F^{-1}(t,\mathbf{x}))$ for $\mathbf{x} \in \Gamma_t^n$.

Homework Consider a flow map in 1-D as $x^2 - X^2 = t$ with $\hat{M} = [0,\infty)$, $M_t = \{x | x^2 \geq t\}$ and $t \geq 0$. Check the following expressions

(i) $v := \dot{x} = \frac{1}{2x}$

(ii) $F := \partial x / \partial X = X/x$

(iii) $\dot{F} := \frac{\partial}{\partial t}|_X F = -\frac{1}{2}\frac{X}{(X^2+t)^{3/2}} = -\frac{\sqrt{x^2-t}}{2x^3}$

(iv) Treat F as a function of (t,x). Check $(\partial_t + v\partial_x)F = -\frac{\sqrt{x^2-t}}{2x^3}$.

10.2.2 Formulation of Compressible Simple Elasticity in terms of F^{-1}

It is natural to use the quantity $F^{-1}(t,\mathbf{x})$ as a dependent variable because it is naturally defined in Eulerian coordinate $(t,\mathbf{x})$. Furthermore, the compatibility condition for F^{-1} has a simple form. The evolution equation for F^{-1} is

$$\begin{aligned} \left.\frac{d}{dt}\right|_X (F^{-1}) &= -F^{-1}\dot{F}(F^{-1}) \\ &= -F^{-1}(\nabla_{\mathbf{x}}\mathbf{v})F(F^{-1}) \\ &= -(F^{-1})(\nabla_{\mathbf{x}}\mathbf{v}). \end{aligned}$$

$$\frac{d}{dt}(F^{-1})_i^\alpha = -(F^{-1})_k^\alpha L_i^k, \quad L_i^k := \frac{\partial v^k}{\partial x^i}.$$

In the Eulerian coordinate, we have

$$\partial_t(F^{-1}) + \mathbf{v}\cdot\nabla_{\mathbf{x}}(F^{-1}) = -(F^{-1})(\nabla_{\mathbf{x}}\mathbf{v})^T. \tag{10.25}$$

The compatibility condition for F^{-1} is just

$$\nabla_{\mathbf{x}} \times F^{-T} = 0, \quad \frac{\partial}{\partial x_j}(F^{-T})_\alpha^i = \frac{\partial}{\partial x^i}(F^{-T})_\alpha^j. \tag{10.26}$$

The advection equation for F^{-1} can be written in conservation form:

$$\partial_t (F^{-1})^\alpha_i + \partial_{x^i}\left((F^{-1})^\alpha_j v^j\right) = 0. \tag{10.27}$$

This follows from (10.25) and (10.26):

$$\begin{aligned}\partial_t (F^{-1})^\alpha_i + \partial_{x^i}\left((F^{-1})^\alpha_j v^j\right) &= \partial_t (F^{-1})^\alpha_i + v^j \partial_{x^j}(F^{-1})^\alpha_i - v^j \partial_{x^j}(F^{-1})^\alpha_i + \partial_{x^i}\left((F^{-1})^\alpha_j v^j\right)\\ = -(F^{-1})^\alpha_j \partial_{x^i} v^j - v^j \partial_{x^j}(F^{-1})^\alpha_i + \partial_{x^i}\left((F^{-1})^\alpha_j v^j\right) &= v^j\left(-\partial_{x^j}(F^{-1})^\alpha_i + \partial_{x^i}(F^{-1})^\alpha_j\right) = 0.\end{aligned}$$

Thus, the full set of equations are

$$\begin{cases} \partial_t \rho + \partial_{x^j}(v^j \rho) = 0\\ \partial_t(\rho v^i) + \partial_{x^j}\left(\rho v^i v^j\right) = \partial_{x^j}\sigma^{ij} + f^i\\ \partial_t (F^{-1})^\alpha_k + \partial_{x^k}\left((F^{-1})^\alpha_j v^j\right) = 0. \end{cases} \tag{10.28}$$

Plus the density constraint: $\rho J = \rho_0$ and the compatibility condition

$$\nabla_{\mathbf{x}} \times F^{-T} = 0. \tag{10.29}$$

There are $1+9+3 = 13$ unknowns $(\rho, \mathbf{v}, F^{-1})$ and equations.

Boundary conditions in Euler coordinate

- Dirichlet: $\mathbf{v}(t,\mathbf{x}) = 0$ for $\mathbf{x} \in \Gamma^d_t$;
- Neumann: $\sigma(\mathbf{x})\cdot \nu = \mathbf{g}(F^{-1}(t,\mathbf{x}))$ for $\mathbf{x} \in \Gamma^n_t$.

Remarks [5]

- The continuity equation is redundant because it can be derived from $\rho J = \rho_0$.
- The compatibility condition is satisfied if it holds initially. This is due to the fact that (10.27) preserves the property $\nabla_{\mathbf{x}} \times (F^{-1}) = 0$.

[5]References:

1. Trangenstein and Colella, A Higher-order Godunov method for modeling finite deformation in elastic-plastic solids, Comm. Pure. Appl. Math (1991).
2. Miller & Colella, A high-order Eulerian Godunov method for elastic–plastic flow in solids, J. Comput. Phys. (2001).
3. D.J. Hill , D. Pullin, M. Ortiz, D. Meiron, An Eulerian hybrid WENO centered-difference solver for elastic–plastic solids, J. Comput. Phys. (2010)

10.2.3 Formulation of Compressible Simple Elasticity in terms of B

We shall see in later chapter that the stress σ can be expressed as

$$\sigma = 2\hat{W}_B B,$$

where $B = FF^T$ is the left Cauchy-Green deformation tensor. It satisfies

$$\dot{B} = \dot{F}F^T + F\dot{F}^T = LFF^T + FF^T L = LB + BL^T.$$

Here $L = \nabla\mathbf{v}$ and $\dot{B}$ means the material derivative. In terms of Eulerian coordinate, B satisfies

$$B_{(1)} := \frac{\partial B}{\partial t} + \mathbf{v}\cdot\nabla B - LB - BL^T = 0.$$

The term $B_{(1)}$ is called the first order upper-convected derivative of B. In terms of Lie derivative, this upper convected derivative is the Lie derivative for the tensor $B = B_{ij}dx^i \otimes dx^j$:

$$(\partial_t + \mathscr{L}_{\mathbf{v}})B = 0.$$

In addition, B should satisfy the compatibility condition.

Thus, the equations are

$$\boxed{\begin{array}{rcl} \partial_t\rho + \nabla\cdot(\rho\mathbf{v}) & = & 0 \\ \rho\left(\partial_t\mathbf{v} + \mathbf{v}\cdot\nabla\mathbf{v}\right) & = & \nabla\cdot\sigma + \mathbf{f} \\ \partial_t B + \mathbf{v}\cdot\nabla B & = & (\nabla\mathbf{v})B + B(\nabla\mathbf{v})^T \end{array}} \qquad \text{in } \Omega_t. \tag{10.30}$$

together with the density constraint $\rho J = \rho_0$. Here,

$$\sigma = 2\hat{W}_B B.$$

An expression of σ in terms of B is given by Theorem 9.10. The compatibility for B is more complicated. It can be derived from the compatibility condition for $C = F^T F$. The compatibility condition for C can be found in [Cialet, pp. 55] or [Antman, pp. 423-426].

10.2.4 Formulation of Incompressible Simple Elasticity

If $\mathbf{v}(t,\mathbf{x})$ is the velocity field which generates the flow map $\mathbf{x}(t,X)$, that is, $\dot{\mathbf{x}}(t,X) = \mathbf{v}(t,x(t,X))$, then the incompressibility of $\mathbf{x}(t,X)$ is equivalent to $\nabla\cdot\mathbf{v}(t,x) = 0$. This comes from the following formula

$$\delta\det(A) = tr\left((\delta A)A^{-T}\right)\det(A).$$

and the formula

$$\frac{\partial \dot{\mathbf{x}}}{\partial X} = (\nabla \mathbf{v})\frac{\partial \mathbf{x}}{\partial X},$$

we get

$$\dot{J} = tr\left(\dot{F}F^{-T}\right)J = tr(\nabla \mathbf{v})J = (\nabla \cdot \mathbf{v})J.$$

Thus,

$$\dot{J} = 0 \quad \text{if and only if} \quad \nabla \cdot \mathbf{v} = 0.$$

Similarly, let $\mathbf{x}_\varepsilon(t,X)$ be a perturbation of $\mathbf{x}(t,X)$ satisfying volume preserving property. Let $\delta \mathbf{x}(t,X) := \frac{\partial}{\partial \varepsilon}|_{\varepsilon=0}\mathbf{x}_\varepsilon(t,X)$. Let $\mathbf{w}(t,\mathbf{x}(t,X)) = \delta \mathbf{x}(t,X)$. Let $F_\varepsilon = \partial \mathbf{x}_\varepsilon/\partial X$. $\delta F := \frac{\partial}{\partial \varepsilon}|_{\varepsilon=0}F_\varepsilon$. Then

$$\delta F = (\nabla \mathbf{w})F.$$

Similarly,

$$\delta J = (\nabla \cdot \mathbf{w})J.$$

Thus, the volume preserving of $\mathbf{x}_\varepsilon$ is equivalent to $\delta J = 0$, and is also equivalent to $\nabla \cdot \mathbf{w} = 0$.

Now, for the constraint $\nabla \cdot \mathbf{w} = 0$, we introduce a Lagrange multiplier p. Then we have the constrained variation

$$\begin{aligned} 0 &= \int_{t_0}^{t_1}\int (-\rho \frac{D\mathbf{v}}{Dt} + \nabla \cdot \sigma) \cdot \mathbf{w} + p(\nabla \cdot \mathbf{w})\,dx\,dt \\ &= \int_{t_0}^{t_1}\int (-\rho \frac{D\mathbf{v}}{Dt} + \nabla \cdot \sigma - \nabla p) \cdot \mathbf{w}\,dx\,dt \end{aligned}$$

This gives

$$\rho \frac{D\mathbf{v}}{Dt} + \nabla p = \nabla \cdot \sigma.$$

Here, $\sigma(F) = W'(F)F^T$. We still need an equation for F. From

$$\dot{F} = \left(\frac{\partial \mathbf{x}}{\partial X}\right)_t = \frac{\partial \mathbf{v}}{\partial X} = \frac{\partial \mathbf{v}}{\partial \mathbf{x}}\frac{\partial \mathbf{x}}{\partial X} = (\nabla \mathbf{v})F,$$

we get

$$\frac{DF}{Dt} = (\nabla \mathbf{v})F.$$

Thus, the complete set of equations for incompressible inviscid elasticity are

$$\left\{ \begin{array}{rcl} \frac{D\rho}{Dt} &=& 0 \\ \nabla \cdot \mathbf{v} &=& 0 \\ \rho \frac{D\mathbf{v}}{Dt} &=& -\nabla p + \nabla \cdot \sigma(F) \\ \frac{DF}{Dt} &=& (\nabla \mathbf{v})F. \end{array} \right.$$

with the constitutive equation $\sigma(F) = J^{-1}W'(F)F^T$ and the density constraint $\rho J = \rho_0$. The unknowns are $(\rho, p, \mathbf{v}, F)$. We notice that these equations can be written in conservation form

$$\left\{\begin{array}{rcl} \partial_t\rho + \nabla\cdot(\rho\mathbf{v}) &=& 0 \\ \nabla\cdot\mathbf{v} &=& 0 \\ \partial_t(\rho\mathbf{v}) + \nabla\cdot(\rho\mathbf{v}\mathbf{v}) &=& -\nabla p + \nabla\cdot\sigma(F) \\ \partial_t(F^{-1}) + \nabla\left((F^{-1})\mathbf{v}\right) &=& 0. \end{array}\right.$$

The last equation in component form reads

$$\partial_t(F^{-1})^\alpha_k + \partial_{x^k}\left((F^{-1})^\alpha_j v^j\right) = 0.$$

10.3 Advection Equations and The Compatibility Conditions

Sometimes, it is more convenient to use other types of strain tensors. In that case, the corresponding compatibility conditions and advection equations are needed. We list some of them.

10.3.1 Compatibility condition for the deformation gradients

- For $F^i_\alpha := \frac{\partial x^i}{\partial X^\alpha}$, we have

$$\frac{\partial F^i_\alpha}{\partial X^\beta} = \frac{\partial^2 x^i}{\partial X^\beta \partial \alpha} = \frac{\partial^2 x^i}{\partial X^\alpha \partial \beta} = \frac{\partial F^i_\beta}{\partial X^\alpha}.$$

  This is called the compatibility condition for F. Sometimes, we write it as

$$\nabla_X \times F^T = 0.$$

- For $(F^{-1})^\alpha_i = \frac{\partial X^\alpha}{\partial x^i}$, the corresponding compatibility condition reads

$$\frac{\partial (F^{-1})^\alpha_i}{\partial x^j} = \frac{\partial (F^{-1})^\alpha_i}{\partial x^i}.$$

  or

$$\nabla_\mathbf{x} \times F^{-T} = 0.$$

- For $C := F^T F$, which is the pullback of the metric in M_t, we define

$$\Gamma_{\alpha\gamma\beta} = \frac{1}{2}\left(\partial_\beta C_{\alpha\gamma} - \partial_\alpha C_{\beta\gamma} - \partial_\gamma C_{\alpha\beta}\right), \quad \Gamma^\gamma_{\alpha\beta} = (C^{-1})_{\gamma\delta}\Gamma_{\alpha\delta\beta}.$$

And the corresponding compatibility condition for C reads

$$\partial_\delta \Gamma^\beta_{\alpha\gamma} - \partial_\gamma \Gamma^\beta_{\alpha\delta} + \Gamma^\tau_{\alpha\gamma}\Gamma^\beta_{\tau\delta} - \Gamma^\tau_{\alpha\delta}\Gamma^\beta_{\tau\gamma} = 0.$$

The above expression states that the Riemann-Christoffel curvature tensor is zero. See [Cialet, pp. 55], [Antman pp. 423-426].

Homework: Derive the compatibility condition for $B = FF^T$.

10.4 Geometric Formulation of elasticity

The equations of elasticity consist of continuity equation, equation of motion (momentum equation), energy equation (first law of thermodynamics), and an advection equation for the deformation gradient. We will write them in the Language of differential forms. Recall the following notations:

- Let ρ_t denote for $\rho(t,\cdot)$ and μ_t be the volume form of M_t. Sometimes, we neglect the subscript t.
- $\mathbf{v} = v^i\partial_{x^i}$ is the velocity. $\eta = v_i dx^i = \flat\mathbf{v}$ is the momentum.
- $\sigma = \sigma_i^j(\star dx^j)\otimes dx^i$ is the stress.
- φ_t^* is the pull-back operator. d_t is the time derivative with fixed material coordinate. An important formula is
$$d_t\varphi_t^* = \varphi_t^*(\partial_t + \mathscr{L}_\mathbf{v}).$$

Continuity equation

$$\boxed{(\partial_t + \mathscr{L}_\mathbf{v})(\rho_t\mu_t) = 0.} \tag{10.31}$$

Advection equation for deformation gradient F Recall that

$$F(X) = F^i_\alpha(X)dX^\alpha \otimes \partial_{x^i}, \quad F^i_\alpha := \frac{\partial x^i}{\partial X^\alpha}. \tag{10.32}$$

The advection equation for F is

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

In term of Lie derivative, it is

$$\boxed{\partial_t F + \mathscr{L}_\mathbf{v} F = 0.} \tag{10.33}$$

This follows from

$$\begin{aligned}
\partial_t F + \mathscr{L}_{\mathbf{v}} F &= \frac{d}{dt}\left(F^i_\alpha(X) dX^\alpha \otimes \partial_{x^i}\right) \\
&= \frac{d}{dt}\left(F^i_\alpha(X) dX^\alpha \otimes \frac{\partial X^\beta}{\partial x^i} \partial_{X^\beta}\right) \\
&= \left(\partial_t F^i_\alpha + v^k \partial_{x^k} F^i_\alpha - F^k_\alpha \frac{\partial v^i}{\partial x^k}\right) dX^\alpha \otimes \partial_{x^i} \\
&= 0.
\end{aligned}$$

Note that the pull-back is only for ∂_{x^k}.

Advection of the left Cauchy-Green deformation tensor Define the left Cauchy-Green tensor

$$B(\mathbf{x}) = F^i_\alpha F^j_\alpha \partial_{x^i} \otimes \partial_{x^j},$$

which is a tensor of type $(2,0)$. The Lie derivative of a type $(2,0)$ tensor A is given by

$$\begin{aligned}
\mathscr{L}_{\mathbf{v}} A &= (\mathscr{L}_{\mathbf{v}} A^{ij}) \frac{\partial}{\partial x^i} \otimes \frac{\partial}{\partial x^j} + A^{kj} \mathscr{L}_{\mathbf{v}}\left(\frac{\partial}{\partial x^k}\right) \otimes \frac{\partial}{\partial x^j} + A^{i\ell} \frac{\partial}{\partial x^i} \otimes \mathscr{L}_{\mathbf{v}}\left(\frac{\partial}{\partial x^\ell}\right) \\
&= \left(\partial_t A^{ij} + v^k \partial_{x^k} A^{ij} - A^{kj} \frac{\partial v^i}{\partial x^k} - A^{i\ell} \frac{\partial v^j}{\partial x^\ell}\right) \frac{\partial}{\partial x^i} \otimes \frac{\partial}{\partial x^j}
\end{aligned}$$

This is also known as the upper-convected derivative of the tensor A. Thus,

$$(\partial_t + \mathscr{L}_{\mathbf{v}}) B = (\partial_t + \mathbf{v} \cdot \nabla) B - LB - BL^T = 0.$$

Equation of motion Let $\eta = v_i dx^i$ be the momentum 1-form. The Piola stress has the form

$$P(F) = P^\alpha_i(F)(\star dX^\alpha) \otimes dx^i. \tag{10.34}$$

This means that $P \in \Omega^{n-1}(\hat{M}) \otimes T^*M$, or $\Omega^{n-1}(\hat{M}, T^*M)$. The pairing of P and F is

$$W(F)\hat{\mu} := F \wedge P = F^i_\alpha P^\alpha_i dX^\alpha \wedge (*dX^\alpha) \langle \partial_{x^i} | dx^i \rangle = F^i_\alpha P^\alpha_i \hat{\mu}. \tag{10.35}$$

The equation of motion is

$$\boxed{(\partial_t + \mathscr{L}_{\mathbf{v}})\eta - d\left(\frac{1}{2}|\mathbf{v}|^2\right) = \frac{1}{\rho} \star d\sigma.} \tag{10.36}$$

The connection between P and σ is

$$P = \varphi_t^* \sigma.$$

10.5 Hyperbolicity

10.5.1 Hyperbolicity for Simple Elasticity in the Lagrangian Coordinate

The equation of motion for simple elasticity reads

$$\rho_0 \ddot{\mathbf{x}} = \nabla_X \cdot P, \quad P = \frac{\partial W}{\partial F}. \tag{10.37}$$

In component form, it reads

$$\rho_0 \ddot{x}_i = \partial_{X^\alpha} P_i^\alpha, \quad P_i^\alpha = \frac{\partial W}{\partial F_\alpha^i}.$$

Let

$$a_{ij}^{\alpha\beta}(F) := \frac{\partial^2 W(F)}{\partial F_\alpha^i \partial F_\beta^j}.$$

For stability issue, we consider a linearized equation where the coefficient $a_{\alpha\beta}^{ij}(F_0)$ is frozen at a particular F_0. In this case, the linearized equation reads

$$\rho_0 \ddot{x}_i = \sum_{j,\alpha,\beta=1}^{3} a_{ij}^{\alpha\beta}(F_0) \frac{\partial^2 x^j}{\partial X^\alpha \partial X^\beta}, \quad i = 1,2,3. \tag{10.38}$$

We look for plane-wave solutions of the form $\mathbf{x}(t,X) = \xi e^{i(X\cdot\eta - \lambda t)}$. It means that, given a direction $\eta \in \mathbb{R}^3$, we look for a plane wave with speed $\lambda(\eta)$ and amplitude $\xi(\eta) \in \mathbb{R}^3$. Plugging this expression into the linearized equation (10.38), eliminating $e^{i(X\cdot\eta-\lambda t)}$ on both sides, we get

$$\rho_0 \lambda^2 \xi^i = \sum_{j,\alpha,\beta=1}^{3} a_{ij}^{\alpha\beta} \xi^j \eta_\alpha \eta_\beta = \sum_{j=1}^{3} \left(\sum_{\alpha,\beta=1}^{3} a_{ij}^{\alpha\beta} \eta_\alpha \eta_\beta \right) \xi^j.$$

In matrix form, it is

$$A(\eta)\xi = \rho_0 \lambda^2 \xi, \quad A(\eta)_{ij} := \left(\sum_{\alpha,\beta=1}^{3} a_{ij}^{\alpha\beta} \eta_\alpha \eta_\beta \right)_{3\times 3}.$$

Thus, equation (10.38) supports plane wave solution in direction η if $A(\eta)$ has non-negative eigenvalue $\rho_0 \lambda^2$ with eigenvector ξ. [6]

[6] We will see in the next subsection that there is no zero eigenvalue for matrix A.

Proposition 10.12. *Given a stored energy $W(F)$, define $a_{ij}^{\alpha\beta} = \frac{\partial^2 W}{\partial F_\alpha^i \partial F_\beta^j}$. Then for any $\eta \in \mathbb{R}^3$, the matrix $A(\eta)_{ij} := (\sum_{\alpha,\beta} a_{ij}^{\alpha\beta} \eta_\alpha \eta_\beta)$ is symmetric.*

Proof. This is due to

$$A(\eta)_{ij} = \sum_{\alpha,\beta=1}^{3} a_{ij}^{\alpha\beta} \eta_\alpha \eta_\beta = \sum_{\alpha,\beta=1}^{3} a_{ij}^{\alpha\beta} \eta_\beta \eta_\alpha = \sum_{\alpha,\beta=1}^{3} a_{ij}^{\beta\alpha} \eta_\alpha \eta_\beta = \sum_{\alpha,\beta=1}^{3} a_{ji}^{\alpha\beta} \eta_\alpha \eta_\beta = A(\eta)_{ji}. \tag{10.39}$$

Here, the 2nd equality is due to $\eta_\alpha \eta_\beta = \eta_\beta \eta_\alpha$. The 3rd equality is a change of indices. The 4th equality uses $a_{ij}^{\beta\alpha} = a_{ji}^{\alpha\beta}$, which is resulted in hyper-elasticity assumption:

$$a_{ij}^{\beta\alpha} = \frac{\partial^2 W}{\partial F_\beta^i \partial F_\alpha^j} = \frac{\partial^2 W}{\partial F_\alpha^j \partial F_\beta^i} = a_{ji}^{\alpha\beta}.$$

□

To support plane-wave solutions, we need $A(\eta)$ to be positive definite for $\eta \neq 0$. This means

$$\sum_{i,j,\alpha,\beta=1}^{3} a_{ij}^{\alpha\beta} \xi^i \xi^j \eta_\alpha \eta_\beta > 0, \text{ for all } \eta, \xi \neq 0. \tag{10.40}$$

This condition is called the *strong ellipticity condition* for the tensor $a_{ij}^{\alpha\beta}$.

Definition 10.4. *System (10.37) is called hyperbolic if*

$$\frac{\partial^2 W(F)}{\partial F_\alpha^i \partial F_\beta^j} \xi^i \xi^j \eta_\alpha \eta_\beta > 0, \quad \textit{for every } F \in \mathbb{M}_3^+,\ \xi \neq 0, \eta \neq 0. \tag{10.41}$$

10.5.2 Hyperbolicity for the first-order system in Lagrangian coordinate

Equation of motion in Lagrangian coordinate The equations for elasticity include the evolution equation for F:

$$\dot{F}_\beta^j - \frac{\partial v^j}{\partial X^\beta} = 0, \quad j, \beta = 1,2,3, \tag{10.42}$$

and the equation of motion:

$$\rho_0 \dot{v}_i - \sum_{\alpha=1}^{3} \frac{\partial P_i^\alpha}{\partial X^\alpha} = 0, \quad i = 1,2,3, \tag{10.43}$$

where the first Piola stress P is given by

$$P_i^\alpha = \frac{\partial W}{\partial F_\alpha^i}, \quad i, \alpha = 1, 2, 3. \tag{10.44}$$

for some potential function $W(F)$. Note that the deformation gradient F should satisfy the compatibility condition

$$\frac{\partial F_\alpha^i}{\partial X^\beta} = \frac{\partial F_\beta^i}{\partial X^\alpha}. \tag{10.45}$$

There are 12 equations (10.42) (10.43) for 12 unknowns $(F, \mathbf{v})$. The compatibility condition is automatically satisfied for $t > 0$ if it is satisfied at $t = 0$. Writing these equations in vector form, they are

$$\boxed{\begin{array}{l} \dot{F} = \frac{\partial \mathbf{v}}{\partial X} \\ \rho_0 \dot{\mathbf{v}} = \nabla_X \cdot P(F). \end{array}} \tag{10.46}$$

The compatibility condition reads

$$\nabla \times F^T = 0. \tag{10.47}$$

Hyperbolicity and characteristic modes Let us take $\rho_0 \equiv 1$ for simplicity. It is not hard to put them back in the theory below. The system can be rewritten in the following conservation form

$$\partial_t \mathcal{W} + \sum_{\alpha=1}^{3} \partial_{X^\alpha} \mathcal{G}^\alpha = 0,$$

where

$$\mathcal{W} = \begin{bmatrix} F_1^1 \\ F_1^2 \\ F_1^3 \\ F_2^1 \\ F_2^2 \\ F_2^3 \\ F_3^1 \\ F_3^2 \\ F_3^3 \\ v^1 \\ v^2 \\ v^3 \end{bmatrix}, \quad \mathcal{G}^1 = -\begin{bmatrix} v^1 \\ v^2 \\ v^3 \\ 0 \\ 0 \\ 0 \\ 0 \\ 0 \\ 0 \\ P_1^1 \\ P_2^1 \\ P_3^1 \end{bmatrix}, \quad \mathcal{G}^2 = -\begin{bmatrix} 0 \\ 0 \\ 0 \\ v^1 \\ v^2 \\ v^3 \\ 0 \\ 0 \\ 0 \\ P_1^2 \\ P_2^2 \\ P_3^2 \end{bmatrix}, \quad \mathcal{G}^3 = -\begin{bmatrix} 0 \\ 0 \\ 0 \\ 0 \\ 0 \\ 0 \\ v^1 \\ v^2 \\ v^3 \\ P_1^3 \\ P_2^3 \\ P_3^3 \end{bmatrix}$$

This system can be written as a quasi-linear form

$$\partial_t \mathcal{W} + \sum_{\alpha=1}^{3} \mathcal{B}^\alpha \partial_{X^\alpha} \mathcal{W} = 0, \quad \mathcal{B}^\alpha = \frac{\partial \mathcal{G}^\alpha}{\partial \mathcal{W}}.$$

The matrix $\mathcal{B}^\alpha$ has the form

$$\mathcal{B}^\alpha = -\begin{bmatrix} 0_{9\times 9} & {E^\alpha}_{9\times 3} \\ {A^\alpha}_{3\times 9} & 0_{3\times 3} \end{bmatrix}$$

where

$$E^1 = \begin{bmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 1 \\ 0 & 0 & 0 \\ 0 & 0 & 0 \\ 0 & 0 & 0 \\ 0 & 0 & 0 \\ 0 & 0 & 0 \\ 0 & 0 & 0 \end{bmatrix}, \quad E^2 = \begin{bmatrix} 0 & 0 & 0 \\ 0 & 0 & 0 \\ 0 & 0 & 0 \\ 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 1 \\ 0 & 0 & 0 \\ 0 & 0 & 0 \\ 0 & 0 & 0 \end{bmatrix}, \quad E^3 = \begin{bmatrix} 0 & 0 & 0 \\ 0 & 0 & 0 \\ 0 & 0 & 0 \\ 0 & 0 & 0 \\ 0 & 0 & 0 \\ 0 & 0 & 0 \\ 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 1 \end{bmatrix},$$

$$A^\alpha = \begin{bmatrix} a_{11}^{\alpha 1} & a_{11}^{\alpha 2} & \cdots & a_{13}^{\alpha 3} \\ a_{21}^{\alpha 1} & a_{21}^{\alpha 2} & \cdots & a_{23}^{\alpha 3} \\ a_{31}^{\alpha 1} & a_{31}^{\alpha 2} & \cdots & a_{33}^{\alpha 3} \end{bmatrix}_{3\times 9}, \quad a_{ij}^{\alpha\beta} := \frac{\partial P_i^\alpha}{\partial F_j^\beta} = \frac{\partial^2 W(F)}{\partial F_\beta^j \partial F_\alpha^i}.$$

We shall look for plane wave solution of the form

$$(F, \mathbf{v}) = (\zeta_1, \zeta_2, \zeta_3, \xi^1, \xi^2, \xi^3)^T e^{i(\eta\cdot X - \lambda t)}.$$

Plug this ansatz into the equation. Let us define the matrices

$$\Lambda(\mathcal{W}, \eta) := \sum_{\alpha=1}^{3} \mathcal{B}^\alpha \eta_\alpha$$

and

$$\Lambda(\mathcal{W}, \eta) = -\begin{bmatrix} 0 & 0 & 0 & \eta & 0 & 0 \\ 0 & 0 & 0 & 0 & \eta & 0 \\ 0 & 0 & 0 & 0 & 0 & \eta \\ \mathbf{b}_{11} & \mathbf{b}_{12} & \mathbf{b}_{13} & 0 & 0 & 0 \\ \mathbf{b}_{21} & \mathbf{b}_{22} & \mathbf{b}_{23} & 0 & 0 & 0 \\ \mathbf{b}_{31} & \mathbf{b}_{32} & \mathbf{b}_{33} & 0 & 0 & 0 \end{bmatrix}_{12\times 12} := -\begin{bmatrix} 0_{9\times 9} & C_{9\times 3} \\ B_{3\times 9} & 0_{3\times 3} \end{bmatrix},$$

$$\eta = \begin{bmatrix} \eta_1 \\ \eta_2 \\ \eta_3 \end{bmatrix}_{3\times 1}, \quad \mathbf{b}_{ij}(\eta) = \begin{bmatrix} \sum_\alpha a_{ij}^{\alpha 1}\eta_\alpha & \sum_\alpha a_{ij}^{\alpha 2}\eta_\alpha & \sum_\alpha a_{ij}^{\alpha 3}\eta_\alpha \end{bmatrix}_{1\times 3}$$

The characteristic equation of the matrix $\Lambda(\mathcal{W},\eta)$ is:

$$\det(\lambda-\Lambda(\mathcal{W},\eta)) = \det\begin{bmatrix}\lambda I_{9\times 9} & C_{9\times 3}\\ B_{3\times 9} & \lambda I_{3\times 3}\end{bmatrix} = \det\begin{bmatrix}\lambda I_{9\times 9} & C_{9\times 3}\\ 0_{3\times 9} & -\frac{1}{\lambda}B_{3\times 9}C_{9\times 3}+\lambda I_{3\times 3}\end{bmatrix}$$
$$\lambda^9\det\left(\lambda\delta_{ij}-\frac{1}{\lambda}\sum_{\alpha,\beta=1}^{3} a_{ij}^{\alpha\beta}\eta_\alpha\eta_\beta\right) = \lambda^6\det(\lambda^2 I - A(\eta)) = 0.$$

Strong ellipticity and hyperbolicity

- There are 6 zero eigenvalues of $\Lambda(\mathcal{W},\eta)$.
- The rest 6 eigenvalues are real provided $(A(\eta))$ is positive definite.[7]

The strong ellipticity assumption for $(a_{ij}^{\alpha\beta})$ is equivalent the positive definite assumption for $A(\beta)$, and is equivalent to the existence of 6 real eigenvalues of $\Lambda(\mathcal{W},\eta)$.

Eigenvectors corresponding to 0 eigenvalue Let us find the eigenvector corresponding the 0 eigenvalue:

$$\begin{bmatrix} 0 & 0 & 0 & \eta & 0 & 0\\ 0 & 0 & 0 & 0 & \eta & 0\\ 0 & 0 & 0 & 0 & 0 & \eta\\ \mathbf{b}_{11} & \mathbf{b}_{12} & \mathbf{b}_{13} & 0 & 0 & 0\\ \mathbf{b}_{21} & \mathbf{b}_{22} & \mathbf{b}_{23} & 0 & 0 & 0\\ \mathbf{b}_{31} & \mathbf{b}_{32} & \mathbf{b}_{33} & 0 & 0 & 0\end{bmatrix}\begin{bmatrix}\zeta_1\\ \zeta_2\\ \zeta_3\\ \xi^1\\ \xi^2\\ \xi^3\end{bmatrix} = 0, \quad \text{where } \zeta_i = \begin{bmatrix}\zeta_i^1\\ \zeta_i^2\\ \zeta_i^3\end{bmatrix}, i=1,2,3.$$

The first 9 equations give

$$\eta\xi^i = 0, \quad i=1,2,3$$

Since $\eta\neq 0$, we obtain $\xi^i=0$ for $i=1,2,3$. The last three equation are independent from the strong ellipticity of $(a_{ij}^{\alpha\beta})$. This gives three independent equations for 9 variables $\zeta_i\in\mathbb{R}^3$, $i=1,2,3$. Thus, the dimension of the kernel of $\Lambda(\mathcal{W},\eta)$ is 6. If we assume the material is isotropic, we can just choose direction $\eta=(1,0,0)^T$ to find the eigenvectors. The eigenvectors corresponding to other direction η can be obtained by a rotation. When $\eta=(1,0,0)^T$,

$$\mathbf{b}_{ij} = \begin{bmatrix} a_{ij}^{11} & a_{ij}^{12} & a_{ij}^{13}\end{bmatrix}, \quad i,j=1,2,3. \tag{10.48}$$

[7] Note that the 3×3 matrix

$$A(\eta)_{ij} := \sum_{\alpha,\beta=1}^{3} a_{ij}^{\alpha\beta}\eta_\alpha\eta_\beta$$

is symmetric from (10.12).

The last three equations for ζ_i, $i = 1,2,3$ read

$$\sum_{j=1}^{3} b_{ij}\zeta_j = 0, \quad i = 1,2,3. \tag{10.49}$$

There are 3 independent equations with 9 unknowns. Suppose the first three column vectors are independent, we can set

$$(\zeta_2, \zeta_3) = \begin{bmatrix} X & X \\ X & X \\ X & X \end{bmatrix}$$

with one of X's being 1 and the rests being 0's. There are 6 of them. For each of them, we plug into (10.49) to find the corresponding ζ_1. This gives 6 eigenvectors corresponding to the zero eigenvalue.

Eigenvectors corresponding to the nonzero eigenvalues We solve the eigen system

$$\begin{bmatrix} \lambda I & 0 & 0 & \eta & 0 & 0 \\ 0 & \lambda I & 0 & 0 & \eta & 0 \\ 0 & 0 & \lambda I & 0 & 0 & \eta \\ \mathbf{b}_{11} & \mathbf{b}_{12} & \mathbf{b}_{13} & \lambda & 0 & 0 \\ \mathbf{b}_{21} & \mathbf{b}_{22} & \mathbf{b}_{23} & 0 & \lambda & 0 \\ \mathbf{b}_{31} & \mathbf{b}_{32} & \mathbf{b}_{33} & 0 & 0 & \lambda \end{bmatrix} \begin{bmatrix} \zeta_1 \\ \zeta_2 \\ \zeta_3 \\ \xi^1 \\ \xi^2 \\ \xi^3 \end{bmatrix} = 0, \tag{10.50}$$

for λ and $[\zeta, \xi]^T$ with $\lambda \neq 0$. The first 9 equations give

$$\zeta_k = -\frac{\xi^k}{\lambda}\eta. \tag{10.51}$$

Plugging into the last three equations, from (10.48), the last three equations read

$$\sum_{j=1}^{3}\sum_{\beta=1}^{3}\left(\sum_{\alpha=1}^{3} a_{ij}^{\alpha\beta}\eta_\alpha\right)\left(-\frac{\xi^j}{\lambda}\eta_\beta\right) + \lambda\xi^i = 0, \quad i = 1,2,3.$$

This shows (λ^2, ξ) are eigen pair of the matrix

$$A(\eta) = \sum_{\alpha,\beta=1}^{3} a_{ij}^{\alpha\beta}\eta_\alpha\eta_\beta.$$

Note that A is positive definite from strong ellipticity of $(a_{ij}^{\alpha\beta})$. We thus get $\pm\lambda$ are the eigenvalues of (10.50). The corresponding eigenvectors are also obtained from the eigenvectors of A and (10.51).

Definition 10.5. *System (10.37) is called hyperbolic if*

$$\frac{\partial^2 W(F)}{\partial F^i_\alpha \partial F^j_\beta}\xi^i\xi^j\eta_\alpha\eta_\beta > 0, \quad \textit{for every } F \in \mathbb{M}^+_3,\ \xi \neq 0, \eta \neq 0. \tag{10.52}$$

This hyperbolicity condition is a basic requirement for the restored energy W for the well-posedness of system (10.37).

10.5.3 Hyperbolicity for first-order system in Eulerian formulation

Let us denote

$$G_{\alpha i} = \left(F^{-1}\right)^\alpha_i.$$

The system can be rewritten in the following conservation form

$$\partial_t \mathcal{U} + \sum_{j=1}^{3} \partial_{x^j}\mathcal{F}_\alpha = 0,$$

where

$$\mathcal{U} = \begin{bmatrix} G_{11} \\ G_{21} \\ G_{31} \\ G_{12} \\ G_{22} \\ G_{32} \\ G_{13} \\ G_{23} \\ G_{33} \\ \rho v^1 \\ \rho v^2 \\ \rho v^3 \\ \rho \end{bmatrix}, \quad \mathcal{F}_1 = \begin{bmatrix} G_{11}v^1 \\ G_{12}v^2 \\ G_{13}v^3 \\ 0 \\ 0 \\ 0 \\ 0 \\ 0 \\ 0 \\ \rho v^1 v^1 - \sigma_{11} \\ \rho v^1 v^2 - \sigma_{21} \\ \rho v^1 v^3 - \sigma_{31} \\ \rho v^1 \end{bmatrix}, \quad \mathcal{F}_2 = \begin{bmatrix} 0 \\ 0 \\ 0 \\ G_{21}v^1 \\ G_{22}v^2 \\ G_{23}v^3 \\ 0 \\ 0 \\ 0 \\ \rho v^2 v^1 - \sigma_{12} \\ \rho v^2 v^2 - \sigma_{22} \\ \rho v^2 v^3 - \sigma_{32} \\ \rho v^2 \end{bmatrix}, \quad \mathcal{F}_3 = \begin{bmatrix} 0 \\ 0 \\ 0 \\ 0 \\ 0 \\ 0 \\ G_{31}v^1 \\ G_{32}v^2 \\ G_{33}v^3 \\ \rho v^3 v^1 - \sigma_{13} \\ \rho v^3 v^2 - \sigma_{23} \\ \rho v^3 v^3 - \sigma_{33} \\ \rho v^3 \end{bmatrix}$$

We look for solutions of the form

$$(F, \mathbf{v}) = (\zeta_1, \zeta_2, \zeta_3, \xi^1, \xi^2, \xi^3)^T e^{i(\eta\cdot\mathbf{x}-\lambda t)}.$$

One can use the eigen-decomposition for the Lagrangian system to get the eigen-decomposition for the above Eulerian system. The correspondence are

Lagrangian	Eulerian
$\lambda = 0$	$\lambda = \mathbf{v}\cdot\eta$
$\pm\lambda_p,$	$\mathbf{v}\cdot\eta \pm \lambda_p, p = 1,2,3$

The corresponding eigenvector can be obtained from the Lagrangian-Eulerian transformation formula. We leave the details to students to complete. You can also see Trangenstein and Colella's paper.

Reference

- Trangenstein and Colella, A Higher-order Godunov method for modeling finite deformation in elastic-plastic solids, Comm. Pure. Appl. Math (1991).

Chapter 11

Thermo-elasticity

Reference

- Jacob Lubliner, Plasticity Theory.
- Silhavy, The Mechanics and Thermodynamics of Continuous Media, 1997.
- Li, Tatsien and Tiehu Qin, Physics and PDEs, Vol.II. ,SIAM.

11.1 Constitutive law

11.1.1 First Law of Thermo-Elasticity

State variables

1. To describe a motion of an elastic material, we introduce the flow map φ_t, which maps M_0 to $\mathcal{S}$.

2. The kinetic state variables are fields $(\varphi(t,X), \dot{\varphi}(t,X), F(t,X))$, or $(\mathbf{x}(t,X), \dot{\mathbf{x}}(t,X), \frac{\partial \mathbf{x}}{\partial X}(t,X))$.

3. In addition, there are thermo variables, which are $(\rho_0(X), S(t,X), T(t,X))$, which are scalar fields. We should treat ρ_0 as a measure in the material space M_0 and is independent of time.

4. An adiabatic process is a motion φ_t which is so slow that no energy exchange occurs internally or externally except the work done by the motion φ_t.

Work and stored energy

1. Given a flow map $\mathbf{x}(X)$, consider a one-parameter family of flow map $\mathbf{x}^s(X)$ with $\mathbf{x}^0(X) = \mathbf{x}(X)$. The variation $\frac{d}{ds}\big|_{s=0}\mathbf{x}^s(X)$ is called a variation of $\mathbf{x}(X)$. We denote it by $\mathring{\mathbf{x}}$ (i.e. $\delta\mathbf{x}$). The variation $\mathring{\mathbf{x}}$ induces a variation in the deformation gradient F, denoted by $\mathring{F}$ (i.e. $\mathring{F} = \frac{\partial \mathring{\mathbf{x}}}{\partial X}$). We summary these variations by
$$\mathring{\mathbf{x}} := \frac{d}{ds}\bigg|_{s=0}\mathbf{x}^s(X), \quad \mathring{F} := \frac{\partial \mathring{\mathbf{x}}}{\partial X}.$$

2. When a material undergoes a deformation, a stress (called the first Piola stress) P is induced in response to such a variation. The corresponding variation of work is
$$\mathring{W} = P : \mathring{F}.$$

3. A material is called hyper-elastic if the work done by the material is independent of the path it deforms. We call such P conservative. This is equivalent to the existence of a stored energy $W(F)$ such that first Piola stress P is the derivative of W with respective to F, and W can be obtained from F through integration:
$$P = \frac{\partial W}{\partial F}, \quad W(F) = \int_I^F P : \mathring{F}\, ds.$$
Here,
$$\mathring{F} = \frac{\partial}{\partial X}\frac{\partial \mathbf{x}^s}{\partial s},$$
and $\mathbf{x}^s$ is a path from the identity flow map ($\mathbf{x}(X) = X$) to a given flow map $\mathbf{x}(X)$.

4. The specific internal energy $U(F)$ is defined as
$$\rho_0(X)U(F(X)) = W(F(X)).$$
Then the variation of internal energy is due to the variation of work, which is
$$\rho_0\mathring{U} = P : \mathring{F}. \tag{11.1}$$

5. In Eulerian coordinate, we have
$$\rho\mathring{U} = \sigma : \mathring{\varepsilon}. \tag{11.2}$$
Here,
$$\sigma_{ij} = \rho\frac{\partial U}{\partial F^i_\alpha}F^k_\alpha g_{kj}, \quad \mathring{\varepsilon}_{ij} = \frac{1}{2}\left(\frac{\partial \mathring{x}^i}{\partial x^j} + \frac{\partial \mathring{x}^j}{\partial x^i}\right)$$
are the Cauchy stress and the pseudo-strain, respectively. Formula (11.2) is obtained from (11.1) and the symmetry of σ. [1]

[1]

Heat and the first law of thermo-elasticity

1. The energy exchange of the material internally or externally is characterized by a scalar quantity Q, called *heat*. And the variation of internal energy is then characterized by
$$\rho_0 \mathring{U} = \rho_0 \mathring{Q} + P : \mathring{F}. \tag{11.3}$$
This is called the Gibbs relation.

2. An adiabatic process is a process with $\mathring{Q} = 0$. When the stress P is conservative, then an adiabatic process stays in a hyper-surface in the space $\{(U,F)\}$. It also means that there exists an additive field $S(U,F)$, called the entropy, and a scalar field $T(U,F) > 0$, called the absolute temperature, such that
$$\mathring{Q} = T\mathring{S}.$$
The Gibbs relation is expressed as
$$\boxed{\rho_0 \mathring{U} = \rho_0 T\mathring{S} + P : \mathring{F}.} \tag{11.4}$$
The local existence of S is a theorem, which can be derived from the assumption of the existence of the restored energy W. [2] Thus, the first law of thermo-elasticity can be stated as: there exists an internal energy $U(S,F)$ such that the Gibbs relation (11.4) holds.

3. The Gibbs relation can also be expressed in Eulerian coordinate. Let us still use $U(t,\mathbf{x})$ for the specific internal energy at $(t,\mathbf{x})$. The Gibbs relation is
$$\boxed{\rho \mathring{U} = \rho T\mathring{S} + \sigma : \mathring{\varepsilon}.} \tag{11.5}$$

Representation of stresses in terms of internal energy

- We will assume our world space is the Euclidean space $\mathbb{R}^3$. The metric is $\delta_{ij}dx^i \times dx^j$.
- We have used
$$\mathring{F}^i_\alpha = \frac{\partial \mathring{x}^i}{\partial X^\alpha} = \frac{\partial \mathring{x}^i}{\partial x^k}\frac{\partial x^k}{\partial X^\alpha} = \frac{\partial \mathring{x}^i}{\partial x^k}F^k_\alpha.$$
and
$$\rho \mathring{U} = \rho \frac{\partial U}{\partial F^i_\alpha}\mathring{F}^i_\alpha = \rho \frac{\partial U}{\partial F^i_\alpha}F^k_\alpha \frac{\partial \mathring{x}^i}{\partial x^k} = \sigma_{ik}\frac{\partial \mathring{x}^i}{\partial x^k} = \sigma_{ij}\frac{1}{2}\left(\frac{\partial \mathring{x}^i}{\partial x^j} + \frac{\partial \mathring{x}^j}{\partial x^i}\right).$$

[2] This is due to Carathéodory's theory of geometric thermodynamics.

1. We can invert the relation $S \leftrightarrow U$ in the function relation $S = S(U,F)$ and use (S,F) as the independent state variables. A constitutive law is a function

$$U = U(S,F)$$

which characterizes the internal energy U in terms of the state variables (S,F).

2. From the first law of thermodynamics (Gibbs relation), the constitutive law of two thermo variables are derived:

   - the stress is then given by $P = \rho_0 (U_F)_S$;
   - the absolute temperature $T = (U_S)_F$.

3. The function U should satisfy the frame indifference hypothesis $U(S,OF) = U(S,F)$ for all $O \in O(3)$. This implies that U is a function of $C = F^T F$ and the Cauchy stress $\sigma = 2(U_C)_S C$ is symmetric.

4. If in addition, the material is isotropic, then U satisfies the property: $U(S,FO) = U(S,F)$ for all $O \in O(3)$. The frame-indifference and isotropy imply that U is a function of the invariants $I_k = \iota_k(F^T F)$, $k = 1,2,3$. That is,

$$\boxed{U(S,F) = \bar{U}(S,I_1,I_2,I_3).}$$

5. Using $W = \rho_0 U$, the Piola stress can be represented as

$$P = \rho_0 \left(\frac{\partial U}{\partial F}\right)_S,$$

6. By using $\rho_0 J^{-1} = \rho$ and $\sigma = J^{-1} P F^T$, the Cauchy stress can be represented as:

$$\sigma = \rho U_F F^T, \quad \sigma_i^j = \rho \frac{\partial U}{\partial F_\alpha^i} F_\alpha^j. \tag{11.6}$$

$$\sigma = -\rho (F^{-T}) U_{(F^{-1})}, \quad \sigma_i^j = -\rho (F^{-1})_i^\alpha \frac{\partial U}{\partial (F^{-1})_j^\alpha}. \tag{11.7}$$

$$\sigma = -\rho U_{(F^{-T})} (F^{-1}), \quad \sigma_i^j = -\rho \frac{\partial U}{\partial (F^{-T})_\alpha^i} (F^{-1})_j^\alpha. \tag{11.8}$$

$$\sigma = 2\rho B U_B, \quad \sigma_j^i = 2\rho B^{ik} \frac{\partial U}{\partial B^{kj}}, \quad \text{where } B = F F^T. \tag{11.9}$$

$$\sigma^{ij} = 2\rho \frac{\partial U}{\partial C_{\alpha\beta}} F_\alpha^i F_\beta^j \tag{11.10}$$

7. Using the representation formulae (9.11) and (9.12), the Cauchy stress for an isotropic hyper-elastic material with internal energy function $\bar{U}(S, I_1, I_2, I_3)$ is given by
$$\sigma = 2\rho\left[(I_3\bar{U}_{I_3})I + (\bar{U}_{I_1} + I_1\bar{U}_{I_2})B - \bar{U}_{I_2}B^2\right] \tag{11.11}$$
or
$$\sigma = 2\rho\left[(I_2\bar{U}_{I_2} + I_3\bar{U}_{I_3})I + \bar{U}_{I_1}B - I_3\bar{U}_{I_2}B^{-1}\right]. \tag{11.12}$$

8. Using (9.15) and (9.17), the Piola stress can be represented as
$$P = 2\rho_0 F\left(\psi_0 C^{-1} + \psi_1 I + \psi_2 C\right)$$
with
$$\psi_0 = I_3\bar{U}_{I_3}, \quad \psi_1 = \bar{U}_{I_1} + I_1\bar{U}_{I_2}, \quad \psi_2 = -\bar{U}_{I_2},$$
or
$$P = 2\rho_0 F\left(\gamma_0 I + \gamma_1 C + \gamma_2 C^2\right)$$
with
$$\gamma_0 = \psi_1 + \frac{\psi_0 I_2}{I_3}, \quad \gamma_1 = \psi_2 - \frac{\psi_0 I_1}{I_3}, \quad \gamma_2 = \frac{\psi_0}{I_3}.$$

Summary

- **The first law of thermo-elasticity**: there exists an internal energy $U(S, F)$ such that
$$\boxed{\rho_0\mathring{U} = \rho_0 T\mathring{S} + P : \mathring{F}}$$
where
$$T := \frac{\partial U}{\partial S}, \quad P := \frac{\rho_0 U}{\partial F}.$$
In Eulerian coordinate, it reads
$$\boxed{\rho\mathring{U} = \rho T\mathring{S} + \sigma : \mathring{\varepsilon}.}$$

- **Stability conditions**
  - U_{FF} is strongly elliptic, that is
$$\frac{\partial^2 U}{\partial F^i_\alpha \partial F^j_\beta}\xi^i\xi^j\eta_\alpha\eta_\beta > 0,$$
  - $U_{SS} > 0$

These conditions are necessary and sufficient to support stable plane-wave solutions. These will be discussed in the linear stability analysis later.

First law of thermo-elasticity in terms of Helmholtz free energy In elasticity, it is customary to express constitutive law in terms of temperature T and strain. We thus introduce the Helmholtz free energy

$$\Psi := U - TS.$$

and treat (T,F) as the independent state variables. The first law of thermo-elasticity becomes: there exists a function $\Psi(T,F)$ such that

$$\boxed{\rho_0 \mathring{\Psi} = -\rho_0 S \mathring{T} + P : \mathring{F}.} \tag{11.13}$$

From this formula, we get

$$S = -\left(\frac{\partial \Psi}{\partial T}\right)_F, \quad P = \rho_0 \left(\frac{\partial \Psi}{\partial F}\right)_T. \tag{11.14}$$

We can also express this first law of thermodynamics in Eulerian coordinate:

$$\boxed{\rho \mathring{\Psi} = -\rho S \mathring{T} + \sigma : \mathring{\varepsilon}.} \tag{11.15}$$

Representation of stresses in terms of the Helmholtz free energy

1. The free energy Ψ should satisfy the following condition: Frame indifference $\Psi(T, OF) = \Psi(T,F)$. This implies Ψ is a function of $C = F^T F$, and the Cauchy stress $\sigma$is symmetric.

2. If in addition, the material is isotropic, then Ψ should satisfy $\Psi(T, FO) = \Psi(T,F)$ for all $O \in O(3)$. This implies

$$\Psi = \bar{\Psi}(T, I_1, I_2, I_3), \text{ where } I_k = \iota_k(C).$$

3. The representation of stress is the same as that expressions in terms of internal energy U. We only need to replace $\left(\frac{\partial U}{\partial F}\right)_S$ by $\left(\frac{\partial \Psi}{\partial F}\right)_T$.

Stability condition

- Ψ_{FF} satisfies the strong ellipticity condition
- $\Psi_{TT} < 0$

These conditions are necessary and sufficient to support stable plane-wave solutions. These will be discussed in the linear stability analysis later.

11.1.2 Second Law of Thermo-elasticity

1. The second law of thermo-elasticity characterizes irreversible process of a deformation process. It postulates that there exists a heat flux $\mathbf{Q}(T,\nabla T,F)$ and a heat source r such that
$$\boxed{\rho_0\dot{S}+\nabla_X\cdot\left(\frac{\mathbf{Q}}{T}\right)-\frac{\rho_0 r}{T}\geq 0.} \tag{11.16}$$
This is called the *Clausius-Duhem inequality*. The integral form of the Clausius-Duhem inequality is
$$\frac{d}{dt}\int_{\Omega_0}\rho_0(X)S(t,X)\,dX\geq-\int_{\partial\Omega_0}\frac{\mathbf{Q}\cdot\mathbf{N}}{T}\,dS_0+\int_{\Omega_0}\frac{\rho_0 r}{T}\,dX.$$
The entropy production in Ω_0 is greater than the heat per temperature passing through $\partial\Omega_0$ from outside plus the heat source per temperature produced inside.

2. The above Clausius-Duhem inequality can be expressed in Eulerian coordinate:
$$\boxed{\rho\dot{S}+\nabla_{\mathbf{x}}\cdot\left(\frac{\mathbf{q}}{T}\right)-\frac{\rho r}{T}\geq 0.} \tag{11.17}$$
Here, the Lagrangian heat flux $\mathbf{Q}$ and the Eulerian heat flux $\mathbf{q}$ are related by
$$\mathbf{q}=J^{-1}\mathbf{Q}F^T.$$
The integral form of the Clausius-Duhem inequality in Eulerian coordinate is
$$\frac{d}{dt}\int_{\Omega(t)}\rho S\,d\mathbf{x}+\int_{\partial\Omega(t)}\frac{\mathbf{q}\cdot\nu}{T}\,dS_t-\int_{\Omega(t)}\frac{\rho r}{T}\,d\mathbf{x}\geq 0. \tag{11.18}$$
Here, $\Omega(t)=\varphi_t(\Omega_0)$. The terms $-\int_{\partial\Omega(t)}\frac{\mathbf{q}\cdot\nu}{T}\,dS_t$ is the rate of entropy increase from heat flux. The term $\int_{\Omega(t)}\frac{\rho r}{T}$ is rate of entropy production from heat source.

11.1.3 Entropy Production

The constitutive law is postulated by: there exists a function $U(S,F)$ such that the specific internal energy U is given by the relation $U=U(S,F)$. From the variational approach and the Euler-Lagrange transformation formula, we can get the same equation of motion
$$\partial_t(\rho\mathbf{v})+\nabla\cdot(\rho\mathbf{v}\mathbf{v})=\nabla\cdot\sigma$$
with stress
$$\sigma_{ij}=\rho\frac{\partial U}{\partial F^i_\alpha}F^j_\alpha.$$

Note that the Cauchy stress σ is symmetric. By multiplying the equation of motion by $\mathbf{v}$ and using

$$(\nabla\cdot\sigma)\cdot\mathbf{v} = \nabla\cdot(\sigma\mathbf{v}) - \sigma\cdot\nabla\mathbf{v} = \nabla\cdot(\sigma\mathbf{v}) - \sigma:\dot{\varepsilon},$$

we get an evolution equation for the kinetic energy density $E_k = \frac{1}{2}|\mathbf{v}|^2$:

$$\partial_t(\rho E_k) + \nabla\cdot[(\rho E_k\mathbf{I} - \sigma)\cdot\mathbf{v}] = -\sigma:\dot{\varepsilon}.$$

Here, $\dot{\varepsilon} = \frac{1}{2}\left(\nabla\mathbf{v} + (\nabla\mathbf{v})^T\right)$ is the rate of strain. The term $\sigma:\dot{\varepsilon}$ is the rate of work done by the elastic material.

Next, the energy equation reads

$$\boxed{\frac{\partial(\rho E)}{\partial t} + \nabla\cdot[(\rho E\mathbf{I} - \sigma)\cdot\mathbf{v}] = -\nabla\cdot\mathbf{q}.} \tag{11.19}$$

where the energy density $E := \frac{1}{2}|\mathbf{v}|^2 + U$, and $\mathbf{q}$ is the heat flux. Subtracting the kinetic energy equation from this energy equation, we get an equation for the internal energy

$$\boxed{\rho\dot{U} = \sigma:\dot{\varepsilon} - \nabla\cdot\mathbf{q}.} \tag{11.20}$$

Here, $\dot{U} := (\partial_t + \mathbf{v}\cdot\nabla)U$. This means that the increase of the internal energy is due to the work done by the elastic material and the source from heat diffusion.

On the other hand, differentiate $U = U(S,F)$ in time (with fixed X) and use the first law of thermodynamics, we get

$$\rho\dot{U} = \rho T\dot{S} + \sigma:\dot{\varepsilon}. \tag{11.21}$$

Putting (11.20) and (11.21) together, we get an equation for entropy

$$\boxed{\rho\dot{S} = -\frac{\nabla\cdot\mathbf{q}}{T}, \quad \text{or} \quad \rho\dot{S} + \nabla\cdot\left(\frac{\mathbf{q}}{T}\right) = -\frac{\mathbf{q}\cdot\nabla T}{T^2}.} \tag{11.22}$$

Adding $S(\rho_t + \nabla\cdot(\rho\mathbf{v})) = 0$, we get entropy production equation

$$\partial_t(\rho S) + \nabla\cdot(\rho S\mathbf{v}) + \nabla\cdot\left(\frac{\mathbf{q}}{T}\right) = -\frac{1}{T^2}\mathbf{q}\cdot\nabla T. \tag{11.23}$$

Its integral form reads

$$\boxed{\frac{d}{dt}\int_{\Omega(t)}\rho S\,d\mathbf{x} + \int_{\partial\Omega(t)}\frac{\mathbf{q}\cdot\mathbf{n}}{T}\,dS = -\int_{\Omega(t)}\frac{1}{T^2}\mathbf{q}\cdot\nabla T\,d\mathbf{x}.} \tag{11.24}$$

Thus, the Clausius-Duhem inequality (11.18) with $r = 0$ is equivalent to

$$\boxed{\mathbf{q}\cdot\nabla T \le 0.} \tag{11.25}$$

It means that the heat can only flow from high temperature to low temperature.

We can also write entropy production in Lagrange coordinate as

$$\rho_0 \dot{S} = -\frac{\nabla_X \mathbf{Q}}{T}, \quad \text{or} \quad \rho_0 \dot{S} + \nabla_X \left(\frac{\mathbf{Q}}{T}\right) = -\frac{\mathbf{Q} \cdot \nabla_X T}{T^2},$$

where the Lagrangian heat flux $\mathbf{Q}$ is (2.15)

$$\mathbf{Q} = J\mathbf{q}F^{-T}$$

The integral form of entropy production in Lagrangian coordinate is

$$\frac{d}{dt}\int_{\Omega_0} \rho_0 S\, dX + \int_{\partial\Omega_0} \frac{\mathbf{Q}\cdot\mathbf{N}}{T}\, dS_0 = -\int_{\Omega_0} \frac{1}{T^2}\mathbf{Q}\cdot\nabla T\, dX.$$

Summary

- The first law of thermo dynamics postulates there exists a function $U(S,F)$ such that: $\rho \mathring{U} = \rho T \mathring{S} + \sigma : \mathring{\varepsilon}$. Then the following equations are equivalent:

  Conservation of energy (11.19) $\Leftrightarrow$ Internal energy equation (11.20) $\Leftrightarrow$ Entropy equation (11.22).

- The second law of thermodynamics postulates there exists a function $\mathbf{Q}(T, \nabla_X T, F)$ (or $\mathbf{q}$ in Eulerian frame) such that

  Clausius-Duhem inequality $\Leftrightarrow \mathbf{q}\cdot\nabla T \le 0 \Leftrightarrow \mathbf{Q}\cdot\nabla_X T \le 0.$

- The relations

  $$U = U(S,F), \quad \mathbf{Q} = \mathbf{Q}(T, \nabla T, F)$$

  are called the kinematic constitutive law and the caloric constitutive law of the thermo-elastic material. One can also use (T,F) as the state variables. In this circumstance, the constitutive laws are given by

  $$\Psi = \Psi(T,F), \quad \mathbf{Q} = \mathbf{Q}(T, \nabla_X T, F).$$

11.2 Linear Thermo-elasticity

The main reference of this Linear Thermo-elasticity Theory is

- Li, Tatsien and Tiehu Qin, Physics and PDEs, Vol.II. ,SIAM.

11.2.1 Constitutive laws

There are two constitutive laws: the kinematic constitutive law and the caloric constitutive law.

Kinematic constitutive law Let us consider a linear elastic material which is at temperature T_0 in its natural steady state. This means that the stress satisfies

$$P(T_0, I) = 0.$$

Let us expand Ψ near this natural state in $\theta := T - T_0$ and $F - I$:

$$\Psi(T,F) = \Psi(T_0,I) + \Psi_F (F-I) + \frac{1}{2}\Psi_{FF}(F-I)(F-I) + \Psi_{FT}(F-I)\theta + \frac{1}{2}\Psi_{TT}\theta^2 + h.o.t.$$

where all Taylor coefficients are evaluated at (T_0, I). Let us call

$$\rho_0\Psi_{FF}(T_0,I) = a_{ijkl}, \quad \rho_0\Psi_{FT}(T_0,I) = G = \left(g_{ij}\right), \quad \rho_0\Psi_{TT}(T_0,I) = -a.$$

The term $(F-I)^i_j = \frac{\partial u^i}{\partial X^j}$. As we have seen in the theory of linear elasticity, a_{ijkl} satisfies

$$a_{ijkl} = a_{klij} = a_{ijlk}.$$

From these symmetries, the quadratic term becomes

$$\sum_{i,j,k,l} a_{ijkl}\frac{\partial u^i}{\partial X^j}\frac{\partial u^k}{\partial X^l} = a_{ijkl}e_{ij}e_{kl}, \quad \text{where } e_{ij} = \frac{1}{2}\left(\frac{\partial u^i}{\partial X^j} + \frac{\partial u^j}{\partial X^i}\right).$$

The second Piola stress is

$$\Sigma_{ij} \approx P_{ij} = \rho_0 \frac{\partial \Psi}{\partial F^i_j} = \sum_{k,l} a_{ijkl}e_{kl} + g_{ij}\theta.$$

From the symmetry of Σ, we obtain g_{ij} is also symmetric, thus

$$\sum_{i,j} g_{ij}\frac{\partial u^i}{\partial X^j} = \sum_{i,j} g_{ij}e_{ij} := G : \mathbf{e}.$$

Dropping high-order terms, Ψ can be approximated as

$$\boxed{\rho_0\Psi = \frac{1}{2}\langle A\mathbf{e}, \mathbf{e}\rangle + (\mathbf{G} : \mathbf{e})\,\theta - \frac{a}{2}\theta^2.}$$

for $F \sim I$. The kinematic constitutive laws are

- The Piola stress:

$$P(\theta, \mathbf{e}) = A\mathbf{e} + \mathbf{G}\theta, \quad P_{ij} = \sum_{k,l=1}^{3} a_{ijkl} e_{kl} + g_{ij}\theta. \tag{11.26}$$

- The entropy S:

$$\rho_0 S = -\rho_0 \frac{\partial \Psi}{\partial T} = -\rho_0 \frac{\partial \Psi}{\partial \theta} = -G : \mathbf{e} + a\theta. \tag{11.27}$$

Caloric constitutive law The caloric constitutive law is $\mathbf{Q} = \mathbf{Q}(T, \nabla_X T, \mathbf{e})$. Let us expand it around $(T, \nabla T, F) \sim (T_0, 0, I)$:

$$\mathbf{Q} = \mathbf{Q}(T, 0, I) - K\nabla_X T + h.o.t.$$

When $\nabla_X T = 0$, there is no heat flux. [3] Thus,

$$\mathbf{Q}(T, 0, I) = 0,$$

and dropping h.o.t., we get a linear model, the Fourier law:

$$\mathbf{Q} = -K\nabla_X T. \tag{11.28}$$

From the Clausius-Duhem inequality $\mathbf{Q} \cdot \nabla_X T \leq 0$, we obtain a condition for K:

$$K_{ij}\Theta_i\Theta_j \geq 0 \text{ for any vector } \Theta = (\Theta_i)_{i=1}^{3}.$$

11.2.2 The full set of equations

Momentum equation The equation of motion is

$$\boxed{\rho_0 \ddot{u}^i = \sum_{j,k,l=1}^{3} a_{ijkl} \frac{\partial u^k}{\partial X^j \partial X^l} + \sum_{j=1}^{3} g_{ij} \frac{\partial \theta}{\partial X^j}.} \tag{11.29}$$

Energy equation Recall the energy equation in terms of entropy and the heat flux as:

$$\rho_0 \dot{S} = -\frac{\nabla_X \mathbf{Q}}{T}. \tag{11.30}$$

It can be approximated by

$$\rho_0 \dot{S} = -\frac{\nabla_X \mathbf{Q}}{T_0},$$

[3] This can be obtained from the second law. In fact, let $f(\lambda) := \mathbf{Q}(T, \lambda\nabla_X T, F)$. From hypothesis of the second law, we get $\lambda f(\lambda) \leq 0$ for all $\lambda \in \mathbb{R}$. This implies $f(0) = 0$.

Plug (11.27) and (11.28) into this linear entropy equation, we get

$$\rho_0 \dot{S} = -G : \dot{\mathbf{e}} + a\dot{\theta} = \frac{1}{T_0} \nabla_X \cdot (\nabla_X \theta).$$

or

$$T_0 a\dot{\theta} = \nabla_X \cdot (K \nabla_X \theta) + T_0 G : \dot{\mathbf{e}}.$$

The energy equation for θ is given by

$$\boxed{a\dot{\theta} = \frac{1}{T_0} \sum_{i,j=1}^{3} K_{ij} \frac{\partial^2 \theta}{\partial X^i \partial X^j} + \sum_{i,j=1}^{3} g_{ij} \frac{\partial^2 u^i}{\partial t \partial X^j}} \tag{11.31}$$

The conditions for the coefficients are

- $a_{ijkl} = a_{klij} = a_{ijlk}$,
- $g_{ij} = g_{ji}$,
- $K + K^T \geq 0$,
- $a > 0$.

Energy dissipation Multiplying (11.29) by $\dot{u}^i$, then integrating over the whole material domain Ω_0, assuming no boundary contribution from integration-by-part, we get

$$\begin{aligned}
\frac{d}{dt} \int_{\Omega_0} \frac{1}{2} \rho_0 \sum_i (\dot{u}^i)^2 \, dX &= \int_{\Omega_0} \sum_{i,j,k,l} a_{ijkl} \frac{\partial^2 u^k}{\partial X^j \partial X^l} \frac{\partial u^i}{\partial t} \, dX + \int_{\Omega_0} \sum_{i,j} g_{ij} \frac{\partial \theta}{\partial X^j} \frac{\partial u^i}{\partial t} \, dX \\
&= -\int_{\Omega_0} \sum_{i,j,k,l} a_{ijkl} \frac{\partial u^k}{\partial X^l} \frac{\partial^2 u^i}{\partial t \partial X^j} \, dX + \int_{\Omega_0} \sum_{i,j} g_{ij} \frac{\partial \theta}{\partial X^j} \frac{\partial u^i}{\partial t} \, dX \\
&= -\frac{d}{dt} \int_{\Omega_0} \frac{1}{2} \sum_{i,j,k,l} a_{ijkl} \left(\frac{\partial u^k}{\partial X^l} + \frac{\partial u^i}{\partial X^j} \right) dX + \int_{\Omega_0} \sum_{i,j} g_{ij} \frac{\partial \theta}{\partial X^j} \frac{\partial u^i}{\partial t} \, dX
\end{aligned}$$

Multiplying (11.31) by θ, integrating over Ω_0, we get

$$\frac{d}{dt} \int_{\Omega_0} \frac{a}{2} \theta^2 \, dX = \frac{1}{T_0} \int_{\Omega_0} \theta \nabla_X \cdot K \nabla_X \theta \, dX + \int_{\Omega_0} \sum_{i,j} g_{ij} \theta \frac{\partial^2 u^i}{\partial t \partial X^j} \, dX.$$

Adding these two equations together, we get

$$\boxed{\frac{d}{dt} \int_{\Omega_0} \frac{1}{2} \left(\rho_0 \left| \frac{\partial \mathbf{u}}{\partial t} \right|^2 + \sum_{i,j,k,l} a_{ijkl} \frac{\partial u^i}{\partial X^j} \frac{\partial u^k}{\partial X^l} + a\theta^2 \right) dX = -\int_{\Omega_0} \frac{1}{T_0} \sum_{j,l} k_{jl} \frac{\partial \theta}{\partial X^j} \frac{\partial \theta}{\partial X^l} \, dX.} \tag{11.32}$$

This shows energy dissipation law.

11.2.3 Plane Waves and Linear Stability Analysis

- **Plane Wave Solutions** We look for solution of the form:

$$
\begin{aligned}
u^i &= \xi^i \exp\left(\mathbb{i}(X\cdot\eta - \lambda t)\right), i = 1,2,3,\\
\theta &= \Theta \exp\left(\mathbb{i}(X\cdot\eta - \lambda t)\right).
\end{aligned}
$$

The system is called stable if

$$Im(\lambda) \leq 0.$$

We would like to investigate the stability condition in terms of the coefficients a_{ijkl}, K, G, a. Plug these expressions into (11.29) and (11.31):

$$-\rho_0\lambda^2\xi^i = -\sum_{j,k,l} a_{ijkl}\eta^j\eta^l\xi^k + \sum_j g_{ij}\mathbb{i}\eta^j\Theta$$

$$-\mathbb{i}a\lambda\Theta = -\frac{1}{T_0}\sum_{j,l} K_{jl}\eta^j\eta^l\Theta + \lambda\sum_{i,j} g_{ij}\eta^j\xi^i.$$

In matrix form, it is

$$\begin{bmatrix} A(\eta) - \rho_0\lambda^2 & -\mathbb{i}G\eta \\ -\lambda(G\eta)^T & \frac{1}{T_0}K(\eta) - \mathbb{i}a\lambda \end{bmatrix}\begin{bmatrix}\xi \\ \Theta\end{bmatrix} = 0.$$

The characteristic equation is

$$
\begin{aligned}
0 &= \det\begin{bmatrix} A(\eta) - \rho_0\lambda^2 I & -\mathbb{i}G\eta \\ -\lambda(G\eta)^T & \frac{1}{T_0}K(\eta) - \mathbb{i}a\lambda \end{bmatrix}\\
&= \det\begin{bmatrix} A(\eta) - \rho_0\lambda^2 I & -\mathbb{i}G\eta \\ 0 & \lambda(G\eta)^T\left(A - \rho_0\lambda^2\right)^{-1}(-\mathbb{i}G\eta) + \frac{1}{T_0}K(\eta) - \mathbb{i}a\lambda \end{bmatrix}
\end{aligned}
$$

This leads to

$$\det\left(A(\eta) - \rho_0\lambda^2 I\right) = 0, \tag{11.33}$$

or

$$\det\left(\lambda(G\eta)^T\left(A(\eta) - \rho_0\lambda^2 I\right)^{-1}(-\mathbb{i}G\eta) + \frac{1}{T_0}K(\eta) - \mathbb{i}a\lambda\right) = 0. \tag{11.34}$$

The first set of equation leads to pure elastic waves. The second set of characteristic equation corresponds to thermodynamic elastic waves which decay time asymptotically.

- **Pure Elastic Waves** From hyperbolicity condition of a_{ijkl}, the matrix $A(\eta)$ is symmetric positive definite. Thus, it has the following eigenvalues and eigenvectors:

$$A(\eta)\xi_p = \rho_0\lambda_p^2\xi_p, \qquad p = 1,2,3.$$

The corresponding solutions for thermo elasticity are pure elastic waves, which include

  - forward waves ($\lambda_p > 0$): $\mathbf{u} = \xi_p \exp(\mathbb{i}(X\cdot\eta - \lambda_p t)), \theta_p \equiv 0, p = 1,2,3$
  - backward waves ($\lambda_p < 0$): $\mathbf{u} = \xi_p \exp(\mathbb{i}(X\cdot\eta + \lambda_p t)), \theta_p \equiv 0, p = 1,2,3.$

- **Thermodynamic Elastic Waves** The other family of solutions are obtained by solving equation (11.34). Let (λ_p^2, ξ_p), $p = 1,2,3$ be the eigen-expansion of $A(\eta)$. We expand $G\eta$ in $\{\xi_p\}$ as

$$G\eta = \sum_{p=1}^{3} g_p\xi_p, \quad \text{where } g_p = G\eta\cdot\xi_p.$$

The term

$$(G\eta)^T \left(A(\eta) - \rho_0\lambda^2 I\right)^{-1} G\eta = \sum_{p=1}^{3}\left(\rho_0(\lambda_p^2 - \lambda^2)\right)^{-1} g_p^2.$$

Equation (11.34) becomes

$$a\lambda + \sum_{p=1}^{3}\frac{\rho_0 g_p^2}{(\lambda_p^2 - \lambda^2)} = -\mathbb{i}\frac{K(\eta)}{T_0}. \tag{11.35}$$

Here, $K(\eta) = \sum_{j,l} K_{jl}\eta_j\eta_l > 0$. After rescaling, this equation is equivalent to

$$a\lambda + \mathbb{i} + \sum_{p=1}^{3} b_p\left(\frac{1}{\lambda_p - \lambda} + \frac{1}{\lambda_p + \lambda}\right) = 0,$$

where the coefficients b_p, λ_p are positive.

Proposition 11.13. *The root of the equation (11.35) satisfies $Im(\lambda) < 0$ if and only if $a > 0$.*

Proof. TO BE COMPLETED. □

With this λ, we find the corresponding vector (ξ, Θ) by solving

$$\left(A(\eta) - \rho_0\lambda^2 I\right)\xi - \mathbb{i}G\eta\Theta = 0.$$

We set Θ as a free parameter and find the solution ξ. This thermodynamic elastic wave has negative $Im(\lambda)$. Thus, the corresponding plane wave solution decays to zero as $t \to \infty$.

Remarks

1. The condition
$$\Psi_{TT} < 0 \tag{11.36}$$
is called the thermal stability condition. Indeed,
$$-\left(\frac{\partial^2\Psi}{\partial T^2}\right)_F = \left(\frac{\partial S}{\partial T}\right)_F = \frac{1}{T}\left(\frac{\partial Q}{\partial T}\right)_F.$$
Here, $dQ = TdS$ is the heat added to the system. Thus, the physical meaning of $\left(\frac{\partial Q}{\partial T}\right)_F$ is the specific heat capacity of the material at constant deformation. The parameter a is
$$a := -\rho_0\frac{\partial^2\Psi}{\partial T^2}.$$

2. The thermal stability condition can also expressed in terms of U as
$$(U_{SS})_F = \left(\frac{\partial T}{\partial S}\right)_F = \frac{1}{\left(\frac{\partial S}{\partial T}\right)F} > 0. \tag{11.37}$$

3. For polytropic gases,
$$T = \frac{A(S)}{R}V^{-\gamma+1}, \quad U = c_vT, \quad A(S) = e^{\frac{S-S_0}{c_v}}.$$
Thus,
$$S = S_0 + c_v\ln\left(RTV^{-\gamma+1}\right),$$
$$\Psi = U - TS = c_vT - T\left(S_0 + c_v\ln\left(RTV^{-\gamma+1}\right)\right).$$
$$-\frac{\partial^2\Psi}{\partial T^2} = \frac{\partial S}{\partial T} = \frac{c_v}{T} > 0.$$
See also (1.25).

11.3 Equations for Nonlinear Thermo-elasticity

11.3.1 Lagrangian formulation

The full set of equations are the equation of motion (10.46) + energy equation (11.30):
$$\begin{array}{l} \dot{F} = \frac{\partial \mathbf{v}}{\partial X} \\ \rho_0\dot{\mathbf{v}} = \nabla_X\cdot P \\ \rho_0\dot{S} = -\frac{\nabla_X\mathbf{Q}}{T}. \end{array} \tag{11.38}$$

Here, ρ_0 is a prescribed initial density field. The unknowns are $(\mathbf{v}, F, T)$. The energy equation can also be expressed as

$$\rho_0 S_T \dot{T} = -\rho_0 S_F \frac{\partial \mathbf{v}}{\partial X} - \frac{\nabla_X \mathbf{Q}}{T}.$$

Since F is the differential of the flow map: $F^i_\alpha = \frac{\partial x^i}{\partial X^\alpha}$, it should satisfy the compatibility condition

$$\nabla_X \times F^T = 0.$$

The constitutive laws are given by the two relations

$$\begin{aligned} \Psi &= \Psi(T, F), \\ \mathbf{Q} &= \mathbf{Q}(T, \nabla_X T, F). \end{aligned} \tag{11.39}$$

From Ψ, the Piola stress and the entropy are obtained:

$$P = \rho_0 \frac{\partial \Psi}{\partial F}, \quad S = -\frac{\partial \Psi}{\partial T}.$$

There are 9 equations for F, three equations for $\mathbf{v}$ and one equation for T.

Hyperbolicity The system is called hyperbolic if

$$\rho_0 \left(\frac{\partial^2 \Psi}{\partial F^i_\alpha \partial F^j_\beta} \right)_T \xi^i \xi^j \eta^\alpha \eta^\beta > 0, \text{ for all } \xi = (\xi^1, \xi^2, \xi^3)^T \neq 0 \text{ and } \eta = (\eta^1, \eta^2, \eta^3)^T \neq 0.$$

Thermo stability

$$\rho_0 \left(\frac{\partial^2 \Psi}{\partial T^2} \right)_F < 0. \tag{11.40}$$

Second law of thermodynamics The heat flux should satisfy the requirement of the second law of thermodynamics:

$$\mathbf{Q} \cdot \nabla_X T \leq 0.$$

11.3.2 Eulerian formulation

In Eulerian formulation, we treat ρ as a new unknown and add the continuity equation. However, this is redundant. So we add a constraint: $\rho J = \rho_0$. The full set of equations include 9 equations for F^{-1}, three equations for $\mathbf{v}$, one continuity equation for ρ and one energy equation for T.

$$\begin{cases} \partial_t\rho + \partial_{x^j}(v^j\rho) = 0 \\ \partial_t(\rho v^i) + \partial_{x^j}\left(\rho v^i v^j\right) = \partial_{x^j}\sigma^{ij} + f^i \\ \partial_t(F^{-1})^\alpha_k + \partial_{x^k}\left((F^{-1})^\alpha_j v^j\right) = 0 \\ \partial_t(\rho E) + \partial_{x^j}\left(v^j\rho E - v^i\sigma^{ij}\right) + \partial_{x^j}q^j = v^i f^i \end{cases} \tag{11.41}$$

where E is the specific total energy $E = \frac{1}{2}|\mathbf{v}|^2 + U$. We need the density constraint: $\rho J = \rho_0$ and the compatibility condition

$$\nabla_{\mathbf{x}} \times F^{-T} = 0. \tag{11.42}$$

The constitutive laws are either expressed in terms of (S,F) as

$$U = U(S,F), \quad \mathbf{q} = \mathbf{q}(S, \nabla_{\mathbf{x}}T, F),$$

or in terms of (T,F) as

$$\Psi = \Psi(T,F), \quad \mathbf{q} = \mathbf{q}(T, \nabla_{\mathbf{x}}T, F),$$

where $\Psi = U - ST$ is the Helmholtz energy. The unknowns are $(\mathbf{v}, F^{-1}, \rho, T)$.

Stability conditions The constitutive equations should satisfy

- **Hyperbolicity**

$$\frac{\partial^2\Psi}{\partial F^i_\alpha \partial F^j_\beta}\eta^\alpha\eta^\beta\xi^i\xi^j > 0, \text{ for all } \eta,\xi \in \mathbb{R}^3 \setminus \{0\},$$

  or

$$\frac{\partial^2 U}{\partial F^i_\alpha \partial F^j_\beta}\eta^\alpha\eta^\beta\xi^i\xi^j > 0, \text{ for all } \eta,\xi \in \mathbb{R}^3 \setminus \{0\},$$

- **Thermo stability** $\Psi_{TT} < 0$ or $U_{SS} > 0$.

- **Second law of thermodynamics** $\mathbf{q} \cdot \nabla_{\mathbf{x}} T \leq 0$.

11.4 Thermo-elastic Models

11.4.1 neo-Hookean models

1. Blatz-Ko rubber [Blatz Ko, 1962]

$$U = \frac{\mu_0}{2\rho_0}\left(I_1 + \frac{1}{\alpha}I_3^{-\alpha}\right).$$

2. Aluminum: a compressible neo-Hookean model for aluminum [Miller-Colella, 2001]

$$U = \frac{\mu_0}{2\rho_0}\left(I_1 - 3I_3^{1/3}\right) + \int_{\rho_0}^{\rho} \frac{P(\rho')}{\rho'^2}\,d\rho',$$

where

$$\rho = \rho_0 I_3{}^{-1/2}, \quad P(\rho) = 72\left(\frac{\rho}{\rho_0} - 1\right) + 172\left(\frac{\rho}{\rho_0} - 1\right)^2 + 40\left(\frac{\rho}{\rho_0} - 1\right)^3.$$

$$\rho_0 = 2.7 \times 10^3 kg/m^3, \quad \mu_0 = 24.8GPa.$$

3. Copper [Miller 2004] The internal energy is decomposed into hydrostatic (H), thermo (T), and shear (S) energies:

$$U = U_H(I_3) + U_T(S, I_3) + U_S(I_1, I_2, I_3),$$

$$U_H = -\frac{4K}{\rho_0(K'-1)^2}\left(1 + r(I_3, K')\right)\exp\left(-r(I_3, K')\right),$$

$$U_T = c_v T_0\left[\exp\left(\frac{S - S_0}{c_v}\right) - 1\right]\exp\left(\frac{\gamma_0 - \gamma(I_3)}{q}\right),$$

$$U_S = \frac{G(I_3)}{2\rho_0}\sqrt{I_3}\left[\beta I_1 I_3^{-1/3} + (1-\beta)I_2 I_3^{-2/3} - 3\right]$$

where

$$r(x,y) = \frac{3}{2}(y-1)\left(x^{1/6} - 1\right), \gamma(x) = \gamma_0 x^q,$$

$$G(x) = \exp\left[-r\left(x, \frac{KG'}{G_0}\right)\right] g(x),$$

$$g(x) = G_0\left\{\left[1 - r\left(x, \frac{KG'}{G_0}\right)\right] x^{-1/6} - \frac{4}{3} r\left(x, \frac{KG'}{G_0}\right)\left(\frac{x^{-1/3}}{\frac{KG'}{G_0} - 1}\right)\right\}.$$

Chapter 12

Elastoplasticity

References

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12.1 Flow laws of elastoplasticity

12.1.1 Decomposition of Deformation

In the deformation of an elastoplastic material, the deformation gradient F can be decomposed into elastic part and plastic part: (see Sec. 8.2.2 of Lubliner's book)

$$F = F^e F^p, \quad F^i_\alpha = (F^e)^i_\beta (F^p)^\beta_\alpha.$$

The elastic part is reversible, while the plastic part, a result of dislocation of lattice, is irreversible. The elastic part F^e will relax to an equilibrium state, while F^p follows a dynamic flow law which depends on some internal variable ξ. This internal variable ξ can be a scalar, a vector, or a tensor. It characterizes the restructure of the material, for instance, the work-hardening parameter. The dynamic law of F^p and ξ are described by the following ODEs

$$\begin{cases} \dot{F}^p = K(\rho, F, F^p, U, \xi), \\ \dot{\xi} = h(\rho, F, F^p, U, \xi). \end{cases}$$

The functions K and h can be derived from the following postulates:

- A constitutive law for the internal energy: $U = U(S, F^e, \xi)$;
- A yield surface $f(\sigma, \chi) = 0$, where $\chi := \partial U / \partial \xi$ is the internal force conjugate to the internal variable ξ;
- The maximum plastic dissipation principle, which states that the flow rule of F^p and ξ are determined by maximizing the plastic dissipation.

The region

$$\{(\sigma, \chi) | f(\sigma, \chi) < 0\}$$

is called elastic region, inside which, the material behaves purely elastically and $F = F^e$. As (σ, χ) reaches the boundary $f(\sigma, \chi) = 0$, dislocation of lattice occurs and the material behaves plastically. The system is irreversible. The increase of entropy S is characterized by the power (rate) of plastic dissipation and power of thermal dissipation. The stress in this plastic regime is obtained by the principle of maximal plastic dissipation. Let us explain these in detail below.

12.1.2 Constitutive Law

The first hypothesis is: there exists a function $U(S, F^e, \xi)$ such that the specific internal energy satisfies

$$U = U(S, F^e, \xi).$$

The reversible part of the internal energy depends only on F^e. The irreversible part of the internal energy is characterized by the interval variables ξ.

There are three conjugate variables derived from U:

- temperature $T := \left(\frac{\partial U}{\partial S}\right)_{F^e, \xi}$,
- stress $\sigma := \rho \left(\frac{\partial U}{\partial F}\right)_{S, \xi} F^T$,
- internal force $\chi := \rho \left(\frac{\partial U}{\partial \xi}\right)_{S, F^e}$.

An example of such internal energy is the following modified Mooney-Rivlin equation-of-state:

$$\begin{aligned}\rho U(S,F^e,\xi) = &\frac{\lambda(S)}{2}\left(\ln\sqrt{\det C^e}\right)^2 + \frac{\mu(S)}{2} trC^e \\ &- \frac{\mu(S)}{2}\ln(\det C^e) + \frac{\rho_0}{\vartheta_0}\rho\left(\xi + \frac{1}{\vartheta_1}e^{-\vartheta_1\xi}\right),\end{aligned}$$

where $C^e := F^e(F^e)^T$ is the elastic strain tensor, ξ is the work-hardening variable, and

$$\chi = \rho\frac{\partial U}{\partial \xi} = \vartheta_0\left(1 - e^{-\vartheta_1\xi}\right)$$

is the work-hardening modulus (or the internal force). Here, ϑ_0, ϑ_1 are two positive constants.

Below, we want to derive the dynamic equations for the thermodynamic variables: S, F^p and ξ. The equation for S is equivalent to the energy equation. The equations for F^p and ξ will be derived from the maximum plasticity dissipation law.

Derivation of equation for S We recall the energy equation reads,

$$\partial_t(\rho E) + \nabla\cdot((\rho E\mathbf{I} - \sigma)\mathbf{v}) = \nabla\cdot(\kappa\nabla T),$$

where $E = \frac{1}{2}|\mathbf{v}|^2 + U$, the specific total energy. By multiplying momentum equation by $\mathbf{v}$, we can get the equation for the kinetic energy $E_k := \frac{1}{2}|\mathbf{v}|^2$

$$\partial_t(\rho E_k) + \nabla\cdot[(\rho E_k\mathbf{I} - \sigma)\cdot\mathbf{v}] = -\sigma : D,$$

where $D = \frac{1}{2}(L + L^T)$, $L = \nabla\mathbf{v}$ is the strain rate. By subtracting the kinetic energy equation from the energy equation, we get the dynamic equation for the internal energy:

$$\rho\dot{U} = \sigma : D + \nabla\cdot(\kappa\nabla T). \tag{12.1}$$

On the other hand, we can treat U as a function of (S,F,F^p,ξ) through $F^e = F(F^p)^{-1}$. By differentiating such $U = U(S,F,F^p,\xi)$ in time with fixed material variable, and treating $F^e = F(F^p)^{-1}$ (i.e. $U(S,F(F^p)^{-1},\xi)$, we get [1]

$$\dot{U} = \frac{\partial U}{\partial S}\dot{S} + \frac{\partial U}{\partial F} : \dot{F} + \frac{\partial U}{\partial F^p} : \dot{F}^p + \frac{\partial U}{\partial \xi}\cdot\dot{\xi}.$$

[1]We treat U as a function of F and F^p, instead of F^e. The reason why we want to have $\partial U/\partial F$ is to be able to obtain the total stress, which is derived from F, not just from F^e, see Mandel.

Multiplying this equation by ρ, we get

$$\rho\dot{U} = \rho T\dot{S} + \rho\frac{\partial U}{\partial F}:\dot{F} + \rho\frac{\partial U}{\partial F^p}:\dot{F}^p + \chi\cdot\dot{\xi}. \tag{12.2}$$

Using $\sigma = \rho U_F F^T$, $\dot{F} = LF$ and the symmetry property of σ, the term

$$\rho\frac{\partial U}{\partial F}:\dot{F} = \rho\frac{\partial U}{\partial F}:LF = \rho U_F F^T:L = \sigma:L = \sigma:D.$$

The term

$$\begin{aligned}
\rho\frac{\partial U}{\partial (F^p)^\alpha_\beta} &= \rho\frac{\partial U}{\partial F^i_\gamma}\frac{\partial F^i_\gamma}{\partial (F^p)^\alpha_\beta} = \left(\rho\frac{\partial U}{\partial F^i_\gamma}\right)\frac{\partial}{\partial (F^p)^\alpha_\beta}\left((F^e)^i_\tau (F^p)^\tau_\gamma\right)\\
&= \left(\rho\frac{\partial U}{\partial F^i_\gamma}\right)(F^e)^i_\tau\delta^{\alpha\tau}\delta_{\beta\gamma} = \left(\rho\frac{\partial U}{\partial F^i_\beta}\right)(F^e)^i_\alpha\\
&= \left(\rho\frac{\partial U}{\partial F^i_\beta}\right)F^i_\gamma((F^p)^{-1})^\gamma_\alpha
\end{aligned}$$

Thus,

$$\rho\frac{\partial U}{\partial F^p}:\dot{F}^p = \left(\rho\frac{\partial U}{\partial F^i_\beta}\right)F^i_\gamma((F^p)^{-1})^\gamma_\alpha(\dot{F}^p)^\alpha_\beta \quad = \left[\left(\rho\frac{\partial U}{\partial F^i_\beta}\right)F^i_\gamma\right]\left[((F^p)^{-1})^\gamma_\alpha(\dot{F}^p)^\alpha_\beta\right]$$

Thus,

$$\rho\frac{\partial U}{\partial F^p}:\dot{F}^p = \rho U_F F:(F^p)^{-1}\dot{F}^p := \Sigma:L^p.$$

Here,

$$\Sigma = \rho U_F F, \quad L^p := (F^p)^{-1}\dot{F}^p.$$

Equating (12.1) and (12.2), we get an evolution equation for the thermo variables:

$$\rho T\dot{S} + \Sigma:L^p + \chi\cdot\dot{\xi} = \nabla\cdot(\kappa\nabla T).$$

The entropy production is

$$\dot{S} = -\frac{1}{\rho T}\left(\Sigma:L^p + \chi\cdot\dot{\xi}\right) + \frac{1}{\rho T}\nabla\cdot(\kappa\nabla T) = \frac{1}{\rho T}\left(\Psi_{plast} + \Psi_{therm}\right)$$

The term

$$\Psi_{plas} := -\Sigma:L^p - \chi\cdot\dot{\xi}$$

is called the power of plastic dissipation. The term

$$\Psi_{therm} := \nabla\cdot(\kappa\nabla T)$$

is called the power of thermo dissipation.

12.1.3 Plastic yield surface

Our second postulate is: there exists a plastic yield function $f(\sigma, \chi)$ such that

- the material behaves elastically when $f(\sigma, \chi) < 0$,
- the material behaves plastically when $f(\sigma, \chi) = 0$.

Example The Mises-Huber constitute model is given by

$$f(\sigma, \chi) = \|dev(\sigma)\| - \sqrt{\frac{2}{3}}(\sigma_Y + \chi). \qquad (12.3)$$

Here, $dev(\sigma) := \sigma - \frac{1}{3}(tr\sigma)I$ is the deviatorial part of σ, σ_Y is a constant yield stress parameter. During material deformation, when the deviatorial stress is greater than $\sqrt{\frac{2}{3}}(\sigma_Y + \chi)$, the material lattice is broken and the material undergoes a plastic deformation. The broken process is described by the internal variable ξ and the plastic deformation F^p. Their dynamics are determined by maximum plastic dissipation law below.

12.1.4 Maximum Plastic Dissipation Law

Our third postulate is that: the dynamics of the plastic variables F^p and ξ are determined by

$$\sup_{\Sigma,\chi} \Psi_{past}(\Sigma, \chi, L^p, \dot{\xi})$$

subject to the constraint

$$f(\sigma(\Sigma), \chi) \le 0.$$

Recall

$$\Psi_{plast} = -\Sigma : L^p - \chi \cdot \dot{\xi}.$$

By using the method of Lagrange multiplier, this is equivalent to the following unconstrained optimization problem:

$$\sup_{\Sigma,\chi} \sup_{\zeta} \left[\Psi_{past}(\Sigma, \chi) + \zeta f(\sigma(\Sigma), \chi)\right].$$

Here, ζ is the Lagrange multiplier. The corresponding Euler-Lagrange equation is

$$\frac{\partial}{\partial \Sigma}\left(\Psi_{plast} + \zeta f\right) = 0, \quad \frac{\partial}{\partial \chi}\left(\Psi_{plast} + \zeta f\right) = 0.$$

Recall $L^p := (F^p)^{-1}\dot{F}^p$, the Euler-Lagrange equations are

$$\dot{F}^p = \zeta F^p \frac{\partial f}{\partial \Sigma}, \tag{12.4}$$

$$\dot{\xi} = \zeta \frac{\partial f}{\partial \chi}. \tag{12.5}$$

The Lagrange multiplier ζ, Σ and χ should satisfy the KKT condition

$$f = 0, \tag{12.6}$$

$$\zeta \geq 0, \tag{12.7}$$

$$\zeta f = 0. \tag{12.8}$$

Its meaning are the follows: (i) $f = 0$ means that it is in plastic regime; (ii) $\zeta \geq 0$ means that it is in either plastic or elastic regimes; (iii) $\zeta f = 0$ means that it can only be in plastic regime ($f = 0$) or elastic regime ($f > 0$ but $\zeta = 0$).

In addition, in the plastic regime (i.e. $f = 0, \zeta > 0$), it should satisfy the consistency condition

$$\zeta \dot{f} = 0 \quad \text{when } f = 0. \tag{12.9}$$

It means that the material stays in plastic mode during $f = 0$ and this gives $\dot{f} = 0$ in this regime.

References

- J. Lubliner, A Maximum-Dissipation Principle in Generalized Plasticity (1984).

Chapter 13

*Hamiltonian Elasticity

Incomplete!

There are two formulations of Hamiltonian elasticity. One is in Lagrange frame of reference. The other is in Euler frame of reference. [1]

Let $\mathbf{q}(t,X)$ be the flow map. The Lagrangian is defined to be

$$L(\mathbf{v},\rho,S,F) := \frac{1}{2}\rho|\mathbf{v}|^2 - \rho U(S,F).$$

$$\mathscr{L}[\mathbf{q}] := \int_{\Omega_0} L(\dot{\mathbf{q}}, \frac{\partial \mathbf{q}}{\partial X})\,dX$$

The momentum

$$\mathbf{p}(X) := \frac{\delta \mathscr{L}}{\partial \mathbf{v}} = \rho_0(X)\mathbf{v}(X).$$

The internal energy U depends on the conformation tensor

$$\mathbf{c}^{ij} = F^i_\alpha F^j_\beta \mathbf{c}_0^{\alpha\beta}.$$

Let us define

$$\mathfrak{s}(\mathbf{x}) = \rho(\mathbf{x})S(\mathbf{x}), \quad \mathfrak{c}(\mathbf{x}) = \rho(\mathbf{x})\mathbf{c}(\frac{\partial \mathbf{x}}{\partial X}), \quad \mathbf{m}(\mathbf{x}) = \rho(\mathbf{x})\mathbf{v}(\mathbf{x}).$$

Then $\mathfrak{s}$ and $\mathfrak{c}$ satisfy

$$\partial_t \mathfrak{s} + \nabla\cdot(\mathbf{v}\mathfrak{s}) = 0, \quad \partial_t \mathfrak{c} + \nabla_{\mathbf{x}}\cdot(\mathbf{v}\mathfrak{c}) - (\nabla\mathbf{v})\mathfrak{c} - \mathfrak{c}(\nabla\mathbf{v})^T = 0.$$

[1] Reference: Beris and Edwards, Thermodynamics of Flowing Systems, pp. 113

We recall the relations between other Eulerian variables $(\rho, \mathfrak{s}, \mathfrak{c}, \mathbf{m})$ and the Lagrangian variables $(\mathbf{q}, \mathbf{p})$ are

$$\begin{aligned}
\rho(\mathbf{x}) &= \int_{\Omega_0} \rho_0(X)\delta(\mathbf{x}-\mathbf{q}(X))\,dX \\
\mathfrak{s}(\mathbf{x}) &= \int_{\Omega_0} \mathfrak{s}_0(X)\delta(\mathbf{x}-\mathbf{q}(X))\,dX \\
\mathbf{m}(\mathbf{x}) &= \int_{\Omega_0} \mathbf{p}(X)\delta(\mathbf{x}-\mathbf{q}(X))\,dX
\end{aligned} \tag{13.1}$$

And

$$\begin{aligned}
\mathfrak{c}(\mathbf{x}) &= \int_{\Omega} \delta(\mathbf{x}-\mathbf{y})\mathfrak{c}(\mathbf{y})\,d\mathbf{y} \\
&= \int_{\Omega_0} \delta(\mathbf{x}-\mathbf{q}(X))\rho(\mathbf{q}(X))\mathbf{c}(\frac{\partial \mathbf{q}}{\partial X})J^{-1}\,dX \\
&= \int_{\Omega_0} \delta(\mathbf{x}-\mathbf{q}(X))\rho_0(X)\mathbf{c}(\frac{\partial \mathbf{q}}{\partial X})\,dX.
\end{aligned}$$

A functional $\mathscr{F}[\mathbf{q},\mathbf{p}]$ can also be represented as a functional of $[\rho, \mathfrak{s}, \mathfrak{c}, \mathbf{m}]$ by

$$\bar{\mathscr{F}}[\rho, \mathfrak{s}, \mathfrak{c}, \mathbf{m}] = \mathscr{F}[\mathbf{q},\mathbf{p}],$$

with variation

$$\begin{aligned}
\delta \mathscr{F} &= \int_{\Omega_0} \left(\frac{\delta \mathscr{F}}{\delta \mathbf{q}} \delta \mathbf{q} + \frac{\delta \mathscr{F}}{\delta \mathbf{p}} \delta \mathbf{p} \right) dX \\
&= \int_{\Omega} \left(\frac{\delta \bar{\mathscr{F}}}{\delta \rho} \delta \rho + \frac{\delta \bar{\mathscr{F}}}{\delta \mathfrak{s}} \delta \mathfrak{s} + \frac{\delta \bar{\mathscr{F}}}{\delta \mathfrak{c}} \delta \mathfrak{c} + \frac{\delta \bar{\mathscr{F}}}{\delta \mathbf{m}} \delta \mathbf{m} \right) d\mathbf{x}
\end{aligned}$$

In this expression, $\frac{\delta \bar{\mathscr{F}}}{\delta \rho}$ is a function of $(\rho, \mathfrak{s}, \mathfrak{c}, \mathbf{m})$, hence a function of $\mathbf{x}$. The variations of $\rho, \mathfrak{s}, \mathfrak{c}$ and $\mathbf{m}$ can be obtained by taking variations on the transformation formulae (13.1). We get

$$\begin{aligned}
\frac{\delta \rho}{\delta \mathbf{q}} &= -\rho_0(X)\nabla_{\mathbf{x}}\delta(\mathbf{x}-\mathbf{q}(X)) \\
\frac{\delta \mathfrak{s}}{\delta \mathbf{q}} &= -\mathfrak{s}_0(X)\nabla_{\mathbf{x}}\delta(\mathbf{x}-\mathbf{q}(X)) \\
\frac{\delta \mathbf{m}}{\delta \mathbf{q}} &= -\mathbf{p}(X)\nabla_{\mathbf{x}}\delta(\mathbf{x}-\mathbf{q}(X)) \\
\frac{\delta \mathbf{m}}{\delta \mathbf{p}} &= \delta(\mathbf{x}-\mathbf{q}(X))
\end{aligned}$$

$$\delta\mathfrak{c}^{ij} = \int_{\Omega_0} -\partial_{x^k}\delta(\mathbf{x}-\mathbf{q}(X))\delta q^k \rho_0(X)\mathbf{c}(\frac{\partial \mathbf{q}}{\partial X}) + \delta(\mathbf{x}-\mathbf{q}(X))\rho_0(X)\delta c^{ij}\, dX.$$

Recall that $c^{ij} = F^i_\alpha F^j_\beta c_0^{\alpha\beta} = \frac{\partial x^i}{\partial X^\alpha}\frac{\partial x^j}{\partial X^\beta} c_0^{\alpha\beta}(X)$. With $\mathbf{x} = \mathbf{q}(t,X)$, we have

$$\delta c^{ij} = \frac{\partial \delta q^i}{\partial X^\alpha} F^j_\beta c_0^{\alpha\beta} + \frac{\partial \delta q^j}{\partial X^\beta} F^i_\alpha c_0^{\alpha\beta} = \left(\delta^i_k F^j_\beta c_0^{\alpha\beta} + \delta^j_k F^i_\beta c_0^{\beta\alpha}\right)\frac{\partial}{\partial X^\alpha}\delta q^k.$$

Thus,

$$\begin{aligned}
\frac{\delta \mathfrak{c}^{ij}}{\delta q^k} &= -\frac{\partial}{\partial x^k}\delta(\mathbf{x}-\mathbf{q}(X))\rho_0 c^{ij} - \frac{\partial}{\partial X^\alpha}\left[\delta(\mathbf{x}-\mathbf{q}(X))\rho_0\left(\delta^i_k F^j_\beta c_0^{\alpha\beta} + \delta^j_k F^i_\beta c_0^{\beta\alpha}\right)\right] \\
&= -\frac{\partial}{\partial x^k}\delta(\mathbf{x}-\mathbf{q}(X))\rho_0 c^{ij} - J\frac{\partial}{\partial x^m}\left[\delta(\mathbf{x}-\mathbf{q}(X))J^{-1}\rho_0(X)\left(\delta^i_k F^j_\beta c_0^{\alpha\beta} + \delta^j_k F^i_\beta c_0^{\beta\alpha}\right)F^m_\alpha\right] \\
&= -\frac{\partial}{\partial x^k}\delta(\mathbf{x}-\mathbf{q}(X))\rho_0 c^{ij} - J\frac{\partial}{\partial x^m}\left[\delta(\mathbf{x}-\mathbf{q}(X))\rho\left(\delta^i_k c^{mj} + \delta^j_k c^{im}\right)\right].
\end{aligned}$$

Here, we have used

$$\frac{\partial}{\partial X^\alpha}P^i_\alpha = J\frac{\partial}{\partial x^m}\sigma^i_m, \quad \sigma^i_m = J^{-1}P^i_\alpha F^m_\alpha.$$

The function $\bar{\mathscr{F}}$ maps $(\rho, \mathfrak{s}, \mathfrak{c}, \mathbf{m})$ to $\mathbb{R}$ and $\mathscr{F} = \bar{\mathscr{F}} \circ \mathbf{q}$ maps $\mathbf{q}$ to $\mathbb{R}$. Therefore, $\frac{\delta \mathscr{F}}{\delta \mathbf{q}}$ and $\frac{\delta \mathscr{F}}{\delta \mathbf{p}}$, which are functions of X, can be expressed as

$$\begin{aligned}
\frac{\delta \mathscr{F}}{\delta \mathbf{q}}(X) &= \int_{\Omega_0}\left(\frac{\delta \bar{\mathscr{F}}}{\delta \rho}\frac{\delta \rho}{\delta \mathbf{q}} + \frac{\delta \bar{\mathscr{F}}}{\delta \mathfrak{s}}\frac{\delta \mathfrak{s}}{\delta \mathbf{q}} + \frac{\delta \bar{\mathscr{F}}}{\delta \mathfrak{c}}\frac{\delta \mathfrak{c}}{\delta \mathbf{q}} + \frac{\delta \bar{\mathscr{F}}}{\delta \mathbf{m}}\frac{\delta \mathbf{m}}{\delta \mathbf{q}}\right) d\mathbf{x} \\
&= I + II. \\
I &= -\int_\Omega \left(\rho_0 \frac{\delta \bar{\mathscr{F}}}{\delta \rho} + \mathfrak{s}_0 \frac{\delta \bar{\mathscr{F}}}{\delta \mathfrak{s}} + \rho_0 \mathbf{c}\frac{\delta \bar{\mathscr{F}}}{\delta \mathfrak{c}} + \mathbf{p}\cdot\frac{\delta \bar{\mathscr{F}}}{\delta \mathbf{m}}\right)\cdot\nabla_{\mathbf{x}}\delta(\mathbf{x}-\mathbf{q}(X))\, d\mathbf{x} \\
&= \int_\Omega \left(\rho_0 \nabla_{\mathbf{x}}\cdot\frac{\delta \bar{\mathscr{F}}}{\delta \rho} + \mathfrak{s}_0 \nabla_{\mathbf{x}}\cdot\frac{\delta \bar{\mathscr{F}}}{\delta \mathfrak{s}} + \rho_0 \mathbf{c}\cdot\frac{\delta \bar{\mathscr{F}}}{\partial \mathfrak{c}} + \mathbf{p}\cdot\nabla_{\mathbf{x}}\frac{\delta \bar{\mathscr{F}}}{\delta \mathbf{m}}\right)\delta(\mathbf{x}-\mathbf{q}(X))\, d\mathbf{x} \\
II &= -\int_\Omega \frac{\delta \bar{\mathscr{F}}}{\delta \mathfrak{c}^{ij}}\frac{\delta \mathfrak{c}^{ij}}{\delta \mathbf{q}}\, d\mathbf{x} \\
&= -\int_\Omega \frac{\delta \bar{\mathscr{F}}}{\delta \mathfrak{c}^{ij}} J\frac{\partial}{\partial x^m}\left[\delta(\mathbf{x}-\mathbf{q}(X))\rho\left(\delta^i_k c^{mj} + \delta^j_k c^{im}\right)\right] d\mathbf{x} \\
\frac{\delta \mathscr{F}}{\delta \mathbf{p}}(X) &= \int_\Omega \frac{\delta \bar{\mathscr{F}}}{\delta \mathbf{m}}\delta(\mathbf{x}-\mathbf{q}(X))\, d\mathbf{x} = \frac{\delta \bar{\mathscr{F}}}{\delta \mathbf{m}}(\mathbf{q}(X))
\end{aligned}$$

The Poisson bracket $\{\mathscr{F}, \mathscr{G}\}$ defined by

$$\{\mathscr{F}, \mathscr{G}\} := \int_{\Omega_0}\left(\frac{\delta \mathscr{F}}{\delta \mathbf{q}}\cdot\frac{\delta \mathscr{G}}{\delta \mathbf{p}} - \frac{\delta \mathscr{G}}{\delta \mathbf{q}}\cdot\frac{\delta \mathscr{F}}{\delta \mathbf{p}}\right) dX$$

can be expressed in terms of $(\rho, \mathfrak{s}, \mathfrak{c}, \mathbf{m})$ as

$$
\begin{aligned}
\{\bar{\mathscr{F}}, \bar{\mathscr{G}}\} &= \{\mathscr{F}, \mathscr{G}\} \\
&= \int_{\Omega_0}\int_{\Omega} \delta(\mathbf{x}-\mathbf{q}(X))\left(\rho_0 \nabla_{\mathbf{x}} \frac{\delta \bar{\mathscr{F}}}{\delta \rho} + \mathfrak{s}_0 \nabla_{\mathbf{x}} \frac{\delta \bar{\mathscr{F}}}{\delta \mathfrak{s}} + \rho_0 \mathbf{c} \nabla_{\mathbf{x}} \frac{\delta \bar{\mathscr{F}}}{\delta \mathfrak{c}} + \mathbf{p} \cdot \nabla_{\mathbf{x}} \frac{\delta \bar{\mathscr{F}}}{\delta \mathbf{m}}\right) \cdot \frac{\delta \bar{\mathscr{G}}}{\delta \mathbf{m}} \\
&\qquad - \delta(\mathbf{x}-\mathbf{q}(X))\left(\rho_0 \nabla_{\mathbf{x}} \frac{\delta \bar{\mathscr{G}}}{\delta \rho} + \mathfrak{s}_0 \nabla_{\mathbf{x}} \frac{\delta \bar{\mathscr{G}}}{\delta \mathfrak{s}} + \rho_0 \mathbf{c} \nabla_{\mathbf{x}} \frac{\delta \bar{\mathscr{G}}}{\delta \mathfrak{c}} + \mathbf{p} \cdot \nabla_{\mathbf{x}} \frac{\delta \bar{\mathscr{G}}}{\delta \mathbf{m}}\right) \cdot \frac{\delta \bar{\mathscr{F}}}{\delta \mathbf{m}} \, d\mathbf{x}\, dX \\
&+ \int_{\Omega_0}\int_{\Omega} \frac{\delta \bar{\mathscr{F}}}{\delta \mathfrak{c}^{ij}} J \frac{\partial}{\partial x^m}\left[\delta(\mathbf{x}-\mathbf{q}(X))\rho\left(\delta^i_k c^{mj} + \delta^j_k c^{im}\right)\right] d\mathbf{x} \frac{\delta \bar{\mathscr{G}}}{\delta \mathbf{m}^k}\, dX \\
&- \int_{\Omega_0}\int_{\Omega} \frac{\delta \bar{\mathscr{G}}}{\delta \mathfrak{c}^{ij}} J \frac{\partial}{\partial x^m}\left[\delta(\mathbf{x}-\mathbf{q}(X))\rho\left(\delta^i_k c^{mj} + \delta^j_k c^{im}\right)\right] d\mathbf{x} \frac{\delta \bar{\mathscr{F}}}{\delta \mathbf{m}^k}\, dX
\end{aligned}
$$

We use (5.6) and a lemma below to get

$$
\begin{aligned}
\{\mathscr{F}, \mathscr{G}\} = \int_{\Omega} &\left(\rho \nabla_{\mathbf{x}} \frac{\delta \bar{\mathscr{F}}}{\delta \rho} + \mathfrak{s} \nabla_{\mathbf{x}} \frac{\delta \bar{\mathscr{F}}}{\delta \mathfrak{s}} + \mathbf{m} \cdot \nabla_{\mathbf{x}} \frac{\delta \bar{\mathscr{F}}}{\delta \mathbf{m}}\right) \cdot \frac{\delta \bar{\mathscr{G}}}{\delta \mathbf{m}} \\
&- \left(\rho \nabla_{\mathbf{x}} \frac{\delta \bar{\mathscr{G}}}{\delta \rho} + \mathfrak{s} \nabla_{\mathbf{x}} \frac{\delta \bar{\mathscr{G}}}{\delta \mathfrak{s}} + \mathbf{m} \cdot \nabla_{\mathbf{x}} \frac{\delta \bar{\mathscr{G}}}{\delta \mathbf{m}}\right) \cdot \frac{\delta \bar{\mathscr{F}}}{\delta \mathbf{m}} \, d\mathbf{x} \\
+ \int_{\Omega} &\mathfrak{c} \nabla_{\mathbf{x}} \frac{\delta \bar{\mathscr{F}}}{\delta \mathfrak{c}} \cdot \frac{\delta \bar{\mathscr{G}}}{\delta \mathbf{m}} - \mathfrak{c} \nabla_{\mathbf{x}} \frac{\delta \bar{\mathscr{G}}}{\delta \mathfrak{c}} \cdot \frac{\delta \bar{\mathscr{F}}}{\delta \mathbf{m}} \, d\mathbf{x} \\
+ \int_{\Omega} &\left(\frac{\partial}{\partial x^m} \frac{\delta \bar{\mathscr{F}}}{\delta \mathfrak{c}^{ij}}\right)\left(\delta^i_k \mathfrak{c}^{mj} + \delta^j_k \mathfrak{c}^{im}\right) \frac{\delta \bar{\mathscr{G}}}{\delta \mathbf{m}^k} \\
&- \left(\frac{\partial}{\partial x^m} \frac{\delta \bar{\mathscr{G}}}{\delta \mathfrak{c}^{ij}}\right)\left(\delta^i_k \mathfrak{c}^{mj} + \delta^j_k \mathfrak{c}^{im}\right) \frac{\delta \bar{\mathscr{F}}}{\delta \mathbf{m}^k} \, d\mathbf{x}
\end{aligned}
$$

Here,

$$
\left(\mathbf{m} \cdot \nabla_{\mathbf{x}} \frac{\delta \bar{\mathscr{G}}}{\delta \mathbf{m}}\right) \cdot \frac{\delta \bar{\mathscr{F}}}{\delta \mathbf{m}} := \mathbf{m}^i \left(\frac{\partial}{\partial x^j} \frac{\delta \bar{\mathscr{G}}}{\delta \mathbf{m}^i}\right) \frac{\delta \bar{\mathscr{F}}}{\delta \mathbf{m}^j}
$$

We need a lemma.

Lemma 13.8. *It holds that*

$$
\int_{\Omega_0}\int_{\Omega} \delta(\mathbf{x}-\mathbf{q}(X))\rho_0(X)\phi(\mathbf{x})\psi(\mathbf{q}(X))\, d\mathbf{x}\, dX = \int_{\Omega} \rho(\mathbf{x})\phi(\mathbf{x})\psi(\mathbf{x})\, d\mathbf{x}.
$$

$$
\int_{\Omega_0}\int_{\Omega} \phi(\mathbf{x}) J(X) \nabla_{\mathbf{x}}[\delta(\mathbf{x}-\mathbf{q}(X))\theta(\mathbf{x})]\psi(\mathbf{q}(X))\, d\mathbf{x}\, dX = -\int_{\Omega} \nabla_{\mathbf{x}}\phi(\mathbf{x})\theta(\mathbf{x})\psi(\mathbf{x})\, d\mathbf{x}
$$

Proof. Let $\mathbf{y} = \mathbf{q}(X)$. Then the above integral is

$$\begin{aligned}
&\int_\Omega \int_\Omega \delta(\mathbf{x}-\mathbf{y})\rho_0(\mathbf{q}^{-1}(\mathbf{y}))\phi(\mathbf{x})\psi(\mathbf{y})\,d\mathbf{x}J^{-1}(\mathbf{q}^{-1}(\mathbf{y}))d\mathbf{y} \\
&= \int_\Omega \int_\Omega \delta(\mathbf{x}-\mathbf{y})\rho(\mathbf{y})\phi(\mathbf{x})\psi(\mathbf{y})\,d\mathbf{x}\,d\mathbf{y} \\
&= \int_\Omega \rho(\mathbf{x})\phi(\mathbf{x})\psi(\mathbf{x})\,d\mathbf{x}.
\end{aligned}$$

$$\int_{\Omega_0}\int_\Omega \phi(\mathbf{x})J(X)\nabla_{\mathbf{x}}[\delta(\mathbf{x}-\mathbf{q}(X))\theta(\mathbf{x})]\psi(\mathbf{q}(X))\,d\mathbf{x}\,dX = \int_\Omega\int_\Omega \phi(\mathbf{x})\nabla_{\mathbf{x}}[\delta(\mathbf{x}-\mathbf{y})\theta(\mathbf{x})]\psi(\mathbf{y})\,d\mathbf{x}\,d\mathbf{y}$$
$$= -\int_\Omega\int_\Omega \nabla_{\mathbf{x}}\phi(\mathbf{x})[\delta(\mathbf{x}-\mathbf{y})\theta(\mathbf{x})]\psi(\mathbf{y})\,d\mathbf{x}\,d\mathbf{y} = -\int_\Omega \nabla_{\mathbf{x}}\phi(\mathbf{x})\theta(\mathbf{x})\psi(\mathbf{x})\,d\mathbf{x}$$

□

13.1 Poisson bracket formulation

Reference:

- Antony N. Beris and Brian J. Edwards, Poisson bracket formulation of viscoelastic flow equations of differential type: A unified approach (1989).
- Miroslev Grmela, Hamiltonian Dynamics of Incompressible Elastic Fluids, Phys. Lett A (1988).

Lagrangian formulation

1. The space we consider is

$$\mathcal{Q} := \{\mathbf{q} : \hat{M} \to M \text{ is 1-1, onto and Lipschitz continuous.}\}$$

An element $\mathbf{q} \in \mathcal{Q}$ is called a flow map. Its gradient $F := \frac{\partial \mathbf{q}}{\partial X}$ is called the deformation gradient.

2. The Lagrangian $L : \mathcal{TQ} \to \mathbb{R}$ is defined by

$$L(\mathbf{q}, \frac{\partial \mathbf{q}}{\partial X}, \mathbf{v}) := \frac{1}{2}\rho|\mathbf{v}|^2 - \rho A(\frac{\partial \mathbf{q}}{\partial X})$$

where A is the Helmholtz energy per unit mass. It depends on $\frac{\partial \mathbf{q}}{\partial X}$ through $\mathbf{c}$, the conformation tensor. A and $\mathbf{c}$ are defined by

$$A(\mathbf{c}) = E(\mathbf{c}) - TS(\mathbf{c}), \quad \mathbf{c} := \frac{\partial \mathbf{q}}{\partial X}\mathbf{c}_0(X)\left(\frac{\partial \mathbf{q}}{\partial X}\right)^T = F\mathbf{c}_0F^T.$$

Here, $\mathbf{c}_0(X)$ is the initial conformation tensor. The function E is the internal energy and S the entropy, both are per unit volume. They are modeled for different types of materials. For example, in a simple dumbbell model,

$$E(\mathbf{c}) = \frac{1}{2} nK(Tr(\mathbf{c}))$$

$$S(\mathbf{c}) = \frac{1}{2} nk_B \ln det(\mathbf{c}).$$

Here n is number density of polymer spring and K is the spring constant.

The action is defined as

$$\begin{aligned}
\mathcal{S}[\mathbf{q}, \frac{\partial \mathbf{q}}{\partial X}, \dot{\mathbf{q}}] &= \int_\Omega \frac{1}{2}\rho(\mathbf{q})|\dot{\mathbf{q}}|^2\, d\mathbf{x} - \int_\Omega A(\mathbf{c})\, d\mathbf{x} \\
&= \int_{\Omega_0} \frac{1}{2}\rho_0(X)|\dot{\mathbf{q}}|^2\, dX - \int_{\Omega_0} A(F\mathbf{c}_0F^T)J\, dX \\
&= \mathscr{K}[\dot{\mathbf{q}}] - \mathscr{A}[\mathbf{q}, F]
\end{aligned}$$

Note that both $\mathbf{c}$ and $\mathbf{c}_0$ are symmetric. The variation of $\mathscr{A}$ w.r.t. $\mathbf{q}$ gives the stress term:

$$\begin{aligned}
\delta\mathscr{A} &= \delta \int_{\Omega_0} A(F\mathbf{c}_0F^T)J\, dX \\
&= \int_{\Omega_0} \left[A'(\mathbf{c}) : \big((\delta F)\mathbf{c}_0F^T + F\mathbf{c}_0(\delta F^T)\big) J + A\delta J\right]\, dX
\end{aligned}$$

Let us assume the fluid is incompressible. We thus neglect δJ term. Since $\mathbf{c}$ is symmetric, $A'(c) := \frac{\partial A}{\partial c_{ij}}$ is also symmetric. Note that

$$(F\mathbf{c}_0(\delta F^T))^T = (\delta F)\mathbf{c}_0F^T \quad \because \mathbf{c}_0 \text{ is symmetric}$$

We then get

$$A'(\mathbf{c}) : \big((\delta F)\mathbf{c}_0F^T + F\mathbf{c}_0(\delta F^T)\big) = 2A'(\mathbf{c}) : (\delta F)\mathbf{c}_0F^T.$$

$$\begin{aligned}
\delta\mathscr{A} &= 2\int_{\Omega_0} A'_{ij}(\delta F)^i_k \mathbf{c}_0^{k\ell}(F^T)^\ell_j J\, dX \\
&= 2\int_{\Omega_0} A'_{ij} \frac{\partial \delta x^i}{\partial X^k} \mathbf{c}_0^{k\ell} F^j_\ell J\, dX \\
&= -2\int_{\Omega_0} \frac{\partial}{\partial X^k}\left(A'_{ij}\mathbf{c}_0^{k\ell}F^j_\ell J\right)\delta q^i\, dX \\
&:= -\int_{\Omega_0} \frac{\partial}{\partial X^k} P \cdot \delta\mathbf{q}\, dX
\end{aligned}$$

Here,

$$P_i^k := 2A'_{ij}\mathbf{c}_0^{k\ell}F_\ell^j J$$

is the first Piola stress.

3. The variation of action gives

$$\delta\mathcal{S} = \int_{t_0}^{t_1}\int_{\Omega_0}(-\rho_0\ddot{\mathbf{q}} + \nabla_X P)\cdot\delta\mathbf{q}\,dX\,dt$$

The corresponding Euler-Lagrange equation is

$$\rho_0\ddot{\mathbf{q}} = \nabla_X P.$$

4. The corresponding Cauchy stress is

$$\sigma = J^{-1}PF^T.$$

In component form, we get

$$\begin{aligned}\sigma_i^j &= P_i^k(F^T)_j^k\\ &= 2A'_{im}\mathbf{c}_0^{k\ell}F_\ell^m F_k^j\\ &= 2A'_{im}c^{mj}\\ &= 2A'\mathbf{c}.\end{aligned}$$

Note that both $\mathbf{c}$, $A' := \frac{\partial A}{\partial \mathbf{c}}$ and σ are symmetric. We have

$$\sigma = 2A'\mathbf{c} = 2\mathbf{c}A'.$$

In the case of viscosity, we add the rate-of-strain to the extra stress. Thus

$$\sigma = 2\mathbf{c}A' + \eta_p\left(\nabla\mathbf{v} + (\nabla\mathbf{v})^T\right).$$

Hamiltonian Dynamics in Lagrangian coordinate

1. We can express the above Euler-Lagrange equation as a Hamiltonian equation. First, let us take Legendre transform of $\mathscr{L}$, which is equivalent to take Legendre transform of L w.r.t. $\mathbf{v}$. This defines the momentum

$$\mathbf{p}(X) = \frac{\partial L}{\partial \mathbf{v}} = \rho_0(X)\mathbf{v}(X).$$

The Hamiltonian is then defined to be the Legendre transform of L. This gives

$$H(\mathbf{q},\frac{\partial\mathbf{q}}{\partial X},\mathbf{p}) = \frac{|\mathbf{p}|^2}{2\rho_0} + A(\mathbf{c}),$$

and

$$\mathscr{H}[\mathbf{q},\frac{\partial\mathbf{q}}{\partial X},\mathbf{p}] := \int_{\Omega_0} H(\mathbf{q},\frac{\partial\mathbf{q}}{\partial X},\mathbf{p})\,dX.$$

2. The Lagrangian dynamics is equivalent to the following Hamiltonian dynamics:

$$\dot{\mathbf{q}} = \frac{\delta \mathscr{H}}{\delta \mathbf{p}} = \rho_0 \mathbf{v}$$
$$\dot{\mathbf{p}} = -\frac{\delta \mathscr{H}}{\partial \mathbf{q}} = \nabla_X P.$$

This equation can also be formulated in terms of Poisson bracket. Namely

$$\dot{\mathbf{q}} = \{\mathbf{q}, \mathscr{H}\}, \quad \dot{\mathbf{p}} = \{\mathbf{p}, \mathscr{H}\},$$

where the Poisson bracket is defined by

$$\{\mathscr{F}, \mathscr{G}\} := \int_{\Omega_0} \left(\frac{\partial \mathscr{F}}{\partial \mathbf{q}} \frac{\partial \mathscr{G}}{\partial \mathbf{p}} - \frac{\partial \mathscr{G}}{\partial \mathbf{q}} \frac{\partial \mathscr{F}}{\partial \mathbf{p}} \right) dX$$

Hamiltonian dynamics in Eulerian variables

1. The Eulerian variables are $(\rho, \mathbf{m}, \mathbf{c})$, where $\mathbf{m} = \rho \mathbf{v}$ and $\mathbf{c} = F\mathbf{c}_0 F^T$ is the conformation tensor. The transformation between $(\mathbf{q}, \mathbf{p})$ and $(\rho, \mathbf{m}, \mathbf{c})$ is

$$\rho(\mathbf{x}) = \int_{\Omega_0} \rho_0(X) \delta(\mathbf{x} - \mathbf{q}(X))\, dX$$
$$\mathbf{m}(\mathbf{x}) = \int_{\Omega_0} \mathbf{p}(X) \delta(\mathbf{x} - \mathbf{q}(X))\, dX$$
$$\mathbf{c}(\mathbf{x}) = \left(\frac{\partial \mathbf{q}}{\partial X} \mathbf{c}_0(X) (\frac{\partial \mathbf{q}}{\partial X})^T \right)_{X = \mathbf{q}^{-1}(\mathbf{x})}$$

Here, we have assumed that ρ_0 and $\mathbf{c}_0$ are pregiven function on Ω_0.

2. Variations

$$\delta \rho = -\int_{\Omega_0} \rho_0(X) \nabla_{\mathbf{x}} \delta(\mathbf{x} - \mathbf{q}(X)) \cdot \delta \mathbf{q}(X)\, dX$$
$$\delta \mathbf{m} = \int_{\Omega_0} (-\mathbf{p} \nabla_{\mathbf{x}} \delta(\mathbf{x} - \mathbf{q}(X))) \cdot \delta \mathbf{q} + \delta(\mathbf{x} - \mathbf{q}(X)) \delta \mathbf{p}\, dX$$

For

$$c^{ij}(\mathbf{q}(X)) := \frac{\partial q^i}{\partial X^k} \frac{\partial q^j}{\partial X^\ell} C^{k\ell}(X)$$

its variation is

$$\delta c^{ij}(\mathbf{q}(X)) = \frac{\partial \delta q^i}{\partial X^k} \frac{\partial q^j}{\partial X^\ell} C^{k\ell} + \frac{\partial \delta q^j}{\partial X^\ell} \frac{\partial q^i}{\partial X^k} C^{k\ell}$$
$$= \frac{\partial (\delta q^m)}{\partial X^k} \left((\delta^{im} \frac{\partial q^j}{\partial X^\ell} + \delta^{jm} \frac{\partial q^i}{\partial X^\ell}) C^{k\ell} \right)$$

Here, we have used $C^{k\ell} = C^{\ell k}$. Hence, for a functional $\mathscr{F}[\mathbf{q},\mathbf{p}] = \bar{\mathscr{F}}[\rho,\mathbf{m},\mathbf{c}] = \int F(\rho,\mathbf{m},\mathbf{c})\,dX$, we have

$$\begin{aligned}
\delta\mathscr{F} &= \int_{\Omega_0}\left(\frac{\delta\mathscr{F}}{\delta\mathbf{q}}\delta\mathbf{q} + \frac{\delta\mathscr{F}}{\delta\mathbf{p}}\right) dX \\
&= \int_{\Omega}\left(\frac{\delta\bar{\mathscr{F}}}{\delta\rho}\delta\rho + \frac{\delta\bar{\mathscr{F}}}{\delta\mathbf{m}}\delta\mathbf{m} + \frac{\delta\bar{\mathscr{F}}}{\delta\mathbf{c}}\delta\mathbf{c}\right) d\mathbf{x} \\
&= \int_{\Omega}\frac{\partial F}{\partial\rho}\int_{\Omega_0} -\rho_0(X)\nabla_{\mathbf{x}}\delta(\mathbf{x}-\mathbf{q}(X))\cdot\delta\mathbf{q}(X)\,dX\,d\mathbf{x} \\
&\quad + \int_{\Omega}\frac{\partial F}{\partial\mathbf{m}}\int_{\Omega_0}(-\mathbf{p}\nabla_{\mathbf{x}}\delta(\mathbf{x}-\mathbf{q}(X)))\cdot\delta\mathbf{q} + \delta(\mathbf{x}-\mathbf{q}(X))\delta\mathbf{p}\,dX\,d\mathbf{x} \\
&\quad + \int_{\Omega}\frac{\partial F}{\partial c^{ij}}\frac{\partial(\delta q^m)}{\partial X^k}\left(\frac{\partial\delta q^i}{\partial X^k}\frac{\partial q^j}{\partial X^\ell}C^{k\ell} + \frac{\partial\delta q^j}{\partial X^\ell}\frac{\partial q^i}{\partial X^k}C^{k\ell}\right) d\mathbf{x} \\
&= \int_{\Omega_0}\int_{\Omega}\left(\delta(\mathbf{x}-\mathbf{q}(X))\rho_0(X)\nabla_{\mathbf{x}}\frac{\partial F}{\partial\rho}\right) d\mathbf{x}\cdot\delta\mathbf{q}(X)\,dX \\
&\quad + \int_{\Omega_0}\int_{\Omega}\left(\delta(\mathbf{x}-\mathbf{q}(X))\mathbf{p}\nabla_{\mathbf{x}}\frac{\partial F}{\partial\mathbf{m}}\right)\cdot\delta\mathbf{q} + \frac{\partial F}{\partial\mathbf{m}}\delta(\mathbf{x}-\mathbf{q}(X))\delta\mathbf{p}\,d\mathbf{x}\,dX \\
&\quad - \int_{\Omega_0}\left[\frac{\partial}{\partial X^k}\left(\frac{\partial F}{\partial c^{\alpha j}}\frac{\partial q^j}{\partial X^\ell}C^{k\ell}J\right) + \frac{\partial}{\partial X^\ell}\left(\frac{\partial F}{\partial c^{i\alpha}}\frac{\partial q^i}{\partial X^k}C^{k\ell}J\right)\right]\cdot\delta q^\alpha\,dX
\end{aligned}$$

Thus,

$$\begin{aligned}
\frac{\delta\mathscr{F}}{\delta\mathbf{q}} &= \int_{\Omega}\delta(\mathbf{x}-\mathbf{q}(X))\left[\rho_0(X)\left(\nabla_{\mathbf{x}}\frac{\partial F}{\partial\rho}\right) + \mathbf{p}\left(\nabla_{\mathbf{x}}\frac{\partial F}{\partial\mathbf{m}}\right)\right] d\mathbf{x} \\
&\quad - \frac{\partial}{\partial X^k}\left(\frac{\partial F}{\partial c^{\alpha j}}\frac{\partial q^j}{\partial X^\ell}C^{k\ell}J + \frac{\partial F}{\partial c^{i\alpha}}\frac{\partial q^i}{\partial X^\ell}C^{\ell k}J\right) \\
\frac{\delta\mathscr{F}}{\delta\mathbf{p}} &= \int_{\Omega}\frac{\partial F}{\partial\mathbf{m}}\delta(\mathbf{x}-\mathbf{q}(X))\,d\mathbf{x} = \frac{\partial F}{\partial\mathbf{m}}|_{\mathbf{x}=\mathbf{q}(X)}
\end{aligned}$$

3. The inner product

$$\begin{aligned}
\int_{\Omega_0}\frac{\delta\mathscr{F}}{\delta\mathbf{q}}\frac{\delta\mathscr{G}}{\delta\mathbf{p}}\,dX &= \int_{\Omega_0}\left[\int_{\Omega}\delta(\mathbf{x}-\mathbf{q}(X))\left(\rho_0(X)\nabla_{\mathbf{x}}\frac{\partial F}{\partial\rho} + \mathbf{p}\nabla_{\mathbf{x}}\frac{\partial F}{\partial\mathbf{m}}\right) d\mathbf{x}\right]\cdot\frac{\partial G}{\partial\mathbf{m}}\,dX \\
&\quad - \int_{\Omega_0}\frac{\partial}{\partial X^k}\left(\frac{\partial F}{\partial c^{\alpha j}}\frac{\partial q^j}{\partial X^\ell}C^{k\ell}J + \frac{\partial F}{\partial c^{i\alpha}}\frac{\partial q^i}{\partial X^\ell}C^{\ell k}J\right)\cdot\frac{\partial G}{\partial\mathbf{m}^\alpha}dX \\
&= \int_{\Omega}\left(\rho\nabla_{\mathbf{x}}\frac{\partial F}{\partial\rho} + \mathbf{m}\nabla_{\mathbf{x}}\frac{\partial F}{\partial\mathbf{m}}\right)\frac{\partial G}{\partial\mathbf{m}}\,d\mathbf{x} \\
&\quad - \int_{\Omega}\frac{\partial}{\partial x^i}\left(\frac{\partial F}{\partial c^{\alpha j}}c^{ij} + \frac{\partial F}{\partial c^{j\alpha}}c^{ji}\right)\cdot\frac{\partial G}{\partial\mathbf{m}^\alpha}\,d\mathbf{x}
\end{aligned}$$

In the last step, we use the following lemma

Lemma 13.9.

$$J\nabla_{\mathbf{x}}\sigma = \nabla_X P,$$

where

$$\sigma = J^{-1}PF^T, \quad \sigma^i_\alpha = J^{-1}P^k_\alpha F^i_k.$$

By setting

$$P^k_\alpha := \frac{\partial F}{\partial c^{\alpha j}}\frac{\partial q^j}{\partial X^\ell}C^{k\ell}J,$$

we get

$$\sigma^i_\alpha = \frac{\partial F}{\partial c^{\alpha j}}F^j_\ell F^i_k C^{k\ell} = \frac{\partial F}{\partial c^{\alpha j}}c^{ij}$$

Thus, the last term in the inner product formula is

$$-\int_\Omega \frac{\partial}{\partial x^i}\left(\frac{\partial F}{\partial c^{\alpha j}}c^{ij} + \frac{\partial F}{\partial c^{j\alpha}}c^{ji}\right)\cdot\frac{\partial G}{\partial \mathbf{m}^\alpha}\,d\mathbf{x}$$

4. The Poisson bracket is

$$\begin{aligned}\{\mathscr{F},\mathscr{G}\} = &\int_\Omega\left(\rho\nabla_{\mathbf{x}}\frac{\partial F}{\partial\rho} + \mathbf{m}\nabla_{\mathbf{x}}\frac{\partial F}{\partial\mathbf{m}}\right)\frac{\partial G}{\partial\mathbf{m}}\,d\mathbf{x} - \int_\Omega\frac{\partial}{\partial x^i}\left(\frac{\partial F}{\partial c^{\alpha j}}c^{ij} + \frac{\partial F}{\partial c^{j\alpha}}c^{ji}\right)\cdot\frac{\partial G}{\partial\mathbf{m}^\alpha}\,d\mathbf{x}\\ &-\int_\Omega\left(\rho\nabla_{\mathbf{x}}\frac{\partial G}{\partial\rho} + \mathbf{m}\nabla_{\mathbf{x}}\frac{\partial G}{\partial\mathbf{m}}\right)\frac{\partial F}{\partial\mathbf{m}}\,d\mathbf{x} + \int_\Omega\frac{\partial}{\partial x^i}\left(\frac{\partial G}{\partial c^{\alpha j}}c^{ij} + \frac{\partial G}{\partial c^{j\alpha}}c^{ji}\right)\cdot\frac{\partial F}{\partial\mathbf{m}^\alpha}\,d\mathbf{x}\end{aligned}$$

Incomplete, some terms are missing.

Ref. Juan C. Simo, Jerrold E. Marsden and P.S. Krishnaprasad, The Hamiltonian structure of nonlinear elasticity: The material and convective representations of solids, rods, and plates (1988)

Chapter 14

Mathematical Theory for Simple Elasticity

Simple elasticity only consider mechanical property of an elastic material, no thermodynamics is under consideration. Mathematical theory for simple elasticity includes

- Initial boundary value problems: elastic wave theory
  - Hyperbolicity and rank-1 convexity
  - Linear elasticity
  - Linear isotropic elasticity
  - Nonlinear elasticity, hyperbolic conservation laws
- Steady state problems:
  - non-uniqueness and uniqueness,
  - poly-convexity, existence and uniqueness
- Stability and Bifurcation theory

References

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14.1 Linear Elasticity

14.1.1 Dynamics of linear elasticity

In simple elasticity, as assuming the strain $\mathbf{e} = \frac{1}{2}\left(\nabla_X \mathbf{u} + (\nabla_X \mathbf{u})^T\right)$ being small, the equation of motion can be approximated by

$$\rho_0 \ddot{u}^i = \sum_{jkl} a_{ijkl} \frac{\partial^2 u^k}{\partial X^j \partial X^l}, \; i = 1,2,3, \quad X \in \Omega_0, \tag{14.1}$$

where the coefficients

$$a_{ijkl} := \frac{\partial^2 W(I)}{\partial F^i_j \partial F^k_l} \tag{14.2}$$

satisfies

$$a_{ijkl} = a_{ijlk} = a_{klij} = a_{jikl}. \tag{14.3}$$

The first equality is due to $C = F^T F$ being symmetric. The second equality is from $\frac{\partial^2 W(I)}{\partial F^i_j \partial F^k_l} = \frac{\partial^2 W(I)}{\partial F^k_l \partial F^i_j}$. The third equality is a consequence of the first two equalities.

14.1.2 Hyperbolicity of linear elasticity

We look for plane wave solution for equation (14.1). We plug the ansatz $\mathbf{u} = \xi e^{i(\eta \cdot X - \lambda t)}$ into (14.1) to get

$$\rho_0 \lambda^2 \xi_i = \sum_{j,k,l=1}^{3} a_{ijkl} \xi_k \eta_j \eta_l. \tag{14.4}$$

Thus, equation (14.1) supports plane wave solution in direction η if the 3×3 matrix

$$A(\eta)_{ik} := \sum_{j,l=1}^{3} a_{ijkl} \eta_j \eta_l$$

has positive eigenvalue $\rho_0 \lambda^2$ with eigenvector ξ.

Lemma 14.10. *The matrix $A(\eta)_{ik} := \sum_{j,l=1}^{3} a_{ijkl} \eta^j \eta^l$ is symmetric.*

This is due to $a_{ijkl} = a_{klij}$ (hyper-elasticity) and

$$A(\eta)_{ik} = \sum_{j,l=1}^{3} a_{ijkl} \eta_j \eta_l = \sum_{j,l=1}^{3} a_{ijkl} \eta_l \eta_j = \sum_{j,l=1}^{3} a_{ilkj} \eta_j \eta_l = \sum_{j,l=1}^{3} a_{kjil} \eta_j \eta_l = A(\eta)_{ki}.$$

Thus, A has real eigenvalues. To support plane wave solutions, we need A to be positive definite. The definition of positivity of A is the follows.

Definition 14.6 (Strong ellipticity)**.** *The 4-tensor (a_{ijkl}) with symmetry property (14.3) is said to satisfy strong ellipticity condition if there exists a positive constant α such that for any $\xi \in \mathbb{R}^3$, $\eta \in \mathbb{R}^3$,*
$$\sum_{ijkl} a_{ijkl}\xi_i\xi_k\eta_j\eta_l \geq \alpha|\xi|^2|\eta|^2. \tag{14.5}$$

From the above discussion, we have the following proposition.

Proposition 14.14. *Strong ellipticity for the 4-tensor (a_{ijkl}) is equivalent to the hyperbolicity of system (14.1).*

Remarks

- Condition (14.5) is also called Legendre-Hadamard condition in Calculus of Variations.

Definition 14.7. *Let $\mathbb{M}_n$ be the space of $n\times n$ matrices. Let $W:\mathbb{M}_n\to\mathbb{R}$. Such function W is called rank-one convex if it is convex along all directions spanned by matrices of rank 1. That is,*
$$W(\lambda\mathbf{F}+(1-\lambda)\mathbf{G}) \leq \lambda W(\mathbf{F})+(1-\lambda)W(\mathbf{G}),$$
for all
$$\mathbf{F},\mathbf{G}\in\mathbb{M}_n, \quad rank(\mathbf{F}-\mathbf{G})\leq 1.$$

Proposition 1. *The matrix $(\xi_i\eta_j) := \xi\eta^T$ is a rank-1 matrix. Indeed, all rank-1 matrix has this form. $W(F) := a_{ijkl}F^i_jF^k_l$ is rank-1 convex $\Leftrightarrow$ a_{ijkl} is strongly elliptic.*

14.1.3 Energy law

We want to study how energy changes in time. From the symmetry property of a_{ijkl}, we have
$$\sum_{kl} a_{ijkl}\frac{\partial u^l}{\partial X^k} = \sum_{kl} a_{ijkl}\frac{\partial u^k}{\partial X^l}.$$
The dynamic equation can be written as
$$\rho_0\ddot{u}^i = \frac{1}{2}\sum_j\sum_{kl}\partial_j a_{ijkl}\left(\frac{\partial u^k}{\partial X^l}+\frac{\partial u^l}{\partial X^k}\right).$$
In vector form, it reads
$$\rho_0\ddot{\mathbf{u}} = \frac{1}{2}\nabla_{\mathbf{x}}\cdot\left[A\left(\nabla_X\mathbf{u}+(\nabla_X\mathbf{u})^T\right)\right] = \nabla_X\cdot A\mathbf{e}. \tag{14.6}$$

By multiplying (14.6) by $\dot{\mathbf{u}}$ then integrating in X, we get

$$\begin{aligned}\frac{d}{dt}\int_{\Omega_0}\left(\frac{1}{2}\rho_0|\dot{\mathbf{u}}|^2\right)dX &= \int_{\Omega_0}\frac{1}{2}\nabla_{\mathbf{x}}\cdot\left[A\left(\nabla_X\mathbf{u}+(\nabla_X\mathbf{u})^T\right)\right]\cdot\dot{\mathbf{u}}\,dX\\ &= -\int_{\Omega_0}\frac{1}{2}\left[A\left(\nabla_X\mathbf{u}+(\nabla_X\mathbf{u})^T\right)\right]\cdot\nabla_X\dot{\mathbf{u}}\,dX\end{aligned}$$

Note from $a_{ijkl}=a_{jikl}$ we obtain

$$\begin{aligned}\frac{1}{2}\sum_{ijkl}a_{ijkl}\left(\frac{\partial u_l}{\partial X^k}+\frac{\partial u_k}{\partial X^l}\right)\frac{\partial\dot{u}_i}{\partial X^j} &= \frac{1}{4}\sum_{ijkl}a_{ijkl}\left(\frac{\partial u_l}{\partial X^k}+\frac{\partial u_k}{\partial X^l}\right)\left(\frac{\partial\dot{u}_i}{\partial X^j}+\frac{\partial\dot{u}_j}{\partial X^i}\right)\\ &= \int\sum_{ijkl}a_{ijkl}e_{kl}\dot{e}_{ij}=\langle A\mathbf{e},\dot{\mathbf{e}}\rangle=\frac{d}{dt}\left(\frac{1}{2}\langle A\mathbf{e},\mathbf{e}\rangle\right)\end{aligned}$$

The energy law reads

$$\frac{d}{dt}\int_{\Omega_0}\left(\frac{1}{2}\rho_0|\dot{\mathbf{u}}|^2\right)d\mathbf{x}+\frac{d}{dt}\int_{\Omega_0}W(\mathbf{e})\,d\mathbf{x}=0,$$

where

$$W(\mathbf{e}):=\frac{1}{2}\langle A\mathbf{e},\mathbf{e}\rangle.$$

14.1.4 Dynamics of linear elasticity

Existence theory for linear elasticity with hyperbolicity condition The initial-boundary value problem for linear elasticity is posed as the follows. The evolution equation is

$$\rho_0\ddot{u}^i=\sum_{jkl}a_{ijkl}\frac{\partial^2u^k}{\partial X^j\partial X^l},\ i=1,2,3,\quad X\in\Omega_0. \tag{14.7}$$

The boundary conditions are

$$\begin{cases}\mathbf{u}(X)=\mathbf{h}(X)\text{ on }\partial\Gamma_0^D\\ \sum_{j,k,l=1}^3a_{ijkl}\frac{\partial u^k}{\partial X^l}N^j=t^i(X),i=1,2,3,\text{ on }\partial\Gamma_0^N\end{cases} \tag{14.8}$$

where $\partial\Omega_0=\Gamma_0^D\cup\Gamma_0^N$, $\mathbf{N}=(N^1,N^2,N^3)$ is the outer normal of Γ_0^N. The initial conditions are

$$\mathbf{u}(0,X)=\mathbf{u}_0(X),\quad\partial_t\mathbf{u}(0,X)=\mathbf{u}_1(X),\quad X\in\Omega_0. \tag{14.9}$$

Standard semigroup theory gives L^2 existence theorem under the strong ellipticity condition for (a_{ijkl}).

Remarks

1. For the whole domain problem, one can write the equation as a first-order system

$$\frac{d}{dt}\begin{bmatrix} u \\ \dot{u} \end{bmatrix} = \begin{bmatrix} 0 & I \\ \mathscr{A} & 0 \end{bmatrix}\begin{bmatrix} u \\ \dot{u} \end{bmatrix}, \quad (\mathscr{A}u)^i := \sum_{jkl} a_{ijkl}\frac{\partial^2 u^k}{\partial X^j \partial X^l}.$$

   The Fourier method gives a representation of the solution operator. From which, one can perform L^2 estimate, or Strichartz estimates (L^p-L^q estimates) to obtain L^2 solution or a L^p theory.

2. For bounded-domain problems, operator theory and Hilbert space method can be applied.

14.1.5 Steady state problem for linear elasticity

Outline

- The steady state problem is the boundary value problem of

$$-\sum_{jkl} a_{ijkl}\frac{\partial^2 u^k}{\partial X^j \partial X^l} = \rho_0(X) b_i(\mathbf{x}(X)), i = 1,2,3,\ X \in \Omega_0,$$

  with boundary condition (14.8). Here $\mathbf{b}$ is the body force.

- Stability condition $\Rightarrow$ existence and uniqueness of steady state problem.
- The key step is the Korn's inequality and Lax-Milgram Theorem is used for existence.
- The uniqueness follows from the fact that the solution which minimizes $\int_{\Omega_0} W(\mathbf{e})\,dX$ is the trivial solution. This again follows from Korn's inequality.

Ref. Ciarlet

Definition 14.8 (Stability)**.** *The 4-tensor (a_{ijkl}) is stable if there exists a positive constant $\tilde{\alpha}$ such that for any symmetric matrix (e_{ij}), we have*

$$\sum_{ijkl} a_{ijkl} e_{ij} e_{kl} \geq \tilde{\alpha} \sum_{kl} e_{kl}^2. \tag{14.10}$$

Proposition 14.15. *Assuming a_{ijkl} satisfies*

$$a_{ijkl} = a_{klij} = a_{ijlk}$$

then we have

$$\textit{Stability} \Rightarrow \textit{Strong Ellipticity}.$$

Proof. Choose $e_{kl} = \frac{1}{2}(\xi_k\eta_l + \xi_l\eta_k)$. we get

$$\begin{aligned}\sum_{ijkl} a_{ijkl}e_{ij}e_{kl} &= \frac{1}{4}\sum_{ijkl} a_{ijkl}(\xi_i\eta_j + \xi_j\eta_i)(\xi_k\eta_l + \xi_l\eta_k) \\ &= \sum_{ijkl} a_{ijkl}\xi_i\xi_k\eta_j\eta_l\end{aligned}$$

Here, we used the symmetric property of a_{ijkl}:

$$a_{ijkl} = a_{jikl} = a_{ijlk} = a_{jilk}.$$

We also note that

$$\begin{aligned}\sum_{ij}|e_{ij}|^2 &= \frac{1}{4}\sum_{ij}(\xi_i\eta_j + \xi_j\eta_i)^2 \\ &= \frac{1}{4}\sum_{ij}\left(\xi_i^2\eta_j^2 + \xi_j^2\eta_i^2 + 2\xi_i\eta_i\xi_j\eta_j\right) \\ &= \frac{1}{2}\left(|\xi|^2|\eta|^2 + (\xi\cdot\eta)^2\right) \\ &\geq \frac{1}{2}|\xi|^2|\eta|^2.\end{aligned}$$

If (a_{ijkl}) satisfies stability condition, then

$$\sum_{ijkl} a_{ijkl}\xi_i\xi_k\eta_j\eta_l = \sum_{ijkl} a_{ijkl}e_{ij}e_{kl} \geq \tilde{\alpha}\sum_{k,l} e_{kl}^2 \geq \frac{\tilde{\alpha}}{2}|\xi|^2|\eta|^2.$$

Thus, it also satisfies strong ellipticity condition. □

Remark The stability condition (14.10) is that

$$\sum_{ijkl} a_{ijkl}e_{ij}e_{kl} \geq \tilde{\alpha}\sum_{kl} e_{kl}^2$$

holds for all matrix $e \in \mathbb{M}_n$. The strong ellipticity condition is the same condition holds but only for rank-1 matrices (i.e. $\xi\eta^T$).

Theorem 14.13 (Korn's inequality)**.** *Let $u : \Omega \to \mathbb{R}^3$ and $e = \frac{1}{2}(\partial\mathbf{u}/\partial X + (\partial\mathbf{u}/\partial X)^T)$. It holds that*

$$\int_\Omega \sum_{ij}\left(\frac{\partial u_i}{\partial X^j}\right)^2 dx \leq 2\int \sum_{ij} e_{ij}^2\, dx \ \text{ for all } \ u \in H_0^1(\Omega).$$

Proof. We have that

$$\begin{aligned}\sum_{ij} e_{ij}^2 &= \frac{1}{4}\sum_{ij}\left(\frac{\partial u_i}{\partial X^j}+\frac{\partial u_j}{\partial X^i}\right)^2\\ &= \frac{1}{2}\sum_{ij}\left(\left(\frac{\partial u_i}{\partial X^j}\right)^2+\frac{\partial u_i}{\partial X^j}\frac{\partial u_j}{\partial X^i}\right)\end{aligned}$$

We integrate this equality over Ω. Note that

$$\frac{\partial u_i}{\partial X^j}\frac{\partial u_j}{\partial X^i} = \frac{\partial}{\partial X^j}\left(u_i\frac{\partial u_j}{\partial X^i}\right) - u_i\frac{\partial^2 u_j}{\partial X^i \partial X^j}$$

$$\frac{\partial u_i}{\partial X^i}\frac{\partial u_j}{\partial X^j} = \frac{\partial}{\partial X^i}\left(u_i\frac{\partial u_j}{\partial X^j}\right) - u_i\frac{\partial^2 u_j}{\partial X^i \partial X^j},$$

subtracting these two equations, we get

$$\int_\Omega \frac{\partial u_i}{\partial X^j}\frac{\partial u_j}{\partial X^i}\,dX = \int_\Omega \frac{\partial u_i}{\partial X^i}\frac{\partial u_j}{\partial X^j}\,dX$$

for all $u \in H_0^1(\Omega)$. Thus,

$$\begin{aligned}\int_\Omega \sum_{ij} e_{ij}^2\,dx &= \frac{1}{2}\int_\Omega \sum_{ij}\left(\left(\frac{\partial u_i}{\partial X^j}\right)^2+\frac{\partial u_i}{\partial X^i}\frac{\partial u_j}{\partial X^j}\right)dx\\ &= \frac{1}{2}\int_\Omega \sum_{ij}\left(\frac{\partial u_i}{\partial X^j}\right)^2+\left(\sum_i \frac{\partial u_i}{\partial X^i}\right)^2 dx\\ &\geq \frac{1}{2}\int_\Omega \sum_{ij}\left(\frac{\partial u_i}{\partial X^j}\right)^2 dx\end{aligned}$$

□

Existence theory with stability condition Stability condition gives existence and uniqueness in $H^1(\Omega_0)$. Standard energy method can be applied to prove this result. The key step is the Korn's inequality.

14.2 Linear isotropic elasticity

14.2.1 Characteristic wave modes

For linear isotropic material

$$a_{ijkl} = \lambda\delta_{ij}\delta_{kl} + \mu(\delta_{ik}\delta_{jl} + \delta_{il}\delta_{jk}), \tag{14.11}$$

the matrix $A(\eta)$ is

$$A(\eta)_{ik} = \sum_{ijkl} a_{ijkl}\eta_j\eta_l = (\lambda+\mu)\eta_i\eta_k + \mu|\eta|^2\delta_{ik}.$$

The equation of motion reads

$$\boxed{\rho_0\ddot{u}^i = \mu \triangle u^i + (\lambda+\mu)\partial_i(\partial_k u^k).} \tag{14.12}$$

To find the eigenvalues of $A(\eta)$, using isotropy property, we may choose $\eta = (0,0,1)$. The eigenvalues of $A(\eta)$ in direction η can be obtained by rotating $(0,0,1)$ to η. The corresponding eigenvectors can be obtained by the same rotation. Now, for $\eta = (0,0,1)$,

$$A((0,0,1)) = (\lambda+\mu)\begin{bmatrix} 0 & 0 & 0 \\ 0 & 0 & 0 \\ 0 & 0 & 1 \end{bmatrix} + \mu\begin{bmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 1 \end{bmatrix}.$$

The eigenvalues are

$$\rho_0\lambda_i^2 = \mu, i = 1,2, \quad \rho_0\lambda_3^2 = \lambda+2\mu. \tag{14.13}$$

The eigenvectors are the Cartesian unit vectors E_1, E_2 and E_3.

- **Longitudinal wave** is the eigen-mode

$$E_3 e^{i(X^3 \pm \lambda_3 t)}.$$

  The material oscillates in the direction of wave propagation (i.e. $\eta = (0,0,1)$ and $E_3 = (0,0,1)$). It is also called the *primary wave*, or the *P-wave*:.

- **Transverse wave** is the eigenmode

$$E_k e^{i(X^3 \pm \lambda_k t)}, k = 1,2.$$

  The material oscillates orthogonal to the direction of wave propagation (i.e. $\eta = (0,0,1)$, whereas $E_1 = (1,0,0)$, $E_2 = (0,0,1)$). It is also called the *secondary wave*, or the *S-wave*.

Proposition 14.16. *For linear isotropic elastic material, the strong ellipticity of*

$$a_{ijkl} = \lambda\delta_{ij}\delta_{kl} + \mu(\delta_{ik}\delta_{jl} + \delta_{il}\delta_{jk})$$

is equivalent to

$$\lambda+2\mu > 0, \quad \mu > 0. \tag{14.14}$$

In terms of the Young modulus E and Poisson ratio ν, we have

$$(\lambda > 0,\ \mu > 0) \Leftrightarrow (0 < \nu < \frac{1}{2},\ E > 0) \Rightarrow (\lambda+2\mu > 0,\ \mu > 0). \tag{14.15}$$

Proof. 1. (14.14) follows from (14.13).

2. (14.15) follows from (9.40).

□

14.2.2 Dynamics of linear isotropic elasticity

Equation (14.12) in vector form reads

$$\rho_0 \partial_t^2 \mathbf{u} = \mu \triangle \mathbf{u} + (\lambda + \mu)\nabla(\nabla \cdot \mathbf{u}).$$

Let us decompose the displacement $\mathbf{u}$ into

$$\mathbf{u} = \mathbf{v} + \mathbf{w},$$

with

$$\mathbf{v} = \nabla \phi, \quad \nabla \cdot \mathbf{w} = 0.$$

Such decomposition is called Hodge decomposition. [1] With Hodge decomposition, the equation becomes

$$\rho_0 \partial_t^2 (\nabla \phi + \mathbf{w}) = \mu \triangle (\nabla \phi + \mathbf{w}) + (\lambda + \mu)\nabla(\nabla \cdot \nabla \phi) = \mu \triangle (\nabla \phi + \mathbf{w}) + (\lambda + \mu)\nabla \triangle \phi.$$

We get

$$\rho_0 \partial_t^2 (\mathbf{v} + \mathbf{w}) = (\lambda + 2\mu) \triangle \mathbf{v} + \mu \triangle \mathbf{w}.$$

Note that the Hodge decomposition is preserved under the operations $\triangle$ and ∂_t^2. Thus, we obtain

$$\boxed{\rho_0 \partial_t^2 \mathbf{v} = (\lambda + 2\mu) \triangle \mathbf{v}, \quad \rho_0 \partial_t^2 \mathbf{w} = \mu \triangle \mathbf{w}.} \tag{14.16}$$

Thus, the longitudinal waves and transverse waves are decoupled. To solve the initial value problem

$$\mathbf{u}(0, X) = \mathbf{u}_0(X), \quad \partial_t \mathbf{u}(0, X) = \mathbf{u}_1(X), \quad X \in \Omega_0,$$

we perform Hodge decomposition for both $\mathbf{u}_0$ and $\mathbf{u}_1$ as

$$\mathbf{u}_0 = \mathbf{v}_0 + \mathbf{w}_0, \quad \mathbf{u}_1 = \mathbf{v}_1 + \mathbf{w}_1.$$

Then solve the initial value problems for both $\mathbf{v}$ and $\mathbf{w}$ separately.

Stability of linear isotropic material For linear isotropic material (14.11),

$$\langle A\mathbf{e}, \mathbf{e} \rangle = \lambda (Tr\,\mathbf{e})^2 + \mu \mathbf{e} : \mathbf{e}$$

The stability condition (14.10) reads

$$\langle A\mathbf{e}, \mathbf{e} \rangle \geq \tilde{\alpha} \|\mathbf{e}\|_F^2.$$

[1]When the domain is simply connected, we can have such decomposition. When the domain is multiple connected, then $\mathbf{u} = \mathbf{v} + \mathbf{w} + \mathbf{h}$ The term $\mathbf{h}$ is a harmonic function, i.e. $\triangle \mathbf{h} = 0$.

For the off-diagonal component, it gives

$$\mu e_{ij}^2 \geq \tilde{\alpha} e_{ij}^2.$$

For the diagonal part, it is

$$\lambda(e_{11}+e_{22}+e_{33})^2 + 2\mu e_{kk}^2 \geq \tilde{\alpha} e_{kk}^2, \quad k = 1,2,3,$$

for some $\tilde{\alpha} > 0$. Summing this equation over $k = 1,2,3$, we get

$$3\lambda(e_{11}+e_{22}+e_{33})^2 + 2\mu(e_{11}^2+e_{22}^2+e_{33}^2) \geq \tilde{\alpha}(e_{11}^2+e_{22}^2+e_{33}^2)$$

for any e_{11}, e_{22}, e_{33}. TOBE COMPLETED This is equivalent to

$$3\lambda + 2\mu > 0.$$

Thus, the *stability condition* for linear isotropic material is

$$\boxed{3\lambda + 2\mu > 0, \quad \mu > 0.} \tag{14.17}$$

In terms of shear modulus μ and bulk modulus $K = \lambda + \frac{2}{3}\mu$, stability condition reads

$$\mu > 0, \quad K > 0. \tag{14.18}$$

Let us summarize the stability and hyperbolicity conditions for linear isotropic materials

- Hyperbolicity: $(\lambda + 2\mu > 0,\ \mu > 0) \Leftrightarrow \mu, K \Leftrightarrow E, \nu.$

14.2.3 Steady state problem for linear isotropic material

Given a material in domain Ω_0. Suppose the material has stored energy function $W(X,F)$. Let $P = \frac{\partial W}{\partial F}$ be the first Piola stress. The boundary-value problem for such simple elasticity is to find solution $\mathbf{x}(X)$ which satisfies

$$\begin{cases} -\nabla_X P(X, \mathbf{x}(X)) = \rho_0(X)\mathbf{b}(\mathbf{x}(X)), \quad X \in \Omega_0, \\ \mathbf{x}(X) = \mathbf{x}_0(X), \quad X \in \Gamma_D, \\ P(X, \mathbf{x}(X)) \cdot N(X) = \mathbf{t}_0(X, \mathbf{x}(X)), \quad X \in \Gamma_N. \end{cases} \tag{14.19}$$

Here, N is the outer normal of Γ_N, $\partial\Omega_0 = \Gamma_D \cup \Gamma_N$, $\mathbf{x}_0$ is a prescribed Dirichlet and $\mathbf{t}$ is a prescribed traction.

Cf. Cialet pp. 295

Theorem 14.14. *Consider the boundary value problem for a linear isotropic material with* $W(\mathbf{e}) = \lambda Tr(\mathbf{e})^2 + 2\mu \mathbf{e}:\mathbf{e}$. *We assume*

$$\mu > 0, \quad \lambda > 0. \tag{14.20}$$

Then for the body force $\mathbf{b} \in L^{6/5}(\Omega_0)$ *and traction* $\mathbf{t} \in L^{4/3}(\Gamma_N)$*, there exists a unique solution* $\mathbf{u}$ *in*

$$V = \{\mathbf{v} \in H^1(\Omega_0) : \mathbf{v} = 0 \text{ on } \Gamma_D\}$$

14.3 Hyperbolic System of Nonlinear Elasticity in Lagrangian Coordinate

14.4 Steady State Solutions of Nonlinear Elasticity

14.4.1 Displacement-traction problems

Given a material in domain Ω_0. Suppose the material has stored energy function $W(X,F)$. Let $P = \frac{\partial W}{\partial F}$ be the first Piola stress. The boundary-value problem for such simple elasticity is to find solution $\mathbf{x}(X)$ which satisfies

$$\begin{cases} -\nabla_X P(X,\mathbf{x}(X)) = \rho_0(X)\mathbf{b}(\mathbf{x}(X)), \quad X \in \Omega_0, \\ \mathbf{x}(X) = \mathbf{x}_0(X), \quad X \in \Gamma_D, \\ P(X,\mathbf{x}(X)) \cdot N(X) = \mathbf{t}_0(X,\mathbf{x}(X)), \quad X \in \Gamma_N. \end{cases} \tag{14.21}$$

Here, N is the outer normal of Γ_N, $\partial\Omega_0 = \Gamma_D \cup \Gamma_N$, $\mathbf{x}_0$ is a prescribed Dirichlet and $\mathbf{t}$ is a prescribed traction.

Variation formulation of the steady-state problem See Cialet, Chapter 5.

14.4.2 Nonuniqueness

Ref. Cialet, Chapter 5.8.

- F. John's example [John 1964]:
- Noll [1978]
- Buckling of a rod

14.4.3 Polyconvexity and uniqueness of steady state problems

Definition 14.9. *Let $\mathcal{M}_n$ be the space of all $n \times n$ matrices. A function $W : \mathcal{M}_n \to \mathbb{R}$ is called polyconvex if $W(F)$ can be expressed as a convex function of the determinants of the submatrices of F.*

Theorem 14.15 (Ball)**.** *If $\mathbf{u}^n \rightharpoonup \mathbf{u}$ in $W^{1,p}(\Omega)$, then $M^n \rightharpoonup M$ in $L^{p/m}(\Omega)$, where M is the determinant of any $m \times m$ submatrix of $\partial\mathbf{u}/\partial\mathbf{x}$.*

Theorem 14.16. *If $W(\mathbf{e}) = \frac{1}{2}\langle A\mathbf{e}, \mathbf{e}\rangle$ is polyconvex, then W is strongly elliptic.*

In general, we have the following results: ???

polyconvexity $\Rightarrow$ quasi-convexity $\Rightarrow$ rank-1 convexity $\Leftrightarrow$???Strong ellipticity

quasi-convexity $\Leftrightarrow$ lower semi-continuity of the energy functional.

14.5 Stability of steady-state solution

TOBE CONTINUED

14.6 Incompressible elasticity

Consider incompressible linear simple elasticity

$$\rho_0 \partial_t^2 u^i + \frac{\partial p}{\partial X^i} = a_{ijkl} \frac{\partial^2 u^k}{\partial X^j \partial X^l}$$

$$\nabla_X \cdot \mathbf{u} = 0.$$

We look for solution of the form $u^i = \xi^i e^{\mathbb{i}(X\cdot\eta - \lambda t)}$, $p = \pi e^{\mathbb{i}(X\cdot\eta-\lambda t)}$. Plug these into the equations, we obtain

$$\begin{cases} A(\eta)\xi = \rho_0 \lambda^2 \xi - \mathbb{i}\pi\eta \\ \xi \cdot \eta = 0. \end{cases}$$

Given $\eta \in \mathbb{R}^3$, we look for solutions $(\xi, \pi) \in \mathbb{C}^3 \times \mathbb{C}$ and $\lambda \in \mathbb{C}$.

- Transverse wave: Given $\eta \in \mathbb{R}^3 \setminus \{0\}$, we look for $\xi \in \mathbb{R}^3$ and $\xi \perp \eta$ such that $A(\eta)\xi = \lambda_p \xi$. There are two such solutions, the transverse wave $(\xi_p, \lambda_p), p = 1, 2$. The corresponding $\pi = 0$.

- Longitudinal wave goes to infinity.

TOBE CONTINUED

Chapter 15

Membrane and Shell

15.1 Membrane

15.1.1 Surface geometry

We assume $X = (X^1, X^2)$ be two dimensional and $\mathbf{x} = (x^1, x^2, x^3)$ be three dimensional. The deformation gradient $F = \partial\mathbf{x}/\partial X$ is a 3×2 matrix. The metric $\langle d\mathbf{x}, d\mathbf{x}\rangle$ in $\mathbb{R}^3$ induces a metric

$$C_{\alpha\beta} = \frac{\partial \mathbf{x}}{\partial X^\alpha} \cdot \frac{\partial \mathbf{x}}{\partial X^\beta}$$

on the manifold $\Sigma_t = \{\mathbf{x}(t,\cdot)\}$. That is,

$$(d\mathbf{x}, d\mathbf{x}) = (F\,dX, F\,dX) = (F^T F\,dX, dX) = \sum_{jk} C_{\alpha\beta}\, dX^\alpha dX^\beta.$$

The matrix $C := F^T F$ is called the first fundamental form of the surface Σ_t. It is also the Cauchy-Green tensor of the deformation $\mathbf{x}(X)$. The area spanned by the vectors $\partial\mathbf{x}/\partial X^\alpha$ and $\partial\mathbf{x}/\partial X^\beta$ is

$$\sqrt{\langle \partial\mathbf{x}/\partial X^\alpha, \partial\mathbf{x}/\partial X^\alpha\rangle \langle \partial\mathbf{x}/\partial X^\beta, \partial\mathbf{x}/\partial X^\beta\rangle - \langle \partial\mathbf{x}/\partial X^\alpha, \partial\mathbf{x}/\partial X^\beta\rangle^2} = \sqrt{\det(F^T F)}.$$

Thus, we define $J = \sqrt{\det(F^T F)}$. Then $dS_t = J\,dS_0$.

15.1.2 Energy law of membranes

We want to define an elastic energy $W(F)$ on the manifold Σ_t.

1. **Frame-indifference and isotropicity conditions**

- Frame indifference condition reads

$$W(OF) = W(F), \quad \text{for all } O \in O(3).$$

- Isotropic condition is

$$W(FO_1) = W(F), \quad \text{for all } O_1 \in O(2).$$

2. Taking singular value decomposition of F, i.e. $F = O_{\mathbf{n}} \Lambda O_{\mathbf{N}}^T$, where $O_{\mathbf{n}} \in O(3)$, $O_{\mathbf{N}} \in O(2)$ and Λ is a 3×2 matrix

$$\Lambda = \begin{pmatrix} \lambda_1 & 0 \\ 0 & \lambda_2 \\ 0 & 0 \end{pmatrix},$$

we then have

$$W(F) = W(O_{\mathbf{n}} \Lambda O_{\mathbf{N}}^T) = W(\Lambda).$$

That is, W only depends on the singular values of F.

3. The singular values of F are the square roots of the eigenvalues of $C := F^T F$. Thus, the energy potential W can be expressed in terms of $(F^T F)_{2\times 2}$:

$$\overline{W}(C) := W(F) = W(\Lambda), \quad C = F^T F.$$

4. The energy W can be expressed in terms of principal invariants of $F^T F$: We define

$$\overline{W}(I_1, I_2) = \overline{W}(C) = W(F)$$

where

$$I_k := \iota_k(C), \quad \iota_1(C) := tr(C), \quad \iota_2(C) := det(C).$$

Examples

- Hookean law:

$$W(F) = \overline{W}(I_1, I_2) := \frac{H}{2} I_1 = \frac{H}{2} tr(F^T F) = \frac{H}{2} \sum_{\alpha=1}^{2} \sum_{i=1}^{3} |F_\alpha^i|^2,$$

where $H > 0$ is a constant. The corresponding Piola stress is

$$P_\alpha^i = \frac{\partial W}{\partial F_\alpha^i} = H F_\alpha^i, \alpha = 1, 2, \ i = 1, 2, 3.$$

- Minimal surface

$$W(F) := \sigma I_2 = \sigma\sqrt{\det(C)} = \sigma\sqrt{\det(F^TF)} = \sigma J.$$

Here, σ is a constant, called the surface tension. The energy is

$$\int_{\Omega_0} W(F)\,dX = \int_{\Omega_0} \sigma J\,dX = \int_{\Omega_t} \sigma\,dS_t$$

- Fabric:

$$W(F) := a(I_1-2)^2 + b(\sqrt{I_2}-1)^2 = a(tr(F^TF)-2)^2 + b(\sqrt{\det(F^TF)}-1)^2.$$

Note that when $F = I$ (i.e. the membrane is at rest), we have $tr(I) = 2$ and $\det I = 1$. Another fabric model is to decompose $C = F^TF$ into a trace part and a trace-free part. That is,

$$C = \frac{1}{2}tr(C)I + \left(C - \frac{1}{2}tr(C)I\right)$$

The first part is related to the expansion or shrinking of the surface, while the second is related to the distortion of the surface. We can design the energy to be

$$W(F) = a(tr(C)-2)^2 + b\left\|C - \frac{1}{2}tr(C)I\right\|_F^2. \tag{15.1}$$

The norm here is the Frobenius norm. [1]

Exercise Express (15.1) in terms of I_1 and I_2.

Piola stress $P^i_\alpha = \frac{\partial P}{\partial F^i_\alpha}$, $i = 1,2,3$, $\alpha = 1,2$.

Cauchy stress The Piola stress is convenient in the Lagrange coordinate system. In Eulerian coordinate system, the corresponding stress is the Cauchy stress σ.

$$\sigma = J^{-1}P\cdot F^T.$$

Since $P_{3\times 2}\cdot(F^T)_{2\times 3}$, we have $\sigma_{3\times 3}$ matrix.

[1] For membrane model, a reference book is: Statistical Mechanics of Membranes and Surfaces, 2nd edition, edited by D. Nelson, T. Piran and S. Weinberg (2004).

15.1.3 Equation of Motion

Lagrange formulation

The action is

$$\mathcal{S}[\mathbf{x}] = \int_0^T \int_{\Sigma_0} \frac{1}{2}\rho_0(X)|\dot{\mathbf{x}}(t,X)|^2 - W\left(\frac{\partial \mathbf{x}}{\partial X}\right) dX\, dt$$

The variation of the action with respective to the membrane motion $\mathbf{x}(t,X)$ gives the momentum equation. One can see the previous Euler-Lagrange equation is still the same:

$$\rho_0(X)\ddot{\mathbf{x}}(t,X) = \nabla_X \cdot P\left(\frac{\partial \mathbf{x}}{\partial X}\right)$$

where $P = W'$. Let $\mathbf{v}(t,X) := \dot{\mathbf{x}}(t,X)$. The equation of motion becomes

$$\begin{cases} \rho_0(X)\dot{v}^i(t,X) & = & \frac{\partial}{\partial X^\alpha} P^i_\alpha(F) \\ \dot{F}^i_\alpha & = & \frac{\partial v^i}{\partial X^\alpha} \end{cases}$$

Euler formulation

Let Σ_t be the membrane at time t. We assume that there is an 1-1 and onto mapping $\mathbf{x}(t,X)$ between Σ_0 and Σ_t. The Jacobian $J \neq 0$. The Cauchy stress σ is pullback of the Piola stress P by

$$\sigma_{3\times 3} = J^{-1} P_{3\times 2} \cdot (F^T)_{2\times 3}.$$

The equation of motion is

$$\rho \frac{D\mathbf{v}}{Dt} = \nabla_{\Sigma_t} \cdot \sigma.$$

Here, $\nabla_{\Sigma_t} \cdot$ is the surface divergence on the surface Σ_t.

Remarks

- If N is the normal of the membrane, we claim that $\sigma \cdot N = 0$.

15.2 Shells

In membrane or fabric, the internal energy is only a function of F, which involves only the first fundament form of the membrane. The stress only gives force in the tangential directions of the membrane, which is intrinsic.

However, for shells, there is a bending energy, which gives a normal force. This involves how the shell embedded into $\mathbb{R}^3$. This is extrinsic, which involves the second fundamental form of the surface. The plate is treated as a special case of shell.

To see how this second fundamental form comes out, let us consider a shell with thickness ε. We extend the material domain to

$$\tilde{\Sigma}_0 := \Sigma_0 \times (-\varepsilon, \varepsilon)$$

and

$$\tilde{\Sigma}_t := \tilde{\varphi}_t(\tilde{\Sigma}_0),$$

where

$$\tilde{\varphi}_t(X_1, X_2, X_3) := \tilde{\mathbf{x}}(X_1, X_2, X_3) := \mathbf{x}(X_1, X_2) + X_3 N(X_1, X_2),$$
$$N(X_1, X_2) = \frac{\frac{\partial \mathbf{x}}{\partial X_1} \times \frac{\partial \mathbf{x}}{\partial X_2}}{\|\frac{\partial \mathbf{x}}{\partial X_1} \times \frac{\partial \mathbf{x}}{\partial X_2}\|}.$$

The extended deformation gradient is

$$\begin{aligned}\tilde{F} = \frac{\partial \tilde{\mathbf{x}}}{\partial X} &= \left(\frac{\partial \mathbf{x}}{\partial X_1}, \frac{\partial \mathbf{x}}{\partial X_2}, N\right) + \left(X_3 \frac{\partial N}{\partial X_1}, X_3 \frac{\partial N}{\partial X_2}, 0\right) \\ &= (F, N) + \left(X_3 \frac{\partial N}{\partial X_1}, X_3 \frac{\partial N}{\partial X_2}, 0\right)\end{aligned}$$

The Cauchy-Green tensor is

$$\tilde{F}^T \tilde{F} = \begin{bmatrix} (F^T F)_{2\times 2} & 0 \\ 0^T & 1 \end{bmatrix} + X_3 \begin{bmatrix} \langle \frac{\partial N}{\partial X_1}, \frac{\partial \mathbf{x}}{\partial X_1} \rangle & \langle \frac{\partial N}{\partial X_1}, \frac{\partial \mathbf{x}}{\partial X_2} \rangle & 0 \\ \langle \frac{\partial N}{\partial X_2}, \frac{\partial \mathbf{x}}{\partial X_1} \rangle & \langle \frac{\partial N}{\partial X_2}, \frac{\partial \mathbf{x}}{\partial X_2} \rangle & 0 \\ 0 & 0 & 0 \end{bmatrix} + X_3^2 \begin{bmatrix} \langle \frac{\partial N}{\partial X_1}, \frac{\partial N}{\partial X_1} \rangle & \langle \frac{\partial N}{\partial X_1}, \frac{\partial N}{\partial X_2} \rangle & 0 \\ \langle \frac{\partial N}{\partial X_2}, \frac{\partial N}{\partial X_1} \rangle & \langle \frac{\partial N}{\partial X_2}, \frac{\partial N}{\partial X_2} \rangle & 0 \\ 0 & 0 & 0 \end{bmatrix}$$

The term $F^T F = C$ is the first fundamental form of the surface Σ_t, while the matrix

$$II := \begin{bmatrix} \langle \frac{\partial N}{\partial X_1}, \frac{\partial \mathbf{x}}{\partial X_1} \rangle & \langle \frac{\partial N}{\partial X_1}, \frac{\partial \mathbf{x}}{\partial X_2} \rangle \\ \langle \frac{\partial N}{\partial X_2}, \frac{\partial \mathbf{x}}{\partial X_1} \rangle & \langle \frac{\partial N}{\partial X_2}, \frac{\partial \mathbf{x}}{\partial X_2} \rangle \end{bmatrix}$$

is the second fundamental form of the surface Σ_t. The eigenvalues/eigenvector of II with respect to the first fundamental form are the principal curvatures and principal directions. It is the eigenvalues of the shape operator

$$S := C^{-1} II.$$

Let us denote them by κ_i, $\mathbf{v}_i$. The mean curvature $H := (\kappa_1 + \kappa_2)/2$. The Gaussian curvature is defined by $K := \kappa_1 \kappa_2$. An important fact found by Gauss is that K depends only on the first fundamental form C. It is called an intrinsic quantity, while H depends how the surface Σ_t is embedded in $\mathbb{R}^3$. It is called an extrinsic quantity.

Energy of a thin shell The energy W is a function of the invariants of $\tilde{F}^T\tilde{F}$. Let us write the invariants of $\tilde{F}^T\tilde{F}$ by $\tilde{I}_k$, $k = 1,2,3$. One can show that

$$\tilde{I}_k = I_k(F^TF) + X_3 I_k(S).$$

The energy can be decoupled into

$$W(\tilde{F}) = W_m(I_1(F^TF), I_2(F^TF)) + W_b(I_1(S), I_2(S)).$$

The first one involves the stretching of the surface. It is called the membrane energy. The second involves how the surface is embedded in the space. It is called the bending energy.

Models involves the second fundamental form

- Bending energy:
  $$W := \frac{1}{2}\int \kappa_1^2 + \kappa_2^2 \, dS$$
  It can also be written as
  $$W = 2\int H^2 - \frac{1}{2}K \, dS$$
  The Willmore energy is a penalized energy which is defined as
  $$W = \frac{1}{2}\int (\kappa_1 - \kappa_2)^2 = 2\int (H^2 - K)$$
  Since $\int K = 2\pi\chi(\Sigma)$, the Gauss-Bonnet theorem, we have the energy is essential a function of the mean curvature H.

- Vesicle model (Canham-Helfrich)
  $$W(F) = \frac{\kappa}{2}(H - H_0)^2 + \bar{\kappa}K.$$
  where H is the mean curvature and K the Gaussian curvature. In this formulation, W depends on the second fundamental form of the surface, which, by the intrincit property of surfaces, involves the derivative of F.

Part III

Complex Fluids

Chapter 16

Viscoelasticity

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- Online note: `https://www.viscoelasticity.info/what-is-viscoelasticity/`

16.1 Physical Phenomena of Viscoelastic media

Newtonian fluid model works remarkable well for fluids consisting of small molecules. Such fluid flow does not change the microstructure of its constituents. However, fluids with long flexible polymers behave very differently. The flow can alter microstructure of the fluid's constituents and the Newtonian fluid model is no longer valid. They can exhibit both viscous and elastic phenomena. Below, we introduce typical phenomena and give a definition of viscoelasticity. The main issue in this chapter is to characterize how materials response to the flow motions.

16.1.1 Basic phenomena of viscoelastic flows: Creep and Relaxation

Creep phenomenon Consider a rod-shape specimen (a viscoelastic material) in rest state (stress-free). At $t \geq 0$, we apply a tensile force to its two ends thus provide a stress σ_0 uniformly in time. We investigate the dynamics of its strain $\varepsilon(t)$. (See Youtube.) If the specimen is an elastic material, we will see that the strain $\varepsilon(t)$ is a constant function ε_0 in time. However, for viscoelastic material, it is found that the strain $\varepsilon(t)$ has an additional strain $\varepsilon(t) > \varepsilon_0$ which is an increasing function of t. Such a phenomenon (growing of the additional strain under a load uniformly in time) is called *creep.* See Figure 16.1. The materials are classified as asymptotic solids (resp. liquids) according to $\dot{\varepsilon}(\infty) = 0$ (resp. $\dot{\varepsilon}(\infty) \neq 0$). They are also classified as instantaneous elasticity (resp. liquid) based on $\varepsilon(0+) \neq 0$ (resp. $\varepsilon(0+) = 0$).

Relaxation phenomenon Consider another experiment, the rod-shape specimen is stretched to ε_0 at $t = 0$ then stays as ε_0 for all later time. We then measure the corresponding stress $\sigma(t)$. If it is a purely elastic material, then $\sigma(t) = \sigma_0$ for all later time. However, for an inelastic material, $\sigma(t)$ decreases monotonically and tends to σ_∞. Such a phenomenon is called *relaxation.*

Viscoelastic materials are materials that exhibits both creep and relaxation phenomena. Or equivalently, they exhibit both elastic and viscous response to flow motions.

16.1.2 Isothermal/Non-isothermal Viscoelasticity

Viscoelastic materials generally involve dissipation of energy, which leads to entropy production. Therefore, strictly speaking, viscoelastic behavior is not adiabatic. Thus, in the study of viscoelasticity, we usually classify it into isothermal case and non-isothermal case. In the stress response models discussed below are usually based on the isothermal assumption.

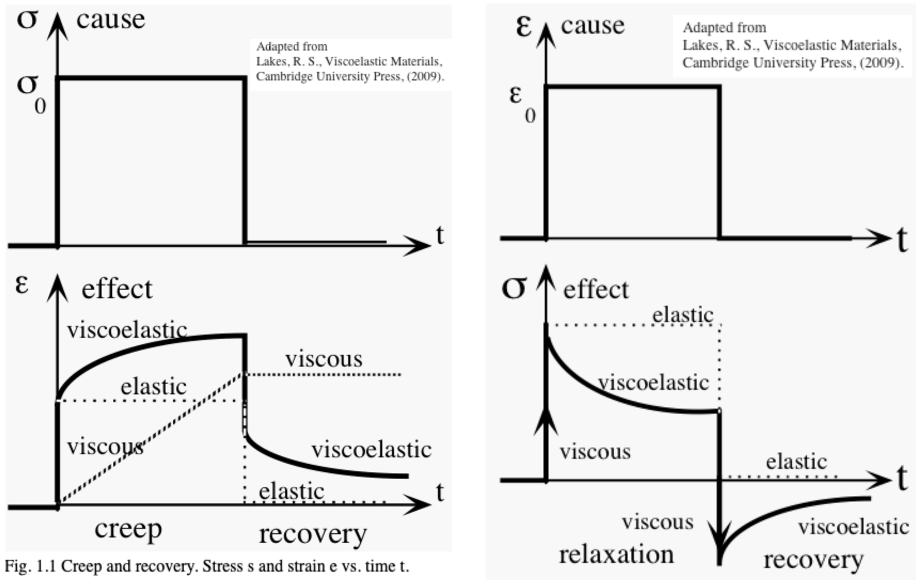

Figure 16.1: Creeping and Relaxation Phenomena. Copied from `http://silver.neep.wisc.edu/~lakes/VEnotes.html`

16.2 Phenomenological Models

16.2.1 Spring-dashpot models

The spring-dashpot model is based on the isothermal assumption. The elastic feature of rheology is modeled by spring, while its viscous feature is modeled by dashpot. The material response to the fluid motion reads

- $\sigma = G\varepsilon$ for elastic effect (the spring part),
- $\sigma = \eta\dot{\varepsilon}$ for viscous effect (the dashpot part).

Here, σ is the stress, ε, the strain, $\dot{\varepsilon}$ the strain rate, G the shear modulus, and η the viscosity.

Two possible ways to combine these two effects: in series, or in parallel. The formal leads to the Maxwell model. The latter gives the Kelvin-Voigat model. Below, let the subscript s and d stand for spring and dashpot, respectively.

Maxwell Model The Maxwell model is a *series connectio*n of spring and dashpot. Thus,

$$\varepsilon = \varepsilon_s + \varepsilon_d, \quad \sigma = \sigma_s = \sigma_d.$$

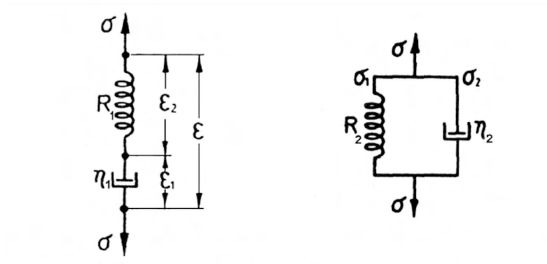

Figure 16.2: Spring-Dashpot models. Left: Maxwell model (solid-like liquids), right: Kelvin-Voigat model (fluid-like solids). Copied from
`https://www.researchgate.net/figure/Simple-two-element-spring-and-dashpo`
`fig1_234027378`

This gives

$$\dot{\varepsilon} = \dot{\varepsilon}_s + \dot{\varepsilon}_d = \frac{\dot{\sigma}_s}{G} + \frac{\sigma_d}{\eta}.$$

Thus, we get

$$\frac{\eta}{G}\dot{\sigma} + \sigma = \eta\dot{\varepsilon}.$$

For short time, the first term on the LHS is more important, the material behaves elastically. For long time, the second term is more important, the material behaves like a viscous liquid. So it is used to model *solid-like liquids.* The ratio $\lambda := \eta/G$ is the relaxation time from solid to fluid.

Kelvin-Voigat model The Kelvin-Voigat model is a parallel connection of spring and dashpot. Thus,

$$\varepsilon = \varepsilon_s = \varepsilon_d, \quad \sigma = \sigma_s + \sigma_d.$$

This gives

$$\sigma = G\varepsilon + \eta\dot{\varepsilon}.$$

For short time, the second term on RHS is more important. Thus, the material behaves like a viscous liquid. For long time, the first term on the RHS is more important. The material behaves like a solid. This model is used to model *fluid-like solids*.

16.2.2 Integral Models

16.3 Dumbbell Model (A Microscopic Model)

This part of note is mainly from:

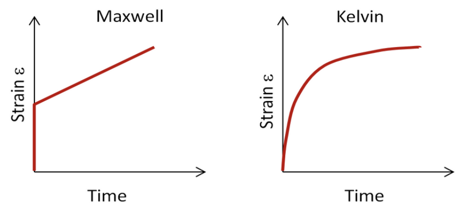

Figure 16.3: Spring-Dashpot models. Copied from `https://polymerdatabase.com/polymer%20physics/Maxwell-Kelvin.html`

- Yn-Hwang Lin with some corrections, Polymer Viscoelasticity, 2nd ed. (2011). Chapter 6.
- Doi and Edwards, The Theory of Polymer Dynamics (1988).

16.3.1 Model set up

1. The fluids are composed of solvent and polymers. For melt polymer, it only consists of polymers. Below, we shall discuss the latter case. But the theory can be extended to fluids with polymer and solvent.

2. We assume the system is *isothermal*.

3. The microscopic analysis is a probability distribution analysis for polymer chains inside a small box $\mathbf{x}+d\mathbf{x}$. Inside the box, a polymer chain is modeled by a dumbbell, which consists of two beads connected by a spring. The beads have mass m and positions $\mathbf{r}_1$ and $\mathbf{r}_2$. Here, $\mathbf{r}_i$, $i=1,2$ represent relative position vectors inside the box $\mathbf{x}+d\mathbf{x}$ with respective to $\mathbf{x}$. We call the configuration space of $\mathbf{r}$ at $\mathbf{x}$ a Fibre space $\mathscr{F}_\mathbf{x}$. In the present case, $\mathscr{F}_\mathbf{x}=\mathbb{R}^3$.

4. We *assume the microscopic fluid inside the box follows the macroscopic fluid*. Thus, the fluid velocity at $\mathbf{r}$ in $\mathscr{F}_\mathbf{x}$ is
$$\mathbf{v}(t,\mathbf{x})+\nabla\mathbf{v}(t,\mathbf{x})\mathbf{r}=\mathbf{v}+\mathbf{L}\mathbf{r}.$$

5. The interaction between the two beads is governed by a spring potential $\Phi(\mathbf{r}_1,\mathbf{r}_2)$, which is assumed to be a central potential (i.e. $\Phi(|\mathbf{r}_1-\mathbf{r}_2|)$). For example, the Hookean potential is
$$\Phi=\frac{3kT}{2R^2}|\mathbf{r}_2-\mathbf{r}_1|^2,$$

where R^2 denotes the mean-square distance between the two beads. The forces on bead 1 and bead 2 respectively are

$$-\frac{\partial \Phi}{\partial \mathbf{r}_1} = -\mathbf{F}, \quad -\frac{\partial \Phi}{\partial \mathbf{r}_2} = \mathbf{F}.$$

6. In addition, the beads are exerted by random forces from surroundings. Thus, $\mathbf{r}_1$ and $\mathbf{r}_2$ are random variables. It is assumed that these two random forces are independent.

7. Let $\Xi(t,\mathbf{x},\mathbf{r}_1,\mathbf{r}_2)$ be the probability density function (pdf) of the dumbbells. Let $\mathbf{r}_c := (\mathbf{r}_1+\mathbf{r}_2)/2$ and $\mathbf{r} = (\mathbf{r}_2-\mathbf{r}_1)/2$. Then the random variables $\mathbf{r}_c$ and $\mathbf{r}$ are independent. This implies that the probability density function Ξ is *separable*, namely,

$$\Xi(t,\mathbf{x},\mathbf{r}_1,\mathbf{r}_2)d\mathbf{r}_1\, d\mathbf{r}_2 = \phi(t,\mathbf{x},\mathbf{r}_c)f(t,\mathbf{x},\mathbf{r})2^3 d\mathbf{r}_c\, d\mathbf{r}.$$

Here, $\phi(t,\mathbf{x},\mathbf{r}_c)$ is the pdf of the centers of dumbbells, and $f(t,\mathbf{x},\mathbf{r})$ is the pdf of random variable $\mathbf{r}$.

16.3.2 Micro Dynamics – the Smoluchowski Equation

1. **Dynamics of the dumbbell.** From the above two forces, the beads satisfy the Langevin equation:

$$\frac{d}{dt}\left(m(\dot{\mathbf{r}}_i - \mathbf{v}_i)\right) + \zeta(\dot{\mathbf{r}}_i - \mathbf{v}_i) = -\nabla_{\mathbf{r}_i}\Phi + \alpha \frac{dB_i}{dt}, \quad i = 1,2. \tag{16.1}$$

Here, $\mathbf{v}_i = \mathbf{v}(t,\mathbf{x}) + \mathbf{L}\mathbf{r}_i$ are the background flow velocity of the beads. $B_i(t)$ are two independent Brownian motions. Assuming small inertia, we thus neglect the inertia term and get the equation, called the damped Langevin equation

$$\zeta(\dot{\mathbf{r}}_i - \mathbf{v}_i) = -\nabla_{\mathbf{r}_i}\Phi + \alpha \frac{dB_i}{dt}, \quad i = 1,2. \tag{16.2}$$

Here, ζ is the damping coefficient, B_i are two independent Brownian motions. By the fluctuation-dissipation theory, the random force and the friction are balanced. This gives

$$\alpha^2 = 2\zeta k_B T,$$

where k_B is the Boltzmann constant and T is the temperature. Note that in this damped dynamics of the dumbbell, it only involves damping, a central forcing and a random forcing.

2. **Relative vector and center of mass** Let $\mathbf{r} := (\mathbf{r}_2 - \mathbf{r}_1)/2$ and $\mathbf{r}_c := (\mathbf{r}_1 + \mathbf{r}_2)/2$. Assuming f and Φ are functions of $r = |\mathbf{r}|$, we then get that the above equation (16.2) for the two beads is equivalent to

$$\begin{cases} \dot{\mathbf{r}} = \mathbf{L}\mathbf{r} + \frac{\mathbf{F}}{\zeta} + \sqrt{\frac{2k_BT}{\zeta}}\frac{dB}{dt}, \\ \dot{\mathbf{r}}_c = \mathbf{v} + \mathbf{L}\mathbf{r}_c + \sqrt{\frac{2k_BT}{\zeta}}\frac{dB_c}{dt}, \end{cases} \tag{16.3}$$

where B and B_c are two independent Brownian motions.

We shall assume the force is a central force, meaning $\Phi(|\mathbf{r}_2 - \mathbf{r}_1|)$. The force

$$\mathbf{F}(\mathbf{r}) := \nabla_{\mathbf{r}}\Phi(|\mathbf{r}|).$$

Note that the center of mass follows the fluid flow without the internal forcing because the central forces are cancelled at the center of mass.

3. **Flux velocities** With the diffusion term in (16.3), the polymer particles will diffuse from higher concentration region to lower concentration region. According to Fick's law, the diffusion velocity is [1]

$$-\frac{k_BT}{\zeta}\frac{\nabla f}{f}.$$

Thus, the *flux velocities* of $\mathbf{r}_c$ and $\mathbf{r}$ are

$$\begin{cases} \dot{\mathbf{r}}_{c,f} := \mathbf{v} + \mathbf{L}\mathbf{r}_c - \frac{k_BT}{\zeta}\frac{\nabla_{\mathbf{r}_c}\phi}{\phi} \\ \dot{\mathbf{r}}_f := \mathbf{L}\mathbf{r} - \frac{1}{\zeta}\nabla_{\mathbf{r}}\Phi - \frac{k_BT}{\zeta}\frac{\nabla_{\mathbf{r}}f}{f}. \end{cases} \tag{16.4}$$

4. **The pdf is separable** From the conservation of polymer particles, the equation for the pdf Ξ is governed by:

$$\dot{\Xi} + \partial_{\mathbf{r}_1} \cdot (\dot{\mathbf{r}}_{1,f}\Xi) + \partial_{\mathbf{r}_2} \cdot (\dot{\mathbf{r}}_{2,f}\Xi) = 0.$$

By changing variables from $(\mathbf{r}_1, \mathbf{r}_2)$ to $(\mathbf{r}_c, \mathbf{r})$, we get

$$\begin{aligned} \dot{\Xi} &= -\partial_{\mathbf{r}_1} \cdot (\dot{\mathbf{r}}_{1,f}\Xi) - \partial_{\mathbf{r}_2} \cdot (\dot{\mathbf{r}}_{2,f}\Xi) \\ &= -\partial_{\mathbf{r}_c} \cdot \left(\dot{\mathbf{r}}_{c,f}\Xi\right) - \partial_{\mathbf{r}} \cdot (\dot{\mathbf{r}}_f\Xi). \end{aligned}$$

Recall Ξ is separable: $\Xi = \phi(t, \mathbf{x}, \mathbf{r}_c) f(t, \mathbf{x}, \mathbf{r})$. We obtain

$$(\phi(\mathbf{r}_c) f(\mathbf{r}))^{\cdot} = -\partial_{\mathbf{r}_c} \cdot (\dot{\mathbf{r}}_{c,f}\phi(\mathbf{r}_c) f(\mathbf{r})) - \partial_{\mathbf{r}} \cdot (\dot{\mathbf{r}}_f \phi(\mathbf{r}_c) f(\mathbf{r}))$$

---

[1] The diffusion coefficient $D = k_BT/\zeta$ can also be obtained from equilibrium state where the drift and diffusion are balanced and the distribution f obey the Gibbs distribution.

$$\Rightarrow \quad \dot{\phi} f + \phi \dot{f} = -\partial_{\mathbf{r}_c} \cdot (\dot{\mathbf{r}}_{c,f}\phi) f - \partial_{\mathbf{r}} \cdot (\dot{\mathbf{r}}_f f)\phi.$$
$$\Rightarrow \quad \left(\dot{\phi} + \partial_{\mathbf{r}_c} \cdot (\dot{\mathbf{r}}_{c,f}\phi)\right) f + \left(\dot{f} + \partial_{\mathbf{r}} \cdot (\dot{\mathbf{r}}_f f)\right)\phi = 0.$$

By separating the variables $\mathbf{r}_c$ and $\mathbf{r}$, we get

$$\begin{cases} \dot{\phi} + \partial_{\mathbf{r}_c} \cdot (\dot{\mathbf{r}}_{c,f}\phi) = 0, \\ \dot{f} + \partial_{\mathbf{r}} \cdot (\dot{\mathbf{r}}_f f) = 0. \end{cases} \tag{16.5}$$

5. **The governing equation for the pdf of center of mass** $\phi(t,\mathbf{x},\mathbf{r}_c)$ To derive the equation for ϕ, we plug (16.4) into the conservation laws (16.5) to get

$$\begin{aligned} \partial_{\mathbf{r}_c} \cdot \left(\dot{\mathbf{r}}_{c,f}\phi\right) &= \partial_{\mathbf{r}_c} \cdot \left(\left(\mathbf{v} + \mathbf{L}\mathbf{r}_c - \frac{k_B T}{\zeta}\frac{\partial_{\mathbf{r}_c}\phi}{\phi}\right)\phi\right) \\ &= (\nabla_{\mathbf{x}} \cdot \mathbf{v})\phi - \frac{k_B T}{\zeta}\partial^2_{\mathbf{r}_c}\phi. \end{aligned}$$

Thus, from (16.5), the equation for ϕ is

$$\boxed{(\partial_t + \mathbf{v}\cdot\nabla_{\mathbf{x}})\phi + (\nabla_{\mathbf{x}}\cdot\mathbf{v})\phi - \frac{k_B T}{\zeta}\partial^2_{\mathbf{r}_c}\phi = 0.} \tag{16.6}$$

This is the *Smoluchowski equation* for $\mathbf{r}_c$. Note that the time derivative "dot" is the material derivative $\partial_t + \mathbf{v}\cdot\nabla_{\mathbf{x}}$. Let us integrate this equation in $\mathbf{r}_c$ over the whole $F_{\mathbf{x}}$, call $\int \phi(t,\mathbf{x},\mathbf{r}_c)\,d\mathbf{r}_c$ by $n(t,\mathbf{x})$, which is the number of polymer particles in $\mathbf{x}+d\mathbf{x}$. Then the equation for $n(t,\mathbf{x})$ is

$$\partial_t n + \mathbf{v}\cdot\nabla_{\mathbf{x}} n + (\nabla_{\mathbf{x}}\cdot\mathbf{v})n = 0.$$

This is the continuity equation for the polymer density $\rho := mn(t,\mathbf{x})$.

6. **The governing equation for the pdf of relative vector** $f(t,\mathbf{x},\mathbf{r})$ To derive an equation for $f(t,\mathbf{x},\mathbf{r})$, using (16.4), we get

$$\partial_{\mathbf{r}} \cdot (\dot{\mathbf{r}}_f f) = \partial_{\mathbf{r}} \cdot \left(\mathbf{L}\mathbf{r} f + \frac{\mathbf{F}}{\zeta} f - \frac{kT}{\zeta}\partial_{\mathbf{r}} f\right).$$

Plug it into (16.5), we arrive at

$$\boxed{\partial_t f + \mathbf{v}\cdot\partial_{\mathbf{x}} f + \partial_{\mathbf{r}}\cdot(\mathbf{L}\mathbf{r} f) = \partial_{\mathbf{r}}\cdot\left(-\frac{\mathbf{F}}{\zeta} f + \frac{kT}{\zeta}\partial_{\mathbf{r}} f\right).} \tag{16.7}$$

This is called the *Smoluchowski equation* for $\mathbf{r}$. [2]

[2] If we define $\mathbf{r} = \mathbf{r}_2 - \mathbf{r}_1$, then we should get

$$\partial_t f + \mathbf{v}\cdot\partial_{\mathbf{x}} f + \partial_{\mathbf{r}}\cdot(\mathbf{L}\mathbf{r} f) = \partial_{\mathbf{r}}\cdot\left(-\frac{2\mathbf{F}}{\zeta} f + \frac{2kT}{\zeta}\partial_{\mathbf{r}} f\right).$$

16.3.3 Constitutive relation – Kramer's formula

Constitutive Equation We shall derive a stress formula for the dumbbell model.

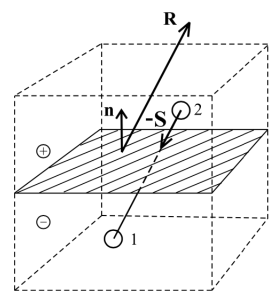

Figure 16.4: Copied from the book by Yn-Hwang Lin, Polymer Viscoelasticity.

1. Let $\mathbf{x} \in \Omega$. We consider a small plane $dA \subset \Omega$ through $\mathbf{x}$ with normal ν ($\mathbf{n}$ is Figure 16.4) pointing from $-$ side to $+$ side. The polymer stress σ_p contains two parts:
   - $\sigma_p^c \cdot \nu$: the tensile force from spring-connector;
   - $\sigma_p^b \cdot \nu$: bead momentum across the surface.
2. **Stress from spring-connector:** We consider a box $\mathbf{x} + d\mathbf{x}$ which has n polymer particles. Assuming they are uniformly distributed in the box. [3] Then, the side length of the cube is $n^{-1/3}$ and the cross-section $dA = n^{-2/3}$. The probability that the dumbbell with direction $\mathbf{r}$ will cross the plane dA is
$$\frac{\text{Projection of } \mathbf{r} \text{ along } \nu}{\text{side length}} = \frac{|\nu \cdot \mathbf{r}|}{n^{-1/3}}.$$
   If the distribution of configuration $\mathbf{r}$ is $f(t, \mathbf{x}, \mathbf{r})$, then the above probability should be
$$\frac{|\nu \cdot \mathbf{r}|}{n^{-1/3}} f(t, \mathbf{x}, \mathbf{r}) d\mathbf{r}.$$
   Now, suppose bead 2 is on $(+)$ side. That is, $\mathbf{r}$ is on the same side of ν. In this case, $|\nu \cdot \mathbf{r}| = \nu \cdot \mathbf{r}$. The force on bead 2 is $-\mathbf{F}$. The force exerted on the $(+)$ side by the spring is $+\mathbf{F}$. Next, suppose bead 1 is on $(+)$ side. That is, $\mathbf{r}$ is on the opposite side of ν. In this case, $|\nu \cdot \mathbf{r}| = -\nu \cdot \mathbf{r}$. The force on bead 1 is $\mathbf{F}$. Thus, the force exerted

[3] This argument may not need. We can still use the pdf ϕ for the center-of-mass to argue the whole thing. The pdf ϕ is a Gaussian distribution.

on the $(+)$ side from the spring is $-\mathbf{F}$. In both cases, the force exerted on the $(+)$ side from dumbbell connectors is

$$n^{1/3}\int \nu\cdot\mathbf{r}\mathbf{F}f(t,\mathbf{r})\,d\mathbf{r}.$$

Dividing this by the area $dA = n^{-2/3}$, we get the tensile force per unit area is

$$n\nu\cdot\int \mathbf{r}\mathbf{F}f(t,\mathbf{r})\,d\mathbf{r} = n\langle\mathbf{r}\mathbf{F}\rangle.$$

Thus,

$$\boxed{\sigma_p^c = n\langle\mathbf{r}\mathbf{F}\rangle.}$$

3. **Stress from momenta of dumbbell beads:** The number of bead 1 passing through a surface dA with normal ν per unit time and per unit area is

$$n(\dot{\mathbf{r}}_1-\mathbf{v}_1)\cdot\nu$$

The momenta that bead 1 carries is

$$n[(\dot{\mathbf{r}}_1-\mathbf{v}_1)\cdot\nu]m(\dot{\mathbf{r}}_1-\mathbf{v}_1).$$

The probability distribution of $\dot{\mathbf{r}}_1-\mathbf{v}_1$ is a Gaussian

$$\Xi(\xi_1) = \frac{\exp\left(-m|\xi_1|^2/2kT\right)}{\iint\exp\left(-m|\xi_1|^2/2kT\right)}, \quad \xi_1 := \dot{\mathbf{r}}_1-\mathbf{v}_1.$$

because

$$\dot{\mathbf{r}}_1-\mathbf{v}_1 = \frac{2kT}{\zeta}\frac{dB_1}{dt},$$

where B_1 is the Brownian motion. The expectation of momentum flux is

$$nm\int[(\dot{\mathbf{r}}_1-\mathbf{v}_1)(\dot{\mathbf{r}}_1-\mathbf{v}_1)\cdot\nu]\Xi(\dot{\mathbf{r}}_1)\,d\dot{\mathbf{r}}_1.$$

For the stress from momentum flux of bead 2, we can get similar formula. Thus, the material responses to the momentum change is

$$\sigma_p^b = -2n\iint[m((\dot{\mathbf{r}}_1-\mathbf{v}_1)(\dot{\mathbf{r}}_1-\mathbf{v}_1)]\,\Xi(\dot{\mathbf{r}}_1)\,d\dot{\mathbf{r}}_1 = -2nkTI.$$

4. **Kramer's formula for polymeric stress**: Combining the formulae of σ_p^c and σ_p^b, we get

$$\boxed{\sigma_p = -2nkTI + n\langle\mathbf{r}\mathbf{F}\rangle.} \tag{16.8}$$

This is called the Kramer's formula for the stress.

5. **Remark.** In the next section, we shall derive the Kramer's formula from micro dynamics. There, the Kramer's formula reads $\sigma_p = -nkTI + n\langle \mathbf{rF}\rangle$. The discrepancy is due to the following reason. Here, σ_p^b counts the randomness contribution from both bead 1 and bead 2, equivalently, randomness of $\mathbf{r}$ and $\mathbf{r}_c$. In the next section, we treat $\mathbf{r}$ as a random variable in an abstract configuration space $\mathscr{F}_{\mathbf{x}}$, and thus neglect the contribution of randomness of the centra $\mathbf{r}_c$. In fact, we should put in the contribution of momentum change from the center-of-mass, or treat such kinds of contribution in abstract way.

The second moment or the conformation tensor For the Hookean potential, the force is

$$\mathbf{F} = \frac{3kT}{R^2}\mathbf{r},$$

the Kramer's formula (16.8) involves to compute $\langle \mathbf{rr}\rangle$. This quantity is called the conformation tensor. We shall use the Smoluchowski equation to derive an evolution equation for the conformation tensor.

1. Define the conformation tensor $\mathbf{c}$ to be the second moment $\langle \mathbf{rr}\rangle$

$$\mathbf{c}(t,\mathbf{x}) := \langle \mathbf{rr}\rangle(t,\mathbf{x}) := \int \mathbf{rr} f(t,\mathbf{x},\mathbf{r})\, d\mathbf{r}.$$

2. Derive an evolution equation for the conformation tensor $\mathbf{c}$. We multiply (16.7) by $M := \mathbf{rr}$, then integrate it in $\mathbf{r}$:

$$\int \mathbf{rr}\left[\partial_t f + \mathbf{v}\cdot\partial_{\mathbf{x}} f + \partial_{\mathbf{r}}\cdot(\mathbf{Lr}f)\right] d\mathbf{r} = \int \mathbf{rr}\left[\partial_{\mathbf{r}}\cdot\left(-\frac{\mathbf{F}}{\zeta}f + \frac{kT}{\zeta}\partial_{\mathbf{r}} f\right)\right] d\mathbf{r} \qquad (16.9)$$

We use the following calculations:

$$\begin{aligned}
&\int \mathbf{rr}\partial_t f\, d\mathbf{r} = \partial_t\langle \mathbf{rr}\rangle \\
&\int \mathbf{rr}(\mathbf{v}\cdot\nabla_{\mathbf{x}} f)\, d\mathbf{r} = \mathbf{v}\cdot\nabla_{\mathbf{x}}\langle \mathbf{rr}\rangle \\
&\int \mathbf{rr}\nabla_{\mathbf{r}}(\mathbf{Lr}f)\, d\mathbf{r} = -\mathbf{L}\langle \mathbf{rr}\rangle - \langle \mathbf{rr}\rangle\mathbf{L}^T \\
&\int \mathbf{rr}\nabla_{\mathbf{r}}\cdot\left(\frac{1}{\zeta}\nabla_{\mathbf{r}}\Phi f\right) d\mathbf{r} = -\frac{2}{\zeta}\langle(\nabla_{\mathbf{r}}\Phi)\mathbf{r}\rangle \\
&\int \mathbf{rr}\nabla_{\mathbf{r}}\cdot\left(\frac{k_BT}{\zeta}\nabla_{\mathbf{r}} f\right) d\mathbf{r} = \frac{2k_BT}{\zeta}I,
\end{aligned}$$

where the third equation in component form is

$$\begin{aligned}\int r_i r_j \partial_{r_k}(L^k_l r_l f)\,dr &= -\int \left(\delta_{ik} r_j L^k_l r_l f + \delta_{kJ} r_i L^k_l r_l f\right) dr\\ &= -\int \left(L^i_l r_l r_j f + L^j_l r_i r_l f\right) dr\end{aligned}$$

Finally, equation (16.9) reads

$$\partial_t \langle \mathbf{rr} \rangle + \mathbf{v} \cdot \partial_{\mathbf{x}} \langle \mathbf{rr} \rangle - (\nabla \mathbf{v}) \cdot \langle \mathbf{rr} \rangle - \langle \mathbf{rr} \rangle \cdot (\nabla \mathbf{v})^T = \frac{2kT}{\zeta} \left(I - \frac{3}{R^2} \langle \mathbf{rr} \rangle \right).$$

In terms of the conformation tensor, it is

$$\boxed{\mathbf{c}_{(1)} := \partial_t \mathbf{c} + \mathbf{v} \cdot \partial_{\mathbf{x}} \mathbf{c} - (\nabla \mathbf{v}) \cdot \mathbf{c} - \mathbf{c} \cdot (\nabla \mathbf{v})^T = \frac{2kT}{\zeta} \left(I - \frac{3}{R^2} \mathbf{c} \right).} \tag{16.10}$$

Here, we abbreviate the left-hand side of (16.10) by $\mathbf{c}_{(1)}$, called the upper convected derivative of the tensor $\mathbf{c}$. Mathematically, it is the Lie derivative of the tensor $\mathbf{c}$ which has type $(2,0)$ (i.e. vector tensor product vector). It is nothing but the time-derivative of the tensor $\mathbf{c}$ with fixed Lagrangian coordinate X. Thus, this evolution equation is a relaxation equation for $\mathbf{c}$. It will relax to $\frac{R^2}{3} I$ as $t \to \infty$, due to the damping, spring forcing and random forcing.

3. Kramer's formula in terms of $\mathbf{c}$. From (16.8), we can express σ_p in terms of $\mathbf{c}$:

$$\boxed{\sigma_p = -2nkTI + \frac{3nkT}{R^2} \mathbf{c}.} \tag{16.11}$$

The first term is from the random forcing to the two beads. The second is from the connecting force between the two beads, which is deterministic. We can also express it as

$$\sigma_p = -nkTI + \tau_p, \quad \tau_p = -nkTI + \frac{3nkT}{R^2} \mathbf{c}.$$

The first term is from the random forcing to the center-of-mass of the dumbbell, whereas the second term is from the spring, which is also random.

Pressure and extra stress Sometimes, we separate pressure from the total stress. The pressure is the stress at equilibrium. The rest is called an extra stress. [4]

[4] It is not necessary to separate pressure from the stress. In fluids, the extra stress is only a function of deviatoric strain. In that case, such decomposition is necessary. Such extra stress is also called the deviatoric stress. In fluids, the trace of the deviatoric stress is zero.

1. The polymer stress σ_p can be decomposed into

$$\sigma_p = -p_p I + \tau_p,$$

where $-p_p I$ is the stress at equilibrium, and τ_p is the extra stress.

2. The equilibrium is the state where $\nabla \mathbf{v} = 0$. At equilibrium, $\mathbf{c}_{(1)} = 0$, we obtain

$$\mathbf{c}_{eq} = \frac{R^2}{3} I. \tag{16.12}$$

Thus,

$$\sigma_{p,eq} := -p_p I = -2nkTI + \frac{3nkT}{R^2}\mathbf{c}_{eq} = -nkTI.$$

Hence,

$$p_p = nkT.$$

And the polymeric extra stress is

$$\tau_p = \sigma_p + p_p I = -nkTI + \frac{3nkT}{R^2}\mathbf{c}. \tag{16.13}$$

This is the Kramer's formula for the extra stress.

Evolution equation for the extra stress Let us take the upper convected derivative on (16.13) to get

$$\tau_{p(1)} = \frac{3nkT}{R^2}\mathbf{c}_{(1)} - nkTI_{(1)} \tag{16.14}$$

Note that

$$-I_{(1)} = (\partial_t + \mathbf{v}\cdot\nabla)(-I) + (\nabla\mathbf{v})I + I(\nabla\mathbf{v})^T = \nabla\mathbf{v} + (\nabla\mathbf{v})^T := \dot{\varepsilon}.$$

By eliminating $\mathbf{c}_{(1)}$ from (16.14) and using (16.10) (16.13), we get

$$\boxed{s\tau_{p(1)} + \tau_p = \eta_p \dot{\varepsilon},} \tag{16.15}$$

where

$$s = \frac{\zeta R^2}{12kT}, \quad \eta_p = nkTs. \tag{16.16}$$

It means that the extra stress will relax to the strain rate $\dot{\varepsilon}$ with relaxation time s. Here, η_p is the polymer viscosity. This is exactly the Maxwell model.

16.4 Micro-Macro Model

16.4.1 Fibre bundle model for rheology

Fibre space We introduce a fibre space $\mathscr{F}_{\mathbf{x}}$ which describes all possible micro configurations at a position $\mathbf{x}$. The element in the fiber space is denoted by $\mathbf{r}$. It represents a micro structure at $\mathbf{x}$. For instance, it is the generalized coordinate of a polymer. In the dumbbell model, the polymer is modeled by a dumbbell with two beads connected by a spring. And $\mathbf{r}$ represents the end-to-end vector of the dumbbell. The fibre bundle $\cup_{\mathbf{x}\in\Omega}\mathscr{F}_{\mathbf{x}}$ forms the configuration space.

Configuration Space and Fibre bundle Consider a region Ω in $\mathbb{R}^3$ and a fiber bundle with base space Ω. The fiber represents some micro configuration. The micro variable is denoted by $\mathbf{r}$ at time t (Eulerian coordinate) and by R at time 0 (Lagrangian coordinate).

16.4.2 Homogeneous micro model

Ref. Doi and Edwards, Chapter 2, Brownian Motion.

Fibre Dynamics We associate $\mathbf{r}$ a potential function $\Phi(\mathbf{r})$, representing interaction potential of polymers. For instance,

$$\Phi(\mathbf{r}) = \frac{3k_BT}{2R^2}|\mathbf{r}|^2$$

is the Hookean model, where R^2 is the mean square distance of the dumbbell. In this micro configuration space, $\mathbf{r}$ satisfies the Langevin equation:

$$m\ddot{\mathbf{r}} + \zeta\dot{\mathbf{r}} + \nabla_{\mathbf{r}}\Phi = \alpha\frac{dB}{dt}.$$

Here, m is the mass, ζ is the damping coefficient, B is the Brownian motion, and α is the strength of the random force. Assuming small inertia, we neglect the inertia term and get the damped Langevin equation

$$\zeta\dot{\mathbf{r}} + \nabla_{\mathbf{r}}\Phi = \alpha\frac{dB}{dt}.$$

According to the fluctuation-dissipation theorem, the strength of the random force and the friction are balanced. This gives

$$\alpha^2 = 2\zeta k_BT, \tag{16.17}$$

where k_B is the Boltzmann constant and T is the temperature. Thus, the damped Langevin equation models the fiber dynamics. It is a stochastic differential equation is usually expressed as

$$\boxed{d\mathbf{r} = -\frac{1}{\zeta}\nabla_{\mathbf{r}}\Phi(\mathbf{r})dt + \sqrt{\frac{2k_BT}{\zeta}}dB.} \tag{16.18}$$

Microscopic pdf and its dynamics The microscopic state is described by a probability density function (pdf) $f(t,\mathbf{r})$ of the random variable $\mathbf{r}(t)$ of (16.18). [5] By applying Ito's formula to (16.18), the pdf f satisfies the Fokker-Planck equation:

$$\boxed{\dot{f} + \nabla_{\mathbf{r}}\cdot[-\frac{1}{\zeta}(\nabla_{\mathbf{r}}\Phi)f] = \frac{k_BT}{\zeta}\triangle_{\mathbf{r}} f.} \tag{16.19}$$

This is also known as the Kolmogorov forward equation. Its derivation is shown in the Appendix of this Chapter. Note that $\int f\,d\mathbf{r} = const$. We also note that this equation can be written as the following conservative transport equation

$$\dot{f} + \nabla_{\mathbf{r}}\cdot(\mathbf{v}_f f) = 0, \tag{16.20}$$

where

$$\mathbf{v}_f := -\frac{1}{\zeta}\left(\nabla_{\mathbf{r}}\Phi + k_BT\frac{\nabla_{\mathbf{r}}f}{f}\right) = -\frac{1}{\zeta}\nabla_{\mathbf{r}}\left(\Phi + k_BT\ln f\right). \tag{16.21}$$

The terms on the right-hand side have the following interpretation:

- The first term $-\nabla_{\mathbf{r}}\Phi$ is called the drift velocity. It drive the fibers from high potential to low potential.
- The second term $-k_BT\frac{\nabla_{\mathbf{r}}f}{f}$ is called the diffusion velocity. It moves the fibers from high density area to low density area.

The dynamics of the particle is a competition between the drift and the diffusion.

Free energy Let us define the Helmholtz free energy density

$$A(f) := \Phi f + k_BT f\ln f,$$

and the specific Helmholtz energy (per unit mass)

$$\mathscr{A}[f] = \int A(f)\,d\mathbf{r}.$$

[5] $f(t,\mathbf{r})\,d\mathbf{r}$ is the probability that $\mathbf{r}(t)$ of (16.18) lies in $\mathbf{r}\,d\mathbf{r}$.

Here, $U = \Phi f$ is the internal energy density. The term $-k_B f \ln f$ is the entropy of the fiber. the Helmholtz free energy density in the fiber is $A = -TS + U$. The free energy of the fiber is the integral of $A(f)$.

From $\mathscr{A}[f]$, we define the chemical potential

$$\mu := \frac{\delta \mathscr{A}}{\delta f} = A_f = k_B T\,(\ln f + 1) + \Phi.$$

Then the flux velocity $\mathbf{v}_f$ is

$$\mathbf{v}_f := -\frac{1}{\zeta}\nabla_{\mathbf{r}}\mu = -\frac{1}{\zeta}\nabla_{\mathbf{r}}A_f. \tag{16.22}$$

Thus, $\mathbf{v}_f$ is small when the damping (friction) coefficient ζ is large.

Dissipation of free energy Multiplying the Fokker-Planck equation (16.20) by A_f

$$A_f \cdot \left(\dot{f} - \nabla_{\mathbf{r}} \cdot \left(f\frac{1}{\zeta}\nabla_{\mathbf{r}}A_f\right) = 0\right)$$

integrating it in $\mathbf{r}$ over the whole fibre space, we get

$$\int A_f\dot{f} - \frac{1}{\zeta}A_f\nabla_{\mathbf{r}} \cdot \left(f\nabla_{\mathbf{r}}A_f\right)\,d\mathbf{r} = 0.$$

Using integration-by-part, one can show that the dynamics (16.19) is a dissipation process:

$$\frac{d}{dt}\int A(f)\,d\mathbf{r} = -\frac{1}{\zeta}\int f|\nabla_{\mathbf{r}}A_f|^2\,d\mathbf{r} = -\frac{1}{\zeta}\int f|\mu|^2\,d\mathbf{r} < 0,$$

which means that the free energy decreases in time, and dissipates to 0 as $t \to \infty$.

Equilibrium distribution As $t \to \infty$, $\mathscr{A}[f(t)] \to \min_f \mathscr{A}[f]$. Note that $\mathscr{A}[f]$ is strictly convex in f. The minimum of $\mathscr{A}[f]$ is unique. It is an equilibrium state. Let us denote it by f_{eq}. The dynamics of the Fokker-Planck equation $f(t) \to f_{eq}$ as $t \to \infty$.

At equilibrium,

$$\frac{\delta \mathscr{A}}{\delta f}[f_{eq}] = 0.$$

That is

$$k_B T f_{eq}\ln f_{eq} + \Phi f_{eq} = 0.$$

Solving this equation, we get an explicit form of f_{eq}:

$$f_{eq}(\mathbf{r}) = \frac{\exp\left(-\Phi(\mathbf{r})/k_B T\right)}{\int \exp\left(-\Phi(\mathbf{r})/k_B T\right)\,d\mathbf{r}}. \tag{16.23}$$

More precisely, we have the following theorem.

Theorem 16.17. *When Φ is strictly convex and $\Phi(\mathbf{r}) \to \infty$ as $\mathbf{r} \to \infty$, then $f(t) \to f_{eq}$ as $t \to \infty$ exponentially fast.*

At equilibrium, it is a state that the diffusion of $\mathbf{r}$ is balanced with the drift term $\nabla\Phi$. The pdf f_{eq} is called the Gibbs distribution.

Fluctuation-dissipation relation Recall that in (16.17), we make an assumption that α, ζ and the fluctuation k_BT are related by (16.17). In the derivation of dissipation limit, we use the parameters ζ and k_BT. The resulting equilibrium f_{eq} is given by the Gibbs distribution (16.23). We can repeat the same procedure using the parameter ζ and α. The resulting f_{eq} is (16.23) with k_BT replaced by $\alpha^2/(2\zeta)$. Thus, at equilibrium, the balance between random force αdB and the friction $\nabla\Phi/\zeta$ gives the equilibrium state (fluctuation is characterized in terms of k_BT).

16.4.3 Microscopic Model – the Smoluchowski Equation

Deformation of micro configuration As the micro dynamics is embedded in a macro flow, it is assumed that *the dynamics of the micro configuration follows the macroscopic deformation*. That is,

$$\mathbf{r} = FR = \frac{\partial \mathbf{x}^i}{\partial X^\alpha}(t,X)R^\alpha. \tag{16.24}$$

Here, R is the Lagrangian coordinate of the micro state variable. The volume form of the microscopic space satisfies

$$d\mathbf{r} = JdR.$$

Probability density function The dynamics of the micro structure is described by (16.18).

$$\dot{\mathbf{r}} = \mathbf{L}\mathbf{r} - \frac{1}{\zeta}\nabla_{\mathbf{r}}\Phi(\mathbf{r}) + \sqrt{\frac{2k_BT}{\zeta}}\frac{dB}{dt}. \tag{16.25}$$

We assume that the microscopic random variable $\mathbf{r}$ is independent of the macroscopic variable $\mathbf{x}$. This implies that the probability distribution function (pdf) of the polymer at $\mathbf{x}+d\mathbf{x}$ is

$$n_p(t,\mathbf{x})\,d\mathbf{x} f(t,\mathbf{x},\mathbf{r})\,d\mathbf{r},$$

where n_p is the number of polymers in $\mathbf{x}+d\mathbf{x}$ and $f(t,\mathbf{x},\mathbf{r})$ is the microscopic probability density function for $\mathbf{r}$ with $\int f\,d\mathbf{r} = 1$. The polymer density is

$$\rho_p(t,\mathbf{x}) = mn_p(t,\mathbf{x}), \quad m \text{ is the polymer mass.}$$

Smoluchowski equation The Fokker-Planck equation (or the Kolmogorov forward equation) for the p.d.f. $f(t,\mathbf{x},\mathbf{r})$ corresponding to the dynamics (16.25) in the background flow $\mathbf{v}(t,x)$ is modified from (16.19) by replacing $\dot{f}$ by the material time-derivative $\partial_t f + \mathbf{v}\cdot\nabla_{\mathbf{x}} f$. It is

$$\boxed{\partial_t f + \mathbf{v}\cdot\nabla_{\mathbf{x}} f + \nabla_{\mathbf{r}}\cdot(\mathbf{L}\mathbf{r}f) = \nabla_{\mathbf{r}}\cdot\frac{1}{\zeta}[(\nabla_{\mathbf{r}}\Phi)f + k_B T\nabla_{\mathbf{r}} f].} \tag{16.26}$$

This equation is also called the Smoluchowski equation. This equation describes the dynamics of spatial dependent micro configuration. This micro dynamics depends on the macro fluid dynamics, which will be derived by the variational approach below.

16.4.4 Stress formula – Lagrangian approach

The trajectory of a parcel of polymer with initial position (X,R) is $(\mathbf{x}(t,X),\mathbf{r}(t,X,R))$, where $\mathbf{r}(t,X,R) = F(t,X)R$. The equation of motion of polymers will be derived by taking variation of action with respect to the path $\mathbf{x}$. The action is defined to be

$$\begin{aligned}
\mathcal{S}[\mathbf{x}] &= \mathscr{K}[\mathbf{x}] - \mathscr{U}[\mathbf{x}],\\
\mathscr{K}[\mathbf{x}] &:= \int_0^t\int \rho(t,\mathbf{x})\frac{1}{2}|\mathbf{v}(t,\mathbf{x})|^2\,d\mathbf{x}\,dt\\
\mathscr{A}[\mathbf{x}] &:= \int_0^t\iint \rho(t,\mathbf{x})A(f(t,\mathbf{x},\mathbf{r}))\,d\mathbf{r}\,d\mathbf{x}\,dt,\\
\mathscr{U}[\mathbf{x}] &:= TS[\mathbf{x}] + \mathscr{A}[\mathbf{x}]
\end{aligned}$$

- We consider the isothermal case. In this case, we use Helmholtz free energy. The temperature of fluid parcel remains constant during fluid motion.

- Note that

  $$\mathscr{A} = -TS + \mathscr{U}$$

  From the Maxwell relation, the stress

  $$P = \left(\frac{\delta\mathscr{A}}{\delta F}\right)_T = \left(\frac{\delta\mathscr{U}}{\delta F}\right)_S.$$

We take variation of $\mathcal{S}$ with respect to flow path $\mathbf{x}(\cdot)$. We claim that the corresponding Euler-Lagrange equation (i.e. $\delta\mathcal{S}[\mathbf{x}] = 0$) has the form

$$\boxed{\rho(\partial_t\mathbf{v} + \mathbf{v}\cdot\nabla\mathbf{v}) = \nabla_{\mathbf{x}}\cdot\sigma,} \tag{16.27}$$

where σ is given by

$$\boxed{\sigma_i^j = \rho\int \mathbf{r}^j(\partial_{\mathbf{r}^i}A_f)f\,d\mathbf{r}} \tag{16.28}$$

We show this result in the following calculations.

1. We denote the variation of the flow map $\mathbf{x}$ by $\mathring{\mathbf{x}}$. [6] Since the fiber follows the macro flow. We thus have
$$\mathring{\mathbf{r}} = \mathring{F}\mathbf{r}, \quad \mathring{F}^i_\alpha = \frac{\partial \mathring{x}^i}{\partial X^\alpha}.$$
The variation of kinetic energy with respect to the flow path $\mathbf{x}$ is
$$\delta\mathscr{K}[\mathbf{x}] = -\int_0^T \int \rho_0(X)\ddot{\mathbf{x}}(X,t)\cdot\mathring{\mathbf{x}}\,dX\,dt.$$
Here, we have taken integration by part for the t-integration and used $\mathring{\mathbf{x}}(0) = \mathring{\mathbf{x}}(T) = 0$.

2. Next, we compute $\mathring{f}$. Note that the variation of F is $\mathring{F}$, which is $\frac{\partial \mathring{\mathbf{x}}}{\partial X}$. From $\mathbf{r} = FR$, we get the variation of dynamic variable $\mathbf{r}(t)$ satisfying
$$\mathring{\mathbf{r}} = \mathring{F}R = \mathring{F}F^{-1}\mathbf{r}.$$
Conservation of micro particles reads
$$\mathring{f} + \nabla_{\mathbf{r}}\cdot(\mathring{\mathbf{r}}f) = 0. \tag{16.29}$$
Combining these two formulae, the variation of f satisfies
$$\mathring{f} = -\nabla_{\mathbf{r}}\cdot\left(\mathring{F}F^{-1}\mathbf{r}f\right).$$

3. Let us compute the variation of the Helmholtz energy
$$\begin{aligned}\mathscr{A}[\mathbf{x}] &= \int_0^T \int_\Omega\int_{\mathbb{R}^3} \rho(t,\mathbf{x})A(f(t,\mathbf{x},\mathbf{r}))\,d\mathbf{r}\,d\mathbf{x}\,dt \\ &= \int_0^T \int_{\Omega_0} \rho_0(X)\int_{\mathbb{R}^3} A(f(t,\mathbf{x}(t,X),\mathbf{r}))\,d\mathbf{r}\,dX\,dt.\end{aligned}$$
Here, we have used $d\mathbf{x} = JdX$ and $\rho J = \rho_0$. We take variation of $\mathscr{A}$ with respect to

[6] Suppose $\mathbf{x}(\cdot)$ is perturbed by a one-parameter family of path $\mathbf{x}^\varepsilon(t)$. Then $\dot{\mathbf{x}}$ denotes the time derivative, while $\mathring{\mathbf{x}}$ denotes the derivative with respective to ε. In our earlier notation, $\mathring{\mathbf{x}}(t) = \delta\mathbf{x}(t)$.

the flow map $\mathbf{x}(\cdot)$:

$$
\begin{aligned}
\delta\mathscr{A}[\mathbf{x}] &= \iint \rho_0(X)\delta\int A(f)\,d\mathbf{r}\,dX\,dt \\
&= \iint \rho_0(X)\left(\int A_f \mathring{f}\,d\mathbf{r}\right)dX\,dt \\
&= -\iint \rho_0(X)\left(\int A_f \nabla_{\mathbf{r}}\cdot(\mathring{F}F^{-1}\mathbf{r}f)\,d\mathbf{r}\right)dX\,dt \\
&= \iint \rho_0(X)\left(\int \left(\nabla_{\mathbf{r}}A_f\right)\cdot(\mathring{F}F^{-1}\mathbf{r}f)\,d\mathbf{r}\right)dX\,dt \\
&= \iint \rho_0(X)\left(\int \left(\nabla_{\mathbf{r}}A_f\right)\cdot(\frac{\partial\mathring{\mathbf{x}}}{\partial X}F^{-1}\mathbf{r}f)\,d\mathbf{r}\right)dX\,dt \\
&= -\iint \left[\nabla_X\cdot\left(\rho_0(X)\int(\nabla_{\mathbf{r}}A_f)(F^{-1}\mathbf{r}f)\,d\mathbf{r}\right)\right]\cdot\mathring{\mathbf{x}}\,dX\,dt
\end{aligned}
$$

Thus,

$$\frac{\delta\mathscr{A}}{\delta\mathbf{x}} = -\nabla_X\cdot P,$$

where

$$P(t,X) := \rho_0(X)\int(\nabla_{\mathbf{r}}A_f)F^{-1}\mathbf{r}f\,d\mathbf{r} = \rho_0(X)\int(\nabla_{\mathbf{r}}A_f)Rf\,JdR,$$

$$P_i^\beta = \rho_0\int \partial_{\mathbf{r}^i}A_f R^\beta f\,JdR,$$

and f is evaluated at $(t,\mathbf{x}(t,X),F(t,X)R)$. This is the *Kramers formula* for the Piola stress.

4. The Euler-Lagrange equation is

$$
\begin{aligned}
\rho_0(X)\ddot{\mathbf{x}} - \nabla_X\cdot P = 0 &\quad \text{(in Lagrangian coordinate)} \\
\rho\dot{\mathbf{v}} - \nabla_{\mathbf{x}}\cdot\sigma = 0 &\quad \text{(in Eulerian coordinate)}
\end{aligned}
$$

where

$$
\begin{aligned}
\sigma &:= J^{-1}PF^T = J^{-1}P_i^\beta F_\beta^j \\
&= J^{-1}\rho_0\int(\partial_{\mathbf{r}^i}A_f)R^\beta f\,JdRF_\beta^j \\
&= \rho\int(\partial_{\mathbf{r}^i}A_f)F_\beta^j R^\beta f\,JdR \\
&= \rho\int(\partial_{\mathbf{r}^i}A_f)\mathbf{r}^j f\,d\mathbf{r}.
\end{aligned}
$$

$$\boxed{\sigma_i^j = \rho \int \mathbf{r}^j (\partial_{\mathbf{r}^i} A_f) f \, d\mathbf{r}} \tag{16.30}$$

This formula is called the Irving-Kirkwood formula or the Kramers formula for the Cauchy stress.

Remarks

- When $A(f) = \Phi(\mathbf{r}) f + k_B T f \ln f$,

$$A_f = \Phi + k_B T (\ln f + 1),$$

and

$$\begin{aligned}
\sigma_i^j &= \rho \int \mathbf{r}^j \partial_{\mathbf{r}^i} \left[\Phi(\mathbf{r}) + T k_B (\ln f + 1)\right] f \, d\mathbf{r} \\
&= \rho \int \left(\mathbf{r}^j \Phi_{\mathbf{r}^i} f + T k_B \mathbf{r}^j f_{\mathbf{r}^i}\right) d\mathbf{r} \\
&= \rho \int \left(\mathbf{r}^j \Phi_{\mathbf{r}^i} f - T k_B \delta^{ij} f\right) d\mathbf{r} \\
&= \rho \langle (\partial_{\mathbf{r}^i} \Phi) \mathbf{r}^j \rangle - \rho T k_B \delta^{ij}
\end{aligned}$$

Thus,

$$\sigma = \rho \langle (\nabla_{\mathbf{r}} \Phi) \otimes \mathbf{r} \rangle - \rho k_B T I, \tag{16.31}$$

where

$$\langle \nabla_{\mathbf{r}} \Phi \otimes \mathbf{r} \rangle := \int (\mathbf{r}^j \partial_{\mathbf{r}^i} \Phi(\mathbf{r})) f(\mathbf{r}) \, d\mathbf{r}.$$

- The term $-\rho k_B T I$ is due to the term $k_B T f \ln f$ in the free energy $A(f)$. It is the energy from random motion of $\mathbf{r}(t)$. It creates this isotropic stress, which we may classify it as a pressure.

- At equilibrium, that is, the right-hand side of (16.26) is zero. In this case, we may show that the resulting stress is isotropic. This is the static pressure term. However, it is not necessary to decompose the polymeric stress into isotropic part and extra stress, unless the latter depends only on the deviatoric strain.

- When $\Phi(\mathbf{r})$ is a central-force potential, that is, $\Phi(\mathbf{r}) = \bar{\Phi}(|\mathbf{r}|)$, then σ is symmetric.

16.4.5 Stress formula – Eulerian approach

This variational approach is taken in the Eulerian frame of reference. The variations of paths cause constraints on the density and the pdf f. Such constrained variation is called dynamically accessible variation.

1. Let $f(t,\mathbf{x},\mathbf{r})$ be the p.d.f. of polymer particles per unit mass. $\rho(t,\mathbf{x})f(t,\mathbf{x},\mathbf{r})$ be the p.d.f. of polymer particles per unit volume. Define the specific Helmholtz energy to be
$$\bar{A}[f](t,\mathbf{x}) = \int A(f)\,d\mathbf{r}, \quad A(f) = \Phi(\mathbf{r})f(t,\mathbf{x},\mathbf{r}) + k_B T f \ln f,$$
The term $\Phi(\mathbf{r})f(t,\mathbf{x},\mathbf{r})$ represents the internal energy. The term $-k_B T f \ln f$ is the energy due to the randomness of the polymer particles at temperature T. The internal energy is
$$\bar{U} = \bar{A} + TS[\mathbf{x}].$$

2. Define the action
$$\mathcal{S}[\rho, f, \mathbf{v}] := \int_{t_0}^{t_1}\int \left(\frac{1}{2}\rho|\mathbf{v}|^2 - \rho\bar{U}[f]\right) d\mathbf{x}\,dt.$$
??? Note that the variation of the term TS is zero under the adiabatic assumption or isothermal assumption. Thus, we shall only consider the variation of the kinetic energy and the Helmholtz energy.

3. Given a flow map $\mathbf{x}(t,X)$, we consider a family of flow maps $\mathbf{x}^s(t,X)$ with $\mathbf{x}^0(t,X) = \mathbf{x}(t,X)$. The two parameters (s,t) are independent. We have defined the velocity field $\mathbf{v}$ as
$$\mathbf{v}(t,\mathbf{x}^s(t,X)) = (\partial_t)_X\,\mathbf{x}^s(t,X).$$
Now, in the s-direction, we define
$$\mathbf{w}(t,\mathbf{x}(t,X)) := (\partial_s|_{s=0})_X\,\mathbf{x}^s(t,X).$$
We call $\mathbf{w}$ a pseudo-velocity. It is a direction of perturbation of the flow map $\mathbf{x}(t,X)$. Indeed, from (4.1),
$$\mathbf{w}(t,\mathbf{x}) = \delta\mathbf{x}(t,\varphi_t^{-1}(\mathbf{x})),$$
where $\varphi_t(X) = \mathbf{x}(t,X)$. *The vector field* $\mathbf{w}$ *is not arbitrary. It comes from a family of flow maps* $\mathbf{x}^s(t,X)$.

4. Let $f^s(t,\mathbf{x},\mathbf{r})$ be defined such that its pullback by the flow $\mathbf{x}^s(t,\cdot)$ is $f_0(X,R)$, where
$$\mathbf{x} = \mathbf{x}^s(t,X), \quad \frac{\partial\mathbf{x}^s(t,X)}{\partial X}R = \mathbf{r}.$$

From conservations of polymer particles in macro and micro scales, ρ^s and f^s satisfy

$$\partial_s \rho^s + \nabla_{\mathbf{x}} \cdot (\mathbf{w}\rho^s) = 0, \tag{16.32}$$

$$\partial_s f^s + \mathbf{w} \cdot \nabla_{\mathbf{x}} f^s + \nabla_{\mathbf{r}} \cdot ((\nabla_{\mathbf{x}} \mathbf{w}) \mathbf{r} f^s) = 0. \tag{16.33}$$

The second equation is from

$$\mathring{f} + \nabla_{\mathbf{r}} \cdot (\mathring{\mathbf{r}} f) = 0,$$

and $\mathbf{r} = FR$,

$$\mathring{\mathbf{r}} = \mathring{F} F^{-1} \mathbf{r} = \nabla_{\mathbf{x}} \mathbf{w} \mathbf{r}.$$

The term $\partial_s|_{s=0}\rho^s$ and $\partial_s|_{s=0} f^s$ are the dynamically accessible variations $\delta\rho$ and δf.

5. Now we take variation of $\mathscr{A}$ with respect to $\mathbf{v}$ in direction $\mathbf{w}$ with ρ and f satisfying the constraints (16.32),(16.33).

$$\delta \int \rho(t,\mathbf{x}) \left(\int A(f(t,\mathbf{x},\mathbf{r}))\, d\mathbf{r} \right) d\mathbf{x} = \int (\delta\rho) \bar{A}\, d\mathbf{x} + \int \rho (\delta \bar{A})\, d\mathbf{x} = I + II.$$

$$\begin{aligned}
I &= \int \delta\rho \bar{A}\, d\mathbf{x} = -\int (\nabla_{\mathbf{x}} \cdot (\rho \mathbf{w})) \bar{A}\, d\mathbf{x} = \int \rho \nabla_{\mathbf{x}} \bar{A} \cdot \mathbf{w}\, d\mathbf{x}. \\
II &= \int \rho (\delta \bar{A})\, d\mathbf{x} = \int \rho \frac{\delta \bar{A}}{\delta f} \cdot \delta f\, d\mathbf{x} \\
&= \int \rho \int A_f \left[-\mathbf{w} \cdot \nabla_{\mathbf{x}} f - \nabla_{\mathbf{r}} \cdot ((\nabla_{\mathbf{x}} \mathbf{w}) \mathbf{r} f) \right] d\mathbf{r}\, d\mathbf{x} \\
&= \int \rho \left[-\int A_f \nabla_{\mathbf{x}} f\, d\mathbf{r} \cdot \mathbf{w} + \int (\nabla_{\mathbf{r}} A_f) \cdot (\nabla_{\mathbf{x}} \mathbf{w}) \mathbf{r} f\, d\mathbf{r} \right] d\mathbf{x} \\
&= -\int \rho \nabla_{\mathbf{x}} \left(\int A\, d\mathbf{r} \right) \cdot \mathbf{w}\, d\mathbf{x} - \int \nabla_{\mathbf{x}} \left[\rho \int (\nabla_{\mathbf{r}} A_f) \mathbf{r} f\, d\mathbf{r} \right] \cdot \mathbf{w}\, d\mathbf{x}
\end{aligned}$$

Here,

$$\int d\mathbf{x} \rho \int d\mathbf{r} \left(-A_f \partial_{\mathbf{r}^i} (\partial_{\mathbf{x}^j} w^i \mathbf{r}^j) \right) = -\int d\mathbf{x} \partial_{\mathbf{x}^j} \left(\rho \int d\mathbf{r} (\partial_{\mathbf{r}^i} A_f) \mathbf{r}^j w^i \right),$$

and the term

$$\nabla_{\mathbf{x}} \bar{A} = \nabla_{\mathbf{x}} \int A(\mathbf{r}, f(t,\mathbf{x},\mathbf{r}))\, d\mathbf{r} = \int A_f \nabla_{\mathbf{x}} f\, d\mathbf{r}.$$

We obtain

$$\begin{aligned}
\delta \int_{t_0}^{t_1} \int \rho \bar{A}[f]\, d\mathbf{x}\, dt &= -\int_{t_0}^{t_1} \int \nabla_{\mathbf{x}} \cdot \left[\rho \int (\nabla_{\mathbf{r}} A_f) \mathbf{r} f\, d\mathbf{r} \right] \cdot \mathbf{w}\, d\mathbf{x}\, dt \\
&= -\int_{t_0}^{t_1} \int \nabla_{\mathbf{x}} \cdot \sigma \cdot \mathbf{w}\, d\mathbf{x}\, dt
\end{aligned}$$

where

$$\sigma = \rho \int (\nabla_{\mathbf{r}} A_f)\mathbf{r} f \, d\mathbf{r}. \tag{16.34}$$

6. Thus, the Euler-Lagrange equation is

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

Formula (16.34) is called the Kramers formula, or the Irving-Kirkwood formula, or the virial stress.

16.4.6 The full set of micro-macro equations

Compressible Viscoelastic flow The full set of micro-macro model for polymeric fluid flow is a differential-integral equation. They include the macroscopic equations

$$\partial_t \rho + \nabla_{\mathbf{x}}\cdot(\rho\mathbf{v}) = 0. \tag{16.35}$$

$$\rho\left(\partial_t \mathbf{v} + \mathbf{v}\nabla_{\mathbf{x}}\mathbf{v}\right) = \nabla_{\mathbf{x}}\cdot\sigma, \tag{16.36}$$

the microscopic equation

$$\partial_t f + \mathbf{v}\cdot\nabla_{\mathbf{x}} f + \nabla_{\mathbf{r}}\cdot(\nabla\mathbf{v}\mathbf{r}f) = \nabla_{\mathbf{r}}\cdot\frac{1}{\zeta}[(\nabla_{\mathbf{r}}\Phi)f + k_B T\nabla_{\mathbf{r}} f]. \tag{16.37}$$

and the coupling between micro and macro dynamics is through

$$\sigma = -\rho k_B T I + \rho\langle\mathbf{r}\nabla_{\mathbf{r}}\Phi\rangle, \quad \text{where } \langle(\cdot)\rangle := \int (\cdot) f \, d\mathbf{r}. \tag{16.38}$$

Incompressible viscoelastic flow [7] In this model, we assume the polymer is in a solvent which is a Newtonian flow with viscosity η. The incompressibility introduces the Lagrangian multiplier p. The model reads

$$\left\{\begin{array}{l} \rho\left(\partial_t\mathbf{v} + \mathbf{v}\cdot\nabla\mathbf{v}\right) + \nabla p = \eta \triangle \mathbf{v} + \nabla\cdot\tau \\ \nabla\cdot\mathbf{v} = 0 \\ \tau = n_p\left(-kTI + \mathbb{E}[\mathbf{r}_t\otimes\mathbf{F}(\mathbf{r}_t)]\right) \\ d\mathbf{r}_t + \mathbf{v}\cdot\nabla_{\mathbf{x}}\mathbf{r}_t\,dt = \left((\nabla_{\mathbf{x}}\mathbf{v})\mathbf{r}_t - \frac{2}{\zeta}\mathbf{F}(\mathbf{r}_t)\right)dt + \sqrt{\frac{4kT}{\zeta}}dW_t \end{array}\right. \tag{16.39}$$

Here n_p is the polymer concentration, which is constant in this model. The density is assumed to be a constant. Otherwise, we should add the continuity and treat ρ as an unknown.

[7] Ref. C. Le Bris, T. Lelièvre, Micro-macro models for viscoelastic fluids: modelling, mathematics and numerics.

The non-dimensional model is

$$\begin{cases} Re\,(\partial_t \mathbf{v} + \mathbf{v}\cdot\nabla\mathbf{v}) + \nabla p = (1-\varepsilon)\,\triangle\,\mathbf{v} + \nabla\cdot\tau \\ \nabla\cdot\mathbf{v} = 0 \\ \tau = \frac{\varepsilon}{We}\,(-kTI + \mathbb{E}[\mathbf{r}_t \otimes \mathbf{F}(\mathbf{r}_t)]) \\ d\mathbf{r}_t + \mathbf{v}\cdot\nabla_{\mathbf{x}}\mathbf{r}_t\,dt = \big((\nabla_x \mathbf{v})\mathbf{r}_t - \frac{1}{2We}\mathbf{F}(\mathbf{r}_t)\big)\,dt + \frac{1}{\sqrt{We}}dW_t \end{cases} \tag{16.40}$$

The parameters are

$$Re = \frac{\rho U L}{\eta}, \quad We = \frac{\lambda U}{L}, \quad \varepsilon = \frac{\eta_p}{\eta}$$

where *Re* is the Renolds number and *We* is the Weisenberg number,

- $L = \sqrt{\frac{kT}{H}}$ the characteristic length scale
- $\lambda = \frac{\zeta}{4H}$ the relaxation time for polymer chain,
- $\eta_p = n_p kT\lambda$ the polymer viscosity
- H the Hookean parameter with $V = \frac{1}{2}H|\mathbf{r}|^2$
- $\mathbf{F}(\mathbf{r}) = \mathbf{r}$ in non-dimensional Hookean model.

The stochastic equation is equivalent to the Fokker-Planck equation. Thus, alternative equations are

$$\begin{cases} Re\,(\partial_t \mathbf{v} + \mathbf{v}\cdot\nabla\mathbf{v}) + \nabla p = (1-\varepsilon)\,\triangle\,\mathbf{v} + \nabla\cdot\tau \\ \nabla\cdot\mathbf{v} = 0 \\ \tau = \frac{\varepsilon}{We}\,(-I + \int(\mathbf{r}_t \otimes \mathbf{F}(\mathbf{r}_t))f\,d\mathbf{r}) \\ \partial_t f + \mathbf{v}\cdot\nabla_{\mathbf{x}} f + \nabla_{\mathbf{r}}\cdot((\nabla_{\mathbf{x}}\mathbf{v})\mathbf{r}f) = \nabla_{\mathbf{r}}\cdot\big(\frac{1}{2We}\mathbf{F}(\mathbf{r})f\big) + \frac{1}{2We}\triangle_{\mathbf{r}} f. \end{cases} \tag{16.41}$$

Energy dissipation The dissipation of energy is

$$\begin{aligned} &\frac{d}{dt}\int_\Omega \left[\frac{1}{2}\rho\mathbf{v}^2 + \left(\int_{\mathbb{R}^3} \frac{\sigma^2}{2} f\ln f + \Phi f\,d\mathbf{r}\right)\right] d\mathbf{x} \\ &= -\int_\Omega\int_{\mathbb{R}^3} f|\nabla_{\mathbf{r}}\mu|^2\,d\mathbf{r}\,d\mathbf{x} \le 0. \end{aligned}$$

16.5 Macro Model – Moment Expansion

The above micro-macro model is still difficult to solve because $f(t,\mathbf{x},\mathbf{r})$ involves 7 variables. Instead, a macroscopic average over the microscopic equation is introduced. To compute the stress, we need to find $\langle \mathbf{r}\nabla_{\mathbf{r}}\Phi(\mathbf{r})\rangle$. The simplest case is Φ is quadratic. This leads to compute $\langle \mathbf{rr} \rangle$, the second moment of the pdf $f(t,\mathbf{x},\mathbf{r})$, called the *conformation tensor*. We will discuss below. In general, we will have moment expansion for Φ and result in moment equations from the Smoluchowski equations. A closure problem is encountered in general. We will leave such theory in the theory of liquid crystals in later chapter. [8]

Conformation tensor Let us define the conformation tensor as

$$\mathbf{c} := \int \mathbf{rr} f(t,\mathbf{x},\mathbf{r})\, d\mathbf{r} := \langle \mathbf{rr} \rangle.$$

It represents the second moment of the micro configuration of the polymeric structure. By Taking $\int \mathbf{rr}(16.26)\, d\mathbf{r}$, we obtain

$$\mathbf{c}_t + \mathbf{v}\cdot\nabla_{\mathbf{x}}\mathbf{c} - (\nabla\mathbf{v})\cdot\mathbf{c} - \mathbf{c}\cdot(\nabla\mathbf{v})^T = \frac{1}{\zeta}\left[2k_BTI - 2\langle(\nabla_{\mathbf{r}}\Phi)\mathbf{r}\rangle\right]. \tag{16.42}$$

In the above formula, we have used the following calculations:

$$\begin{aligned}
&\int \mathbf{rr}\partial_t f\, d\mathbf{r} = \partial_t\langle \mathbf{rr}\rangle \\
&\int \mathbf{rr}(\mathbf{v}\cdot\nabla_{\mathbf{x}} f)\, d\mathbf{r} = \mathbf{v}\cdot\nabla_{\mathbf{x}}\langle \mathbf{rr}\rangle \\
&\int \mathbf{rr}\nabla_{\mathbf{r}}\cdot(\nabla_{\mathbf{x}}\mathbf{v}\mathbf{r}f)\, d\mathbf{r} = -\nabla_{\mathbf{x}}\mathbf{v}\cdot\langle \mathbf{rr}\rangle - \langle \mathbf{rr}\rangle\cdot(\nabla_{\mathbf{x}}\mathbf{v})^T \\
&\int \mathbf{rr}\nabla_{\mathbf{r}}\cdot\left(\frac{1}{\zeta}\nabla_{\mathbf{r}}\Phi f\right)\, d\mathbf{r} = -\frac{2}{\zeta}\langle(\nabla_{\mathbf{r}}\Phi)\mathbf{r}\rangle \\
&\int \mathbf{rr}\nabla_{\mathbf{r}}\cdot\left(\frac{k_BT}{\zeta}\nabla_{\mathbf{r}} f\right)\, d\mathbf{r} = \frac{2k_BT}{\zeta}I.
\end{aligned}$$

In component form, the third equation is

$$\begin{aligned}
\int r_i r_j \partial_{r_k}(L^k_l r_l f)\, dr &= -\int \left(\delta_{ik} r_j L^k_l r_l f + \delta_{kJ} r_i L^k_l r_l f\right)\, dr \\
&= -\int \left(L^i_l r_l r_j f + L^j_l r_i r_l f\right)\, dr \\
&= -L\mathbf{c} - \mathbf{c}L^T.
\end{aligned}$$

[8] Wiki, Sir Sam Edwards, “Edwards worked in the theoretical study of complex materials, such as polymers, gels, colloids and similar systems. His seminal paper[2] came in 1965 which ”in one stroke founded the modern quantitative understanding of polymer matter.”[1] Pierre-Gilles de Gennes notably extended Edwards’s 1965 seminal work, ultimately leading to de Gennes’s 1991 Nobel Prize in Physics. The Doi-Edwards theory of polymer melt viscoelasticity originated from an initial publication of Edwards in 1967,[3] was expanded upon by de Gennes in 1971, and was subsequently formalized through a series of publications between Edwards and Masao Doi in the late 1970s”

We abbreviate (16.42) by

$$\boxed{\mathbf{c}_{(1)} = \frac{2k_BT}{\zeta}I - \frac{2}{\zeta}\langle(\nabla_{\mathbf{r}}\Phi)\mathbf{r}\rangle.} \tag{16.43}$$

where the notation

$$\mathbf{c}_{(1)} := \mathbf{c}_t + \mathbf{v}\cdot\nabla_{\mathbf{x}}\mathbf{c} - (\nabla\mathbf{v})\cdot\mathbf{c} - \mathbf{c}\cdot(\nabla\mathbf{v})^T,$$

is called the upper-convected derivative of the tensor $\mathbf{c}$. It is indeed the Lie derivative of the tensor $\mathbf{c}$.

Hookean potential From $\Phi(\mathbf{r}) = 3k_BT|\mathbf{r}|^2/2R^2$, we obtain

$$\langle(\nabla_{\mathbf{r}}\Phi)\mathbf{r}\rangle = \frac{3k_BT}{R^2}\mathbf{c}.$$

Plug this into (16.43) and (16.38), we obtain the evolution equation of the conformation tensor $\mathbf{c}$:

$$\boxed{\mathbf{c}_{(1)} = \frac{2k_BT}{\zeta}\left(I - \frac{3}{R^2}\mathbf{c}\right).} \tag{16.44}$$

The Kramer's formula for the Hookean potential is

$$\sigma = -\rho k_BTI + \rho\frac{3k_BT}{R^2}\mathbf{c}. \tag{16.45}$$

We can eliminate $\mathbf{c}$ to get an evolution equation for σ:

$$\begin{aligned}
\sigma_{(1)} &= -\rho k_BTI_{(1)} + \rho\frac{3k_BT}{R^2}\mathbf{c}_{(1)} \\
&= \rho k_BT(\nabla\mathbf{v} + (\nabla\mathbf{v})^T) + \rho\frac{3k_BT}{R^2}\frac{2k_BT}{\zeta}\left(I - \frac{3}{R^2}\mathbf{c}\right) \\
&= \rho k_BT(\nabla\mathbf{v} + (\nabla\mathbf{v})^T) - \frac{6k_BT}{R^2\zeta}\sigma.
\end{aligned}$$

This is the evolution equation for σ. It is precisely the Maxwell model.

16.6 Non-isothermal Viscoelasticity

The internal energy consists of heat and work:

$$dU = dQ + dW = \Theta dS + dW,$$

where Θ is the temperature and S the entropy. We assume the energy input from external world is

$$dQ = c\,d\Theta$$

Here, c is heat capacity. Then we have

$$\Theta\,dS = c\,d\Theta$$

This leads to

$$\Theta = \exp\left(\frac{S - S_0}{c}\right).$$

Appendix: Kolmogorov forward equation

Suppose X_t is a time-dependent random variable satisfying

$$dX_t = a(t, X_t)dt + b(t, X_t)dB$$

Here, B is a Brownian motion.

Chapter 17

Two-Phase Flows

17.1 Two-fluid model

17.1.1 Inviscid flows

1. **Governing in the interiors** Consider two simple incompressible fluids occupied region Ω_i, $i = 1,2$ connected by a dynamically moving interface Γ_t. In Ω_i, the fluid is governed by
$$\begin{cases} \nabla \cdot \mathbf{v}_i = 0 \\ \rho_i(\partial_t \mathbf{v}_i + \mathbf{v}_i \cdot \nabla \mathbf{v}_i) + \nabla p_i = 0 \end{cases} \quad \text{in } \Omega_i.$$
Here, we assume that the density ρ_i are constants.

2. **Interface condition** There are two conditions on the interface Γ_t, corresponding the divergence-free equation and the momentum equation.

   - The divergence-free condition ($\nabla \cdot \mathbf{v}_i = 0$) leads to
   $$[\mathbf{v}] \cdot \nu = 0 \quad \text{on } \Gamma_t,$$
   where $[\mathbf{v}] := \mathbf{v}_2 - \mathbf{v}_1$ and ν is the normal of Γ_t pointing from Ω_1 to Ω_2. This implies that the motion of the interface, which can be characterized by its normal velocity $\mathbf{v}_n = v_n \nu$, satifies
   $$v_n = \mathbf{v}_1 \cdot \nu = \mathbf{v}_2 \cdot \nu.$$
   - For force balancing on the interface, we have
   $$[p]\nu = \boldsymbol{\sigma} \cdot \nu$$
   where $\boldsymbol{\sigma}$ is the stress tensor of the interface. It is modeled as $\boldsymbol{\sigma} = \sigma H \nu \otimes \nu$. Here, H is the mean curvature of the surface.

3. **Iterative solver**

   - **Interior solver:** Given v_n, we can solve $(\mathbf{v}_i, p_i)$ in each domains Ω_i with boundary conditions: $\mathbf{v}_i \cdot \nu = v_n$ on the boundary $\partial\Omega_i$.
   - **Interface solver:** On the interface Γ_t, its normal velocity v_n is determined by the other interface condition: $[p] = \sigma H$.

17.1.2 Viscous flows

1. **Interior Equations** We consider two incompressible viscous fluids occupying two domains Ω_i, connected by a dynamically moving interface Γ_t. The governing equations in each region Ω_i are the Navier-Stokes equations

$$\begin{cases} \nabla \cdot \mathbf{v}_i = 0 \\ \rho_i(\partial_t \mathbf{v}_i + \mathbf{v}_i \cdot \nabla \mathbf{v}_i) + \nabla p_i = \nabla \cdot \mu_i \nabla \mathbf{v}_i. \end{cases} \qquad \text{in } \Omega_i$$

   Here, μ_i is the fluid viscosity in region Ω_i.

2. **Interface condition** On the interface Γ_t, due to viscous effect, we impose the condition

$$[\mathbf{v}] = 0.$$

   This leads to

$$\mathbf{v}_1 = \mathbf{v}_2 = \mathbf{v},$$

   where $\mathbf{v}$ is the surface velocity. The surface force on Γ_t coming from the elastic property of the interface is $\sigma H \nu$, σ is the surface tension and H is the mean curvature of the surface. Let $\tau_i := \mu_i \nabla \mathbf{v}_i - p_i I$ be the stress tensor of the fluid i in region Ω_i. Then the force balance law on the interface is

$$[\tau] \cdot \nu = \sigma H \nu.$$

3. **Iterative Solver** If $\mathbf{v}$ is given, then the condition $\mathbf{v}_i = \mathbf{v}$ and Navier-Stokes equation can determine the flow in Ω_i. On the other hand, there are three conditions in $[\tau] \cdot \nu = \sigma H \nu$ to determine the interfacial velocity $\mathbf{v}$.

17.2 Phase field models based on labeled order parameter

17.2.1 Order Parameter and Free Energy

References:

- Gurtin et. al. Two-Phase Binary Fluids and Immiscible Fluids Described by an Order Parameter (1996).
- C. Liu, H. Wu, An Energetic Variational Approach for the Cahn–Hilliard Equation with Dynamic Boundary Condition: Model Derivation and Mathematical Analysis, ARMA (2019)

In some applications (immiscible two-phase flows), we may encounter two different fluids in the same fluid system. For example, oil and water, water and gas, or a system with more components.

We may use a label to indicate the type of phase of the fluid. Such a label is called an *order parameter*. For instance, in a water-oil system, we may use $\phi(t,\mathbf{x}) = 1$ for water and $\phi(t,\mathbf{x}) = -1$ for oil at $(t,\mathbf{x})$.

Types of Order Parameters There are two types of order parameters.

- **Labeled order parameter**: Let ϕ be a phase label of certain type of the fluids. It is advected with the fluids. That is

  $$\partial_t\phi + \mathbf{v}\cdot\nabla\phi = 0.$$

  This is equivalent to

  $$\phi(t,\mathbf{x}(t,X)) = \phi_0(X).$$

- **Concentration order parameter**: $\phi\,d\mathbf{x}$ is a conservative measure. For instance, ϕ is the density or concentration, etc. In this case, ϕ satisfies

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

  This is equivalent to

  $$\phi(t,\mathbf{x}(t,X))J(t,X) = \phi_0(X).$$

Free energy One can associate ϕ with a free energy $\mathscr{F}$ defined by

$$\mathscr{F}[\phi] = \int_\Omega f(\phi,\nabla\phi)\,d\mathbf{x} = \int_\Omega \frac{1}{2}|\nabla\phi|^2 + W(\phi)\,d\mathbf{x}.$$

The energy density W is called a *bulk energy density*. A natural choice of W is a double well potential with minima at -1 and 1. For example, $W(\phi) = \frac{1}{4}(\phi^2-1)^2$. The energy $|\nabla\phi|^2$ is certain kind of kinetic energy. Its effect is to homogenize the fluids. The variation of ϕ causes an energy penalty. When ϕ tends to an equilibrium with 1 and -1 on the two sides of an interface, $\nabla\phi$ becomes the delta function on the interface and $\mathscr{F}[\phi]$ measures the corresponding *surface energy*.

Chemical potential The variation of free energy $\mathscr{F}$ w.r.t. ϕ is called the *chemical potential*

$$\mu := \frac{\delta \mathscr{F}}{\delta \phi} = -\nabla \cdot \frac{\partial f}{\partial \nabla \phi} + \frac{\partial f}{\partial \phi}. \tag{17.1}$$

17.2.2 Labeled Two-Phase Inviscid Flows

Dynamically accessible variations Given a flow map $\mathbf{x}(t,X)$, we shall perturb it by a vector field $\mathbf{w}(\mathbf{x})$. Since the flow satisfies the continuity equation and ϕ satisfies the advection equation. The perturbation $\mathbf{w}$ is required to be a *dynamically accessible variation*, see Subsection 4.2.1.

We define a perturbation of $\mathbf{x}$ in the direction $\mathbf{w}$ as the following flow maps

$$\frac{\partial}{\partial s}\mathbf{x}^s(t,X) = \mathbf{w}(\mathbf{x}^s(t,X)), \quad \mathbf{x}^0(t,X) = \mathbf{x}(t,X). \tag{17.2}$$

The quantity

$$\delta \mathbf{x}(t,X) := \frac{\partial \mathbf{x}^s(t,X)}{\partial s}|_{s=0} = \mathbf{w}(\mathbf{x}(t,X))$$

is called a variation of $\mathbf{x}$, or a pseudo-velocity.

The Eulerian variable ϕ has a constraint

$$\partial_t \phi + \mathbf{v} \cdot \nabla \phi = 0.$$

That is,

$$\phi(t, \mathbf{x}(t,X)) = \phi_0(X).$$

Given an arbitrarily vector field $\mathbf{w}$, we consider the perturbation of $\mathbf{x}(t,\cdot)$ in the direction $\mathbf{w}$. We define a one-parameter family of function ϕ^s by

$$\phi^s(t, \mathbf{x}^s(t,X)) := \phi_0(X).$$

Then the variation

$$\delta \phi := \frac{\partial}{\partial s}|_{t,X} \phi^s(t, \mathbf{x}^s(t,X)) \text{ at } s = 0,$$

is called a dynamically accessible variation of ϕ. It satisfies

$$\delta \phi + \mathbf{w} \cdot \nabla \phi = 0.$$

Variation of free energy $\mathscr{F}$ w.r.t. flow motion The variation of $\mathscr{F}$ at a flow map $\mathbf{x}$ along the tangent direction $\mathbf{w}$ is a Frechet derivative of $\mathscr{F}$ along $\mathbf{x}^s$:

$$\frac{\delta \mathscr{F}}{\delta \phi} \cdot \mathbf{w} = \frac{\delta \mathscr{F}}{\delta \phi^s} \frac{\partial \phi^s}{\partial s} = \mu(-\mathbf{w} \cdot \nabla \phi) = -\mu \nabla \phi \cdot \mathbf{w}.$$

Equation of Motion The action is defined to be

$$\mathcal{S}[\mathbf{x}] = \int_0^T \int_\Omega \left[\frac{1}{2}\rho|\mathbf{v}(t,\mathbf{x})|^2 - f(\phi(t,\mathbf{x}), \nabla\phi(t,\mathbf{x}))\right] d\mathbf{x}\, dt.$$

The variation of action w.r.t. flow map in the direction $\mathbf{w}$ with incompressibility constraint $\nabla \cdot \mathbf{v} = 0$ gives

$$\delta \int_0^T \int_\Omega \frac{1}{2}\rho|\mathbf{v}(t,\mathbf{x})|^2 \, d\mathbf{x}dt = \int_0^T \int_\Omega [-(\rho\mathbf{v})_t - \nabla\cdot(\rho\mathbf{v}\mathbf{v}) - \nabla p]\cdot \mathbf{w}\, d\mathbf{x}\, dt$$

The variation of the bulk free energy $\mathscr{F}$ with respect to $\mathbf{x}(t,\cdot)$ in the direction $\mathbf{w}$ is

$$\frac{\delta\mathscr{F}}{\delta\phi}\cdot\mathbf{w} = -\mu\nabla\phi\cdot\mathbf{w}.$$

Thus, the variation of $\mathcal{S}$ with respect to $\mathbf{x}(t,\cdot)$ in the direction $\mathbf{w}$ is

$$\delta\mathcal{S}[\mathbf{x}] = \int_0^T \int_\Omega [-(\rho\mathbf{v})_t - \nabla\cdot(\rho\mathbf{v}\mathbf{v}) - \nabla p]\cdot\mathbf{w} + \mu\nabla\phi\cdot\mathbf{w}\, d\mathbf{x}\, dt \tag{17.3}$$

This gives the Euler-Lagrange equation

$$(\rho\mathbf{v})_t + \nabla\cdot(\rho\mathbf{v}\mathbf{v}) + \nabla p = \mu\nabla\phi.$$

where μ is given by (17.1)

$$\mu := \frac{\delta\mathscr{F}}{\delta\phi} = -\nabla\cdot\frac{\partial f}{\partial\nabla\phi} + \frac{\partial f}{\partial\phi}.$$

The full set of equations are

$$\begin{cases} \partial_t\phi + \mathbf{v}\cdot\nabla\phi = 0, \\ \partial_t\rho + \nabla\cdot(\rho\mathbf{v}) = 0, \\ \rho(\partial_t\mathbf{v} + \mathbf{v}\nabla\mathbf{v}) + \nabla p = \mu\nabla\phi \\ \nabla\cdot\mathbf{v} = 0 \end{cases}$$

for $(\phi, \rho, \mathbf{v}, p)$.

Conservation of energy We multiply momentum equation by $\mathbf{v}$ then integrate in $\mathbf{x}$ and t to get

$$\frac{d}{dt}\int\frac{1}{2}\rho|\mathbf{v}|^2\, dx = \int\mu\mathbf{v}\cdot\nabla\phi\, dx = -\int\mu\partial_t\phi\, d\mathbf{x} = -\int\frac{\delta\mathscr{F}}{\delta\phi}\cdot\partial_t\phi\, d\mathbf{x} = -\frac{d\mathscr{F}}{dt}$$

That gives

$$\frac{d}{dt}\mathscr{E} = \frac{d}{dt}\left(\int\frac{1}{2}\rho|\mathbf{v}|^2\, dx + \int f(\phi,\nabla\phi)\, d\mathbf{x}\right) = 0.$$

This is the conservation of total energy. It also shows that the force $\mu\nabla\phi$ is the opposite force for the advection of ϕ.

17.2.3 Labeled Two-Phase Viscous Flows

One can add viscous term in the momentum equation:

$$\rho \frac{D\mathbf{v}}{Dt} = \mu \nabla \phi + \nabla \cdot \tau$$

where

$$\tau = \nu \left(\nabla \mathbf{v} + (\nabla \mathbf{v})^T - \frac{2}{3} \nabla \cdot \mathbf{v} I \right) + \lambda \nabla \cdot \mathbf{v} I,$$

is the viscous stress.

Dissipation of order parameter – Allen-Cahn model The order parameter has a tendency to relax to lowest free energy state. This is modeled by the Allen-Cahn model, it is simply a relaxation model defined by

$$\partial_t \phi + \mathbf{v} \cdot \nabla \phi = -\frac{\delta \mathscr{F}}{\delta \phi} = -\mu.$$

Dissipation of the velocity The dissipation of energy can be obtained by multiplying momentum equation by $\mathbf{v}$, multiplying advection equation by μ, then adding them together:

$$(\rho \frac{D\mathbf{v}}{Dt} \cdot \mathbf{v} - \mu \nabla \phi \cdot \mathbf{v}) + (\mu \partial_t \phi + \mu \mathbf{v} \nabla \phi) = \mathbf{v} \cdot \nabla \cdot \tau - \mu^2.$$

This gives

$$\frac{d\mathscr{E}}{dt} = -\tau \cdot \nabla \mathbf{v} - \mu^2.$$

The viscous dissipation becomes

$$-\tau \cdot \nabla \mathbf{v} = -\nu |\nabla \mathbf{v} + (\nabla \mathbf{v})^T|^2 - \lambda |\nabla \cdot \mathbf{v}|^2.$$

17.3 Phase field models based on conservative order parameter – Cahn-Hilliard model

17.3.1 Variation of free energy w.r.t. pre-domain

For ϕ being a concentration such that $\phi\, d\mathbf{x}$ is invariant along the fluid flow, we design one-parameter flow maps $\mathbf{x}^s(t,X)$ such that

$$\phi^s(t, \mathbf{x}^s(t,X)) J^s(t,X) = \phi_0(X).$$

where $J^s(t,X) = det\left(\frac{\partial \mathbf{x}^s(t,X)}{\partial X}\right)$. As in the previous perturbation, we define $\mathbf{w}(t,\mathbf{x}(t,X)) = \delta\mathbf{x}(t,X)$. Then by differentiate the above conservation formula $\phi(t,\mathbf{x}^s(t,X))J^s = \phi_0(X)$ in s, we get

$$\partial_s\phi^s + \nabla\cdot(\mathbf{w}\phi^s) = 0.$$

The variation of $\mathscr{F}$ w.r.t. $\mathbf{x}^s$ is

$$\begin{aligned} \delta\mathscr{F}\cdot\mathbf{w} &= \frac{\delta\mathscr{F}}{\delta\phi^s}\frac{\partial\phi^s}{\partial s} \\ &= \int \mu(-\nabla\cdot(\phi\mathbf{w}))\,d\mathbf{x} \\ &= \int \phi\nabla\mu\cdot\mathbf{w}\,d\mathbf{x} \end{aligned}$$

Conserved order parameter In the case

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

The force from the convection becomes

$$\rho\frac{D\mathbf{v}}{Dt} + \nabla p = -\phi\nabla\mu.$$

The full set of equations are

$$\begin{cases} \partial_t\phi + \nabla\cdot(\phi\mathbf{v}) = 0, \\ \partial_t\rho + \nabla\cdot(\rho\mathbf{v}) = 0, \\ \rho\frac{D\mathbf{v}}{Dt} + \nabla p = -\phi\nabla\mu, \\ \nabla\cdot\mathbf{v} = 0. \end{cases}$$

for $(\phi,\rho,\mathbf{v},p)$.

Conservation of energy For the energy equation, we multiply the above equation by $\mathbf{v}$, take integration by part:

$$\begin{aligned} \frac{d}{dt}\int\frac{1}{2}\rho|\mathbf{v}|^2\,dx = -\int\phi\nabla\mu\cdot\mathbf{v}\,dx = \int\mu\nabla\cdot(\phi\mathbf{v})\,d\mathbf{x} \\ = -\int\mu\partial_t\phi\,d\mathbf{x} = -\int\frac{\delta\mathscr{F}}{\delta\phi}\cdot\partial_t\phi\,d\mathbf{x} = -\frac{d\mathscr{F}}{dt} \end{aligned}$$

We also get same result of conservation of energy:

$$\frac{d}{dt}\int\frac{1}{2}\rho|\mathbf{v}|^2 + f(\phi,\nabla\phi)\,dx = 0.$$

Dissipation

1. Cahn-Hilliard defines the dissipation flux to be

$$-m\nabla\mu,$$

where m is called the mobility. The evolution equation for ϕ is

$$\partial_t\phi + \nabla\cdot(\mathbf{v}\phi) = \nabla\cdot(m\nabla\mu).$$

This is the Cahn-Hilliard equation. The total order parameter is conserved.

2. For Cahn-Hilliard equation, the energy dissipation is

$$\frac{d\mathscr{E}}{dt} = -\tau\cdot\nabla\mathbf{v} - m|\nabla\mu|^2.$$

17.4 Interface structure

17.4.1 Limiting behaviors of the interfacial layers

Interface energy In this section, we shall study the limit of various free energy. We are particularly interested in the kinetic energy part, which is related to the geometry of the interface.

$$\mathscr{F}[\phi] = \int f(\nabla\phi,\phi)\,d\mathbf{x}$$

1. Let

$$f(\nabla\phi,\phi) = \frac{\varepsilon}{2}|\nabla\phi|^2 + \frac{1}{\varepsilon}W(\phi)\,d\mathbf{x}$$

where W is a double well potential. As $\varepsilon\to 0$, $\phi\to\pm1$. The interface energy tends to

$$\mathscr{F}[\phi]\to\sigma_0|\Gamma(t)|.$$

where σ_0 is a constant.

2. Mean curvature:

$$\int_{\Omega(t)}\frac{\eta}{2}\left(\triangle\phi - \frac{1}{\eta^2}W'(\phi)\right)^2 d\mathbf{x} \approx \int_{\Gamma(t)} H^2\,dS.$$

3. Gaussian curvature:

$$\int_{\Omega(t)}\left(\eta\triangle\phi - \frac{1}{\eta}W'(\phi)\right)W'(\phi)\,d\mathbf{x} \approx \int_{\Gamma(t)} K\,dS.$$

Bulk energy The bulk energy also has many choices.

1. Binary system: Consider a binary system with two components A and B with concentration u_A and u_B, where $u_A + u_B = 1$. The bulk energy is

$$W(u_B) = \mu_A u_A + \mu_B u_B + RT(u_A \ln u_A + u_B \ln u_B) + \alpha u_A u_B.$$

   Here, μ_A, μ_B are the chemical potential of components A and B, R the molar gas constant, T the temperature, α the repulsion parameter between A and B.

2. Nernst-Plank-Poisson model: Consider binary charge system. Let p and n are respectively the concentration of positive and negative charges. The bulk energy is

$$W(p,n) = \int_\Omega p \log p + n \log n + \frac{1}{2}(n-p)V[n-p]\, d\mathbf{x}$$

   where $V[n-p]$ is the potential induced by $n-p$, i.e. $\varepsilon \triangle V = n-p$.

17.4.2 Structure of one dimensional interface

Allen-Cahn interface The order parameter satisfies

$$\phi_t = -\frac{\delta \mathscr{F}}{\delta \phi} = \triangle \phi - W'(\phi)$$

where

$$\mathscr{F} = \int \frac{1}{2}|\nabla \phi|^2 + W(\phi)\, d\mathbf{x}$$

$$W(\phi) = \frac{1}{4}(\phi^2 - 1)^2.$$

The interface is assumed to be steady, so $\phi_t = 0$. Thus, we want to solve

$$\triangle \phi - W'(\phi) = 0.$$

Multiplying ϕ on both sides, we get

$$\frac{d}{dx}\left(\frac{1}{2}\phi'^2 - W(\phi)\right) = 0.$$

We look for ϕ which connecting the two equilibria ± 1 at $x = \pm\infty$ and with $\phi'(\pm\infty) = 0$. Thus, the interface we look for satisfies

$$\frac{1}{2}\phi'^2 - W(\phi) = 0.$$

We can solve this ODE:

$$\phi' = \sqrt{2W} \tag{17.4}$$

By separation of variable

$$\frac{d\phi}{\sqrt{2W(\phi)}} = dx$$

When $W(\phi) = \frac{1}{4}(\phi^2-1)^2$, we get

$$\frac{2d\phi}{1-\phi^2} = \pm dx$$

Integrate this, we get

$$\begin{aligned} x+C &= \int \frac{1}{1-\phi} + \frac{1}{1+\phi}\, d\phi \\ &= \ln\left|\frac{1+\phi}{1-\phi}\right| \end{aligned}$$

Thus, let $\xi = e^{x+C}$ We have

$$\frac{1+\phi}{1-\phi} = \pm\xi.$$

Or

$$\phi = \frac{\xi-1}{\xi+1}, \text{ or } \phi = -\frac{\xi+1}{-\xi+1}.$$

For the first solution, we have $\phi(\pm\infty) = \pm 1$, whereas the second solution satisfies $\phi(\pm\infty) = \mp 1$. In general, ϕ can be expressed as $A + B\tanh(x+C)$.

Let us put the scale back. We consider the energy to be

$$\mathscr{F}^\varepsilon[\phi^\varepsilon] = \int \frac{\varepsilon}{2}|\nabla\phi^\varepsilon|^2 + \frac{1}{\varepsilon}W(\phi^\varepsilon)\, dx$$

This gives the traveling wave equation

$$\varepsilon \triangle \phi^\varepsilon - \frac{1}{\varepsilon}W'(\phi^\varepsilon) = 0.$$

Taking $\phi^\varepsilon(x) = \phi(x/\varepsilon)$, we get the rescaled equation. Notice that in $\mathscr{F}$, the energy for the traveling wave solution ϕ^ε is

$$\mathscr{F}^\varepsilon[\phi^\varepsilon] = \mathscr{F}[\phi] = \sigma_0.$$

This is the interface energy in the normal direction of an interface. In multi-dimension, the interface energy is the integration of this value over the whole surface.

Remark. Let us consider a general double well potential W which has two stable equilibria ϕ_a and ϕ_b. Suppose $W(\phi_a) \neq W(\phi_b)$. In this case, we don't have a standing interface. Instead, we have a traveling wave $\phi((x-ct)/\varepsilon)$, where c is the speed of the traveling wave. Plug this ansatz into equation $\delta\mathscr{F}/\delta\phi = 0$, we get

$$-c\phi' - \triangle\phi + W'(\phi) = 0.$$

Cahn-Hilliard interface The Cahn-Hilliard equation is

$$\phi_t = -\nabla \cdot (m\nabla\mu),\ \mu = -\frac{\delta\mathscr{F}}{\delta\phi}.$$

Again, we look for steady interface. This leads to

$$m(\phi)\nabla\mu = C,$$

or

$$\nabla\mu = \frac{C}{m(\phi)}$$

We assume for the moment that the mobility is independent of ϕ. Then we get

$$\mu = \mu_0 \text{ for all } x.$$

Or

$$-\phi'' + W'(\phi) = \mu_0.$$

We look for solution with $\phi(\pm\infty) = \pm 1$ and $\phi'(\pm\infty) = 0$. Multiplying this equation by ϕ', we get

$$\frac{d}{dx}\left(-\frac{1}{2}\phi'^2 + W(\phi) - \mu_0\phi\right) = 0.$$

Using the far field condition, we get

$$-\frac{1}{2}\phi'^2 + W(\phi) - \mu_0\phi = W(1) - \mu_0.$$

Or

$$\phi'^2 = 2(W(\phi) - W(1) - \mu_0(\phi - 1)) = F(\phi)$$

Thus,

$$\phi' = \pm\left(W(\phi) - W(1) - \mu_0(\phi - 1)\right)^{1/2}.$$

In order to have $\phi'(\pm\infty) = 0$, we see that $F(1) = 0$, we also need to require $F(-1) = 0$. This leads to

$$W(-1) - W(1) - \mu_0(-1-1) = 0,$$

which implies

$$\mu_0 = (W(1) - W(-1))/2 = \frac{W(\phi_a) - W(\phi_b)}{\phi_a - \phi_b}.$$

Here, ϕ_a and ϕ_b are the two equilibra of the double well potential W. Thus, the only addimisible chemical potential connecting two equilibra is the relative energy difference between them. With this choice of chemical potential, we see the interface equation is the same as the Allen-Cahn interface equation. Thus, the structure is the same.

Cahn-Hilliard Traveling wave with nonzero speed Suppose the speed is c, then we look for traveling wave solution $\phi(x-ct)$. In this case, the

Combustion front In reaction-diffusion equation

$$u_t = \triangle u + f(u)$$

where $f(u)$ has two equilibra u_a and u_b.

Appendix A

Notations

Coordinates and flow map

- X Lagrange coordinate
- $\mathbf{x}$ Eulerian coordinate
- $\varphi_t(X) = \mathbf{x}(t, X)$ the flow map
- $\mathbf{u} = \mathbf{x} - X$ displacement
- $\mathbf{v} = \dot{\mathbf{x}}(t, X) = \dot{\mathbf{u}}$ velocity

Strain

- $F = \frac{\partial \mathbf{x}}{\partial X}$: Deformation gradient (for the use in Lagrangian coordinate)
- $C = F^T F$: Left Cauchy-Green strain
- $(F^{-1}) = \frac{\partial X}{\partial x}$: inverse deformation gradient (for the use in Eulerian coordinate)
- $B = FF^T$: Right Cauchy-Green strain
- $E = \frac{1}{2}\left(F + F^T\right) - I$: Green-St. Venant strain.
- $(e_{kl}) = \frac{1}{2}\left(\frac{\partial u^k}{\partial X^l} + \frac{\partial u^l}{\partial X^k}\right)$: Infinitesimal strain in Lagrangian coordinate.
- $\varepsilon = \frac{1}{2}\left(\frac{\partial u^i}{\partial x^j} + \frac{\partial u^j}{\partial x^i}\right)$: Infinitesimal strain in Eulerian coordinate.

Strain-rate

- $D = \frac{1}{2}\left(\nabla\mathbf{v} + (\nabla\mathbf{v})^T\right)$: rate-of-strain, strain-rate tensor
- $\dot{\gamma} = 2D = \dot{\varepsilon}$: rate-of-strain
- $S = \frac{1}{2}\left(\nabla\mathbf{v} - (\nabla\mathbf{v})^T\right)$: Spin tensor
- $\omega = 2S = \nabla\mathbf{v} - (\nabla\mathbf{v})^T$: vorticity tensor.

Stress

- P: First Piola stress
- Σ: Second Piola stress
- σ: Cauchy stress
- τ: deviatoric stress

Appendix B

Surface Theory

B.1 Metric, area and first fundamental form

Deformation and parametrization Let $X \mapsto \mathbf{x}$ be a mapping from $\Sigma_0 \subset \mathbb{R}^2$ to a surface $\Sigma \subset \mathbb{R}^3$. Let $F^i_\alpha = \partial x^i/\partial X^\alpha$ be its differential. For a vector field in $T\Sigma_0$ with $\mathbf{v} = v^\alpha \partial/\partial X^\alpha$, the differential F maps it to $\mathbf{w} = w^i \frac{\partial}{\partial x^i}$ with

$$w^i = F^i_\alpha v^\alpha.$$

We denote this by $\mathbf{w} = F\mathbf{v}$.

First fundamental form. The image of Σ_0 by the map φ_t is in $\mathbb{R}^3$, which is called the ambient space. The space $\mathbb{R}^3$ has a Euclidean inner product structure $(\cdot,\cdot)$. We also call it a metric structure. The mapping $\mathbf{x}(\cdot)$ and the metric $(\cdot,\cdot)$ in the ambient space induce an inner product on the tangent space of Σ_0 (denoted by $T\Sigma_0$). Namely, given any $\mathbf{v}_1, \mathbf{v}_2 \in T\Sigma_0$, we define the inner product of $\mathbf{v}_1$ and $\mathbf{v}_2$ by

$$\langle \mathbf{v}_1, \mathbf{v}_2 \rangle := (F\mathbf{v}_1, F\mathbf{v}_2) = (F^T F\mathbf{v}_1, \mathbf{v}_2).$$

Here, $(\cdot,\cdot)$ is the inner product in the ambient Euclidean space. When we use the basis $\frac{\partial}{\partial X^\alpha}$ in $T\Sigma_0$, the metric has the following representation:

$$\langle \mathbf{v}_1, \mathbf{v}_2 \rangle = g_{\alpha\beta} v_1^\alpha v_2^\beta$$

where

$$g_{\alpha\beta} = \left(\frac{\partial \mathbf{x}}{\partial X^\alpha}, \frac{\partial \mathbf{x}}{\partial X^\beta} \right) = (F^T F)_{\alpha\beta},$$

$$\mathbf{v}_i^\alpha = v_i^\alpha \frac{\partial}{\partial X^\alpha}, \quad i = 1,2.$$

In the language of differential geometry, we express the metric $(\cdot,\cdot)$ in the ambient Euclidean space by

$$g_E = \delta_{ij} dx^i \otimes dx^j.$$

The metric g in Σ_0 is

$$g = g_{\alpha\beta} dX^\alpha \otimes dX^\beta.$$

This metric g is called the first fundamental form for the X-coordinate system on Σ. It is used to measure distance, angle and area on the surface Σ. The length of a vector $\mathbf{v}$ is measured by $\langle \mathbf{v}, \mathbf{v} \rangle$, the angle between two unit vectors $\mathbf{v}_1$ and $\mathbf{v}_2$ is $\langle \mathbf{v}_1, \mathbf{v}_2 \rangle$. Thus, a curve $\{X(t) | 0 \le t \le 1\}$ on Σ_0 has length

$$\int_0^1 \sqrt{g_{\alpha\beta}(X(t)) \dot{X}^\alpha(t) \dot{X}^\beta(t)}\, dt.$$

This is indeed the arc length of the curve $\mathbf{x}(X(t))$ in $\mathbb{R}^3$.

The area spaned by two vectors $\mathbf{v}_1$ and $\mathbf{v}_2$ is

$$\sqrt{\langle \mathbf{v}_1, \mathbf{v}_1 \rangle \cdot \langle \mathbf{v}_2, \mathbf{v}_2 \rangle - \langle \mathbf{v}_1, \mathbf{v}_2 \rangle^2} = J |\mathbf{v}_1| |\mathbf{v}_2|.$$

Here, $J = \sqrt{\det g}$ is the Jacobian of the map $\mathbf{x}(\cdot)$. Thus, the area element on Σ under the metric g is

$$dA = J dX_1 dX_2.$$

B.2 Second fundamental form and intrinsic properties

The normal of Σ is

$$N = \frac{\frac{\partial \mathbf{x}}{\partial X^1} \times \frac{\partial \mathbf{x}}{\partial X^2}}{\| \frac{\partial \mathbf{x}}{\partial X^1} \times \frac{\partial \mathbf{x}}{\partial X^2} \|}$$

This normal N maps Σ_0 to S^2. Its differential dN maps $T\Sigma_0$ to the tangent of S^2, which can be identified to be $T\Sigma$. This is because

$$0 = d(N,N)(v) = 2(dN(v), N),$$

that is, for $v \in T\Sigma_0$, we have $dN(v) \perp N$. Hence, we can identify $dN(v) \in T\Sigma$. In particular,

$$dN(\partial/\partial X^\alpha) := \frac{\partial N}{\partial X^\alpha} \in T\Sigma.$$

We define the second fundamental form $II = (L_{\alpha\beta})$ of Σ to be

$$L_{\alpha\beta} = -\left(\frac{\partial N}{\partial X^\alpha}, \frac{\partial \mathbf{x}}{\partial X^\beta} \right).$$

One can immediately see that

$$L_{\alpha\beta} = \left(N, \frac{\partial^2 \mathbf{x}}{\partial X^\alpha \partial X^\beta}\right).$$

Given a curve $C : \mathbf{x}(X(t)), -\varepsilon < t < \varepsilon$ on Σ_0, we parametrize C by its arc length s. We have $(N(s), \mathbf{x}'(s)) = 0$. Hence, $(N(s), \mathbf{x}''(s)) = -(N'(s), \mathbf{x}'(s))$. Therefore,

$$\begin{aligned} I\!I(X'(0)) &:= -L_{\alpha\beta} X'^{\alpha}(0) X'^{\beta}(0) \\ &= -\left(\frac{\partial N}{\partial X^\alpha} X'^{\alpha}(0), \frac{\partial \mathbf{x}}{\partial X^\beta} X'^{\beta}(0)\right) \\ &= -(N'(0), \mathbf{x}'(0)) = (N(0), \mathbf{x}''(0)) = (N, kn) = k_n. \end{aligned}$$

Here, k is the curvature of the curve C and n is its normal. Thus, the second fundamental measures the curvature of curves on the surface passing through at the same point. The eigenvalue of $I\!I$ w.r.t. the first fundamental form g is called the principal curvature of the surface. If we define

$$W := g^{-1} I\!I,$$

called Weingarten matrix, then the eigenvalues of W are the principal curvatures, its trace is called the mean curvature H and its determinant is called the Gaussian curvature K.

B.2.1 Surface energy

- Membrane
- Plate
- Shell

Bending, twist, Willmott energy.

Reference

1. Elasticity of cell membranes

B.3 Vector, Co-vector and Tensor fields

Vector A vector on $T\Sigma_0$ has the form $\mathbf{v} = v^\alpha \partial/\partial X^\alpha$. Its image under $\mathbf{x}(\cdot)$ is $\mathbf{w} = w^i \partial/\partial x^i$ with

$$w^i = F^i_\alpha v^\alpha.$$

That is, $\mathbf{w} = F\mathbf{v}$.

For any $\mathbf{w} \in T\Sigma$, we can find a unique $\mathbf{v} \in T\Sigma_0$ such that $F\mathbf{v} = \mathbf{w}$. To find $\mathbf{v}$ in terms of $\mathbf{w}$, we use

$$F^i_\beta w^i = F^i_\beta F^i_\alpha$$

In matrix form, it is

$$(F^T F)\mathbf{v} = F^T \mathbf{w}$$

Thus,

$$\mathbf{v} = (F^T F)^{-1} F^T \mathbf{w}.$$

We denote $F^\dagger = (F^T F)^{-1} F^T$, the pseudo-inverse of F. The mapping $FF^\dagger$ is the projection from $\mathbb{R}^3$ to the tangent plane of $T\Sigma$.

Co-vector On $T^*\Sigma_0$, we define dX^α such that $dX^\alpha(\partial/\partial X^\beta) = \delta^\alpha_\beta$. A co-vector $\mathbf{v}^* = v^*_\alpha dX^\alpha$ is defined on $T^*\Sigma$. From Riesz representation theorem, there exists a unique $\mathbf{v} \in T\Sigma_0$ such that

$$\mathbf{v}^*(\partial/\partial X^\alpha) = \langle \mathbf{v}, \partial/\partial X^\alpha \rangle.$$

That is, $v^*_\alpha = g_{\alpha\beta} v^\beta$. This leads to

$$v^\alpha = g^{\alpha\beta} v^*_\beta,$$

where

$$g^{\alpha\beta} := (g^{-1})^{\alpha\beta}.$$

A one-form $\omega = \omega_i dx^i$ in $T^*\Sigma$ can be pull back by

$$\omega_i \frac{\partial x^i}{\partial X^\alpha} dX^\alpha = \omega_i F^i_\alpha dX^\alpha$$

or in matrix form, $F^T\omega$.

Given a one-form $\omega_i dx^i$, the vector $\omega = (\omega_i)$ is a co-vector. In the two form $\nu_i dx^j dx^k$, the vecor (ν_i) is also treated as a covector. Therefore, we can pull back them by $F^T\nu$.

If ν is a unit covector in Σ and $\mathbf{n}$ be the normalized pull back of ν under F, then

$$\mathbf{n} = J^{-1} F^T \nu.$$

Tensor A tensor P on Σ_0 maps a co-vector $\mathbf{n} \in T^*\Sigma_0$ to a vector in $\mathbb{R}^3$. P can be represented as $P^{i\alpha}$ and $P\mathbf{n} = P^{i\alpha} n_\alpha \partial/\partial x^i$ If $\mathbf{n}$ is the pullback (with normalization) of a unit co-vector $\nu \in \mathbb{T}^*\Sigma$, then $n = J^{-1} F^T \nu$. Let T be the tensor which maps a co-vector ν to a vector in $T\Sigma$. $T\nu$ can be represented as $T^{ij} n_j \partial/\partial x_i$. If

$$T\nu = P\mathbf{n},$$

then we have the relation
$$T = J^{-1}PF^T.$$
For hyper-elastic material, $P = W'(F)$.

Alternatively, we can define the tensor $\hat{P}$ on Σ_0 which maps $\mathbf{n} \in T^*\Sigma_0$ to $T\Sigma$ and the tensor $P = F\hat{P}$. In this formulation,
$$F\hat{P}F^T = JT$$
In the case of hyper-elastic material, $\hat{P} = W'(F^TF)$.

B.4 Gradient and Divergence

Scalar field A scalar field ϕ_0 defined on Σ_0 can be push forward to a scalar field defined on Σ by
$$\phi(\mathbf{x}) = \phi_0(X) \quad \text{if} \quad \mathbf{x} = \mathbf{x}(X).$$
Alternatively, we can use delta function to express ϕ:
$$\phi(\mathbf{x}) = \int_{\Sigma_0} \phi_0(X)\delta(\mathbf{x} - \mathbf{x}(X))\, dX$$
Physical quantities such as density is treated as a scalar field on Σ. The gradient of a scalar field is defined by the differential of ϕ_0:
$$d\phi_0 = \nabla_X \phi_0(X) \cdot dX.$$
Thus, $\nabla_X \phi_0$ is a co-vector. It is defined to be the co-vector such that it represents the direction derivative:
$$d\phi_0(\mathbf{v}) = (\nabla_X \phi_0, \mathbf{v}).$$
Here, the meaning of $(\cdot, \cdot)$ is the bilinear functional between vector and co-vector, which is defined so that $(dX^\alpha, \partial/\partial X^\beta) = \delta^\alpha_\beta$. We can also define the gradient $\nabla_\mathbf{x}\phi$ to be
$$d\phi(\mathbf{w}) = (\nabla_x \phi, \mathbf{w})$$
for any vector $\mathbf{w} \in T\Sigma$. Since $\mathbf{v} = F^\dagger \mathbf{w}$, we obtain
$$(\nabla_\mathbf{x}\phi, \mathbf{w}) = (\nabla_X \phi_0, F^\dagger \mathbf{w}) = (F^{\dagger T} \nabla_X \phi_0, \mathbf{w})$$
Hence,
$$\nabla_\mathbf{x}\phi = (F^\dagger)^T \nabla_X \phi_0.$$
This is the definition of $\nabla_\mathbf{x}\phi$ on Σ. Since $F^T(F^\dagger)^T = I$, we then get
$$\nabla_X \phi_0 = F^T \nabla_\mathbf{x}\phi.$$
Thus, the co-vector $\nabla_X \phi_0$ is the pullback of $\nabla_\mathbf{x}\phi$.

Appendix C

Tensor Calculus

references

- S. Wang, M.S. Nabizadeh and A. Chern, Exterior Calculus in Graphics, Course Notes for a SIGRAPH 2023 course (2023).

C.1 Vector Space and Dual Space

Vector space

- A vector space V over $\mathbb{R}$ is a set V with two operations: vector addition and scalar multiplication. They satisfy: (1) $(\mathbf{u}+\mathbf{v})+\mathbf{w} = \mathbf{u}+(\mathbf{v}+\mathbf{w})$; (2) $\mathbf{v}+\mathbf{w} = \mathbf{w}+\mathbf{v}$; (3) $\exists 0 \in V$ such that $\mathbf{v}+0 = 0+\mathbf{v}$ for all $\mathbf{v} \in V$; (4) for any $\mathbf{v} \in V$, $\exists(-\mathbf{v}) \in V$ such that $\mathbf{v}+(-\mathbf{v}) = 0$; (5) for any $a,b \in \mathbb{R}$, any $\mathbf{v},\mathbf{w} \in V$, it holds $(a+b)\mathbf{v} = a\mathbf{v}+b\mathbf{v}$, $a(\mathbf{v}+\mathbf{w}) = a\mathbf{v}+a\mathbf{w}$, $(ab)\mathbf{v} = a(b\mathbf{v})$; (6) $1\mathbf{v} = \mathbf{v}$.

- **Dimension** Let V be vector space over $\mathbb{R}$. It is called an n dimensional space if it can be spanned by n independent elements $\{\mathbf{e}_1,...,\mathbf{e}_n\}$. Such a set is called a basis of V. Any two bases of V contains same number of elements. (why?) This number is called the dimension of V. Any vector $\mathbf{v} \in V$ can be represented uniquely as

$$\mathbf{v} = \sum_{i=1}^{n} v^i \mathbf{e}_i := v^i \mathbf{e}_i.$$

  Here, we will use upper index for the coefficient v^i and lower index for the basis e_i. We use Einstein's notation: whenever same upper index and lower index appear in pair, it means that this is a summation over that index.

Dual Space

- A linear functional on V is a linear function $\alpha : V \to \mathbb{R}$. The dual space of V is defined as
$$V^* := \{\alpha : V \to \mathbb{R} \text{ linear}\}.$$
A linear functional is uniquely determined by its values on a basis $\{\mathbf{e}_1, ..., \mathbf{e}_n\}$. Let $\mathbf{e}^i \in V^*$ with
$$\mathbf{e}^i(\mathbf{e}_j) = \delta^i_j := \begin{cases} 1 & i = j \\ 0 & \text{otherwise.} \end{cases}$$
Then $\{\mathbf{e}^1, ..., \mathbf{e}^n\}$ are independent. For any $\alpha \in V^*$, it can be represented uniquely as
$$\alpha = \alpha_i \mathbf{e}^i, \quad \text{where } \alpha_i := \alpha(\mathbf{e}_i).$$
Thus, $dim(V^*) \cong dim(V)$. The basis $\{\mathbf{e}^1, ..., \mathbf{e}^n\}$ is called *the natural dual basis* corresponding to $\{\mathbf{e}_1, ..., \mathbf{e}_n\}$. An element of V is called a vector, while an element of V^* is called a co-vector.

- $V^{**} \cong V$ Any vector $v \in V$ can be viewed as an element of V^{**} by $v(\alpha) := \alpha(v)$ for any $\alpha \in V^*$. Thus, we have $V \subset V^{**}$. Since $dim(V^{**}) = dim(V^*) = dim(V)$, we get $V^{**} = V$.

- Remark. Sometimes, we express $\alpha(\mathbf{v})$ by $\langle \alpha | \mathbf{v} \rangle$.

Inner Product Space

1. An inner product is a bilinear structure on a vector space V. Namely, $\langle \cdot, \cdot \rangle : V \times V \to \mathbb{R}$ which satisfies

   (a) $\langle a\mathbf{u} + b\mathbf{v}, \mathbf{w} \rangle = a\langle \mathbf{u}, \mathbf{w} \rangle + b\langle \mathbf{v}, \mathbf{w} \rangle$

   (b) $\langle \mathbf{u}, \mathbf{v} \rangle = \langle \mathbf{v}, \mathbf{u} \rangle$

   (c) $\langle \mathbf{u}, \mathbf{u} \rangle \geq 0$ for all $\mathbf{u} \in V$. $\langle \mathbf{u}, \mathbf{u} \rangle = 0$ only when $\mathbf{u} = 0$.

   A vector space equipped with an inner product structure is called an *inner product space*.

2. Given an inner product space V. Let us choose a basis $\mathscr{B} = \{\mathbf{e}_1, ..., \mathbf{e}_n\}$. Then the matrix
$$(g_{ij})_{\mathbf{n} \times n} := (\langle \mathbf{e}_i, \mathbf{e}_j \rangle)_{\mathbf{n} \times n}.$$
is called the matrix representation of the inner product under $\mathscr{B}$. For any two vectors
$$\mathbf{u} = \sum_i u^i \mathbf{e}_i, \quad \mathbf{v} = \sum_j v^j \mathbf{e}_j$$

their inner product can be expressed as

$$\langle \mathbf{u}, \mathbf{v} \rangle = \left\langle \sum_i u^i \mathbf{e}_i, \sum_j v^j \mathbf{e}_j \right\rangle = \sum_{i,j} g_{ij} u^i v^j.$$

3. The matrix $(g_{ij})_{n\times n}$ satisfies
   - $g_{ij} = g_{ji}$
   - $\sum_{ij} g_{ij} v^i v^j \geq 0$ for all $\mathbf{v} = \sum_i v^i \mathbf{e}_i$.
   - $\sum_{ij} g_{ij} v^i v^j = 0$ if and only if $\mathbf{v} = 0$.

Riesz representation and the music isomorphism

1. **Music isomorphism**

   Theorem 3.18 (Riesz representation Theorem)**.** *Let V be an inner product space. Then the inner product $\langle \cdot, \cdot \rangle$ induces a natural isomorphism between V and V^*, called music isomorphism:*

   (a) $V \xrightarrow{\flat} V^*$: For any $\mathbf{w} \in V$, it induces a natural linear functional $\mathbf{v} \mapsto \langle \mathbf{w}, \mathbf{v} \rangle$. We denote this linear functional by $\flat(w)$ or $\mathbf{w}^\flat$. That is,

   $$\langle \flat \mathbf{w} | \mathbf{v} \rangle = \langle \mathbf{w}, \mathbf{v} \rangle.$$

   (b) $V^* \xrightarrow{\sharp} V$: For any $\alpha \in V^*$, there exists a unique vector $\mathbf{w}$ such that $\alpha(\mathbf{v}) = \langle \mathbf{w}, \mathbf{v} \rangle$ for all $\mathbf{v} \in V$. We denote $\mathbf{w}$ by $\sharp\alpha$ or $\alpha^\sharp$. That is,

   $$\langle \sharp\alpha, \mathbf{v} \rangle = \langle \alpha | \mathbf{v} \rangle.$$

   (c) It holds $\flat^{-1} = \sharp$.

   Proof. (a) Proof of (b). We shall only prove (b), the rests are easy. Let us assume that we can find an *orthonormal basis* in V, say $\{\mathbf{e}_1, ..., \mathbf{e}_n\}$. Then for any $\mathbf{v} \in V$, it has the representation

   $$\mathbf{v} = \sum_{i=1}^{n} \langle \mathbf{v}, \mathbf{e}_i \rangle \mathbf{e}_i.$$

   Now, for any $\alpha \in V^*$, we define

   $$\sharp\alpha = \alpha(\mathbf{e}_1)\mathbf{e}_1 + \cdots + \alpha(\mathbf{e}_n)\mathbf{e}_n.$$

Then

$$\langle \sharp\alpha, \mathbf{v}\rangle = \sum_{i=1}^{n} \alpha(\mathbf{e}_i)\langle \mathbf{e}_i, \mathbf{v}\rangle = \alpha\left(\sum_{i=1}^{n} \langle \mathbf{v}, \mathbf{e}_i\rangle \mathbf{e}_i\right) = \alpha(\mathbf{v}).$$

Given $\alpha \in V^*$, suppose both $\mathbf{w}_1$ and $\mathbf{w}_2$ satisfy

$$\langle \mathbf{w}_1, \mathbf{v}\rangle = \alpha(\mathbf{v}), \quad \langle \mathbf{w}_2, \mathbf{v}\rangle = \alpha(\mathbf{v}) \text{ for all } \mathbf{v} \in V.$$

Then, we have

$$\langle \mathbf{w}_1 - \mathbf{w}_2, \mathbf{v}\rangle = 0 \text{ for all } \mathbf{v} \in V.$$

This leads to $\mathbf{w}_1 = \mathbf{w}_2$. This shows the uniqueness.

(b) Proof of (c): From (a) and (b), we get that for any $\mathbf{w}$ and $\mathbf{v}$, we have

$$\langle \sharp\flat\mathbf{w}, \mathbf{v}\rangle = \langle \flat\mathbf{w}|\mathbf{v}\rangle = \langle \mathbf{w}, \mathbf{v}\rangle$$

This leads to

$$\sharp\flat\mathbf{w} = \mathbf{w}$$

for any $\mathbf{w} \in V$. Thus, $\sharp\flat = id$.

□

2. Representation of $\flat$: Suppose $\mathscr{B} = \{\mathbf{e}_1, ..., \mathbf{e}_n\}$ is a basis of V and $\mathscr{B}^* = \{\mathbf{e}^1, ..., \mathbf{e}^n\}$ is its natural dual basis in V^*. Let $g_{ij} = \langle \mathbf{e}_i, \mathbf{e}_j\rangle$. Let us express

$$\mathbf{v} = v^j \mathbf{e}_j \quad \flat\mathbf{v} = v_i \mathbf{e}^i,$$

This means that the super index v^i is lower down to a sub index v_i in $\flat\mathbf{v}$. (This is why it is called the *flat* operator.) Then

$$v_i = g_{ij} v^j.$$

3. Let V be an inner product space with the inner product $\langle \cdot, \cdot\rangle_V$. This inner product induces an inner product $\langle \cdot, \cdot\rangle_{V^*}$ in V^*. Let $\alpha, \beta \in V^*$. Let $\sharp : V^* \to V$ be the sharp operator induced by $\langle \cdot, \cdot\rangle_V$. We define

$$\langle \alpha, \beta\rangle_{V^*} := \langle \sharp\alpha, \sharp\beta\rangle_V.$$

Let us denote

$$\langle \mathbf{e}^i, \mathbf{e}^j\rangle_{V^*} = g^{ij}.$$

4. Let $\alpha \in V^*$. Let us express $\alpha \in V^*$ and $\sharp\alpha \in V$ by
$$\alpha = \alpha_i \mathbf{e}^i, \quad \alpha = \alpha^i \mathbf{e}_i.$$
Then
$$\alpha^i = g^{ij}\alpha_j.$$

5. The relation between (g_{ij}) and (g^{ij}) is
$$(g^{ij})_{n\times n} = \left(g_{ij}\right)^{-1}_{n\times n}.$$
This follows from $\sharp\flat = id$: Given $\mathbf{v} = v^i\mathbf{e}_i$. We have
$$(\flat\mathbf{v})_k = g_{kj}v^j, \quad (\sharp(\flat\mathbf{v}))^i = g^{ik}(\flat\mathbf{v})_k = g^{ik}g_{kj}v^j.$$
Since $\sharp\flat = id$, we get
$$v^i = g^{ik}g_{kj}v^j$$
for any $\mathbf{v} = v^i\mathbf{e}_i$. This gives
$$g^{ik}g_{kj} = \delta^i_j.$$

C.2 Tensor Algebra

- **Tensor product and tensor spaces** Tensor product of two vectors: Let U, V be two vector spaces over $\mathbb{R}$. Let $\mathbf{u} \in U$ and $\mathbf{v} \in V$. The tensor product of them, denoted by $\mathbf{u}\otimes\mathbf{v}$ is defined as an operation satisfying linearity in both u and v, associativity, but no commutativity. The tensor product of U and V is defined as
$$U\otimes V := \mathrm{Span}\{\mathbf{u}\otimes\mathbf{v} | \mathbf{u} \in U, \mathbf{v} \in V\}$$
An element in $U\otimes V$ is called a tensor.

- If $\{\mathbf{u}_1, \cdots, \mathbf{u}_m\}$ and $\{\mathbf{v}_1, \cdots, \mathbf{v}_n\}$ are bases of U and V respectively, then $\{\mathbf{u}_i\otimes\mathbf{v}_j | i = 1,...,m, j = 1,...,n\}$ constitutes a basis of $U\otimes V$. Thus, $dim(U\otimes V) = dim(U)\cdot dim(V)$.

- **Tensor Type** Let us introduce the notations:
$$\otimes^r V := \underbrace{V\otimes\cdots\otimes V}_{r \text{ times}}$$
An element T in
$$(\otimes^r V)\otimes(\otimes^s V^*) = \underbrace{V\otimes\cdots\otimes V}_{r \text{ times}}\otimes\underbrace{V^*\otimes\cdots\otimes V^*}_{s \text{ times}}$$
is called a tensor in V of type (r,s).

- **Tensor as a multilinear functional** A tensor on V can also be viewed as a multilinear function on V. For instance, a bilinear function on V is a function

$$A : V \times V \to \mathbb{R},$$

which is linear in both arguments. We denote the set of all bilinear linear functions on V by $\mathscr{L}(V,V)$. We claim that

$$V^* \otimes V^* \cong \mathscr{L}(V,V).$$

To check this claim, we first see that a tensor $T \in V^* \otimes V^*$ is a bilinear function on V. If $T = \alpha \otimes \beta$ with $\alpha, \beta \in V^*$, we define

$$\alpha \otimes \beta(\mathbf{u},\mathbf{v}) := \alpha(\mathbf{u})\beta(\mathbf{v})$$

for vectors $u, v \in V$. If $T = \sum_{i=1}^N a_i \alpha_i \otimes \beta_i$, we define

$$T(\mathbf{u},\mathbf{v}) := \sum_{i=1}^N a_i \alpha_i(\mathbf{u})\beta_i(\mathbf{v}).$$

Thus, a tensor $T \in V^* \otimes V^*$ is a bilinear function on V. Conversely, let $\{\mathbf{e}_1, ..., \mathbf{e}_n\}$ and $\{\mathbf{e}^1, ..., \mathbf{e}^n\}$ are a pair of dual bases in V and V^* with $\mathbf{e}^i(\mathbf{e}_j) = \delta^i_j$. For any bilinear function A, we can define a tensor T_A as

$$T_A := \sum_{i=1}^n \sum_{j=1}^n A(\mathbf{e}_i, \mathbf{e}_j)\mathbf{e}^i \otimes \mathbf{e}^j.$$

Then one can check that

$$T_A(\mathbf{u},\mathbf{v}) = A(\mathbf{u},\mathbf{v})$$

for any $\mathbf{u},\mathbf{v} \in V$. The mapping: $A \mapsto T_A$ is linear. The two spaces $\mathscr{L}(V,V)$ and $V^* \otimes V^*$ have the same dimension. Thus, $\mathscr{L}(V,V) = V^* \otimes V^*$.

- In general, let

$$\mathscr{L}(\underbrace{V^*, \cdots, V^*}_{r \text{ times}}, \underbrace{V, \cdots, V}_{s \text{ times}})$$

be the space of all multilinear functions from $V^* \times \cdots \times V^* \times V \times \cdots \times V \to \mathbb{R}$. Then

$$\mathscr{L}(\underbrace{V^*, \cdots, V^*}_{r \text{ times}}, \underbrace{V, \cdots, V}_{s \text{ times}}) \cong \underbrace{V \otimes \cdots \otimes V}_{r \text{ times}} \otimes \underbrace{V^* \otimes \cdots \otimes V^*}_{s \text{ times}}.$$

An element T there is called a *type* (r,s) *tensor*. It can be expressed as

$$T = T^{i_1,...,i_r}_{j_1,...,j_s} \mathbf{e}_{i_1} \otimes \cdots \otimes \mathbf{e}_{i_r} \otimes \mathbf{e}^{j_1} \otimes \cdots \otimes \mathbf{e}^{j_s}$$

For example, the metric tensor

$$g = g_{ij}\mathbf{e}^i \otimes \mathbf{e}^j$$

is a type-$(0,2)$ tensor.

- **Space of linear maps as a tensor space** Let V, W be two vector spaces. Let

$$Hom(V,W) = \{A : V \to W \text{ linear map}\}.$$

Then

$$Hom(V,W) \cong V^* \otimes W \cong \mathscr{L}(V,W^*). \tag{3.1}$$

For any $A \in Hom(W,W)$ we can identify it as a bilinear functional T_A in $V \times W^*$ by

$$T_A(\mathbf{v}, \mathbf{w}^*) := \mathbf{w}^*(A\mathbf{v}).$$

You can show that $A \mapsto T_A$ is linear, 1-1 and onto.

- **Adjoint operator and symmetric operator:** For $A \in Hom(V,W)$, we define its adjoint $A^* \in Hom(W^*,V^*)$ by

$$\langle A^* w^* | v \rangle := \langle w^* | Av \rangle.$$

If $A \in Hom(V,V^*)$, we call A is symmetric if $A^* = A$. For $A \in Hom(V,V^*)$ which is also $\mathscr{L}(V^*,V^*)$, we can represent A by

$$A = A_{ij}\mathbf{e}^i \otimes \mathbf{e}^j.$$

- **Remark** Let V be a vector space. We have

$$\begin{aligned}
&(1)\ Hom(V,V) \cong V^* \otimes V \cong \mathscr{L}(V,V^*)\\
&(2)\ Hom(V^*,V) \cong V \otimes V \cong \mathscr{L}(V^*,V^*)\\
&(3)\ Hom(V,V^*) \cong V^* \otimes V^* \cong \mathscr{L}(V,V)\\
&(4)\ Hom(V^*,V^*) \cong V \otimes V^* \cong \mathscr{L}(V^*,V)
\end{aligned}$$

When we choose a basis $\mathscr{B}_V$ and its natural dual bases $\mathscr{B}_V^*$, the matrix representations of the above tensors, say A, are

$$(1)\ a_i^j, \quad (2)\ a^{ij}, \quad (3)\ a_{ij}, \quad (4)\ a_j^i.$$

They look similar, but their tensor types are different!

- **Two-point tensors**. Let us consider the tensor space:

$$\underbrace{V \otimes \cdots \otimes V}_{r_1 \text{ times}} \otimes \underbrace{V^* \otimes \cdots \otimes V^*}_{s_1 \text{ times}} \otimes \underbrace{W \otimes \cdots \otimes W}_{r_2 \text{ times}} \otimes \underbrace{W^* \otimes \cdots \otimes W^*}_{s_2 \text{ times}}$$

We call its element a *two-point tensor with type* $(r_1, s_1; r_2, s_2)$.

C.3 Some tensor notations

We shall use a matrix to represent rank 2 tensors and matrix algebra for tensor algebra.

- A rank 1 tensor is a vector, such as the velocity field $\mathbf{v}$, the outer normals $\nu, \mathbf{n}$.
- A rank 2 tensor is a matrix, for example, the stress tensor σ, $\mathbf{I}$.
- Tensor product $\mathbf{vw} := v^i w^j$.
- Scalar product $\mathbf{v}\cdot\mathbf{w} = v^i w^i$, $\sigma\cdot\nu = \sigma^i_j \nu^j$, $\mathbf{A}\cdot\mathbf{B} = A^i_j B^j_k$.
- Scalar product of rank 2 tensors $\mathbf{A}:\mathbf{B} = A_{ij}B_{ij}$.
- Nabla operator ∇:
$$(\nabla\mathbf{v})^i_j := \frac{\partial v^i}{\partial x^j}$$
$$\nabla\cdot\mathbf{v} := \frac{\partial v^j}{\partial x^j},$$
For an $m\times 3$ matrix-valued function $\mathcal{F} = (\mathcal{F}_1, \mathcal{F}_2, \mathcal{F}_3)$,
$$\nabla\cdot\mathcal{F} := \frac{\partial \mathcal{F}_j}{\partial x^j}$$
which is an m-vector.
$$\nabla\times\mathcal{F}^T := \left(\frac{\partial\mathcal{F}_3}{\partial x^2} - \frac{\partial\mathcal{F}_2}{\partial x^3}, \frac{\partial\mathcal{F}_1}{\partial x^3} - \frac{\partial\mathcal{F}_3}{\partial x^1}, \frac{\partial\mathcal{F}_2}{\partial x^1} - \frac{\partial\mathcal{F}_1}{\partial x^2}\right),$$
which is again an $m\times 3$ matrix-valued function.
- Note that for $\mathbf{v}$ being a 3×1 vector, f a scalar function, we have
$$(\mathbf{v}\cdot\nabla)f = (\nabla f)\cdot\mathbf{v} = v^i\partial_i f$$
For $\mathbf{w}$ being an $m\times 1$ vector, we have
$$(\mathbf{v}\cdot\nabla)\mathbf{w} = (\nabla\mathbf{w})\cdot\mathbf{v} = v_j\partial_j w^i.$$
- In the tensor community, ∇ is treated as a column vector and $\nabla\mathbf{v}$ is defined to be $\partial_{x^i} v^j$, which is different from us. Some people uses $\mathbf{v}\otimes\nabla$ to stand for $\partial_{x^j} v^i$. (e.g. Vlado A. Lubarda). We will only use $\nabla\mathbf{v}$ to stand for $\partial_{x^j} v^i$ and $\nabla\cdot\mathcal{F} = \partial_{x^j}\mathcal{F}_j$.

Theorem 3.19 (Divergence theorem)**.** *Let $\mathcal{F}: \Omega(\subset\mathbb{R}^3)\to\mathbb{R}^m\times\mathbb{R}^3$ be a vector field. Then*
$$\int_{\partial\Omega}\mathcal{F}\cdot\nu\, dS = \int_\Omega \nabla\cdot\mathcal{F}\, d\mathbf{x}.$$
Here, $\partial\Omega$ denotes for the boundary of Ω, dS is the surface element, and ν is the outer normal of $\partial\Omega$.

C.4 Tensors in Euler and Lagrange coordinates

C.4.1 Eulerian and Lagrangian coordinates

Let $\hat{M}$ be the initial configuration and M be the current configuration at time t. X be the coordinate on $\hat{M}$ and $\mathbf{x}$ be the coordinate on $M \subset \mathbb{R}^n$. We first make a table of correspondence of notations between vector calculus and differential geometry. The notation of vector calculus we use is from the book: Aleksey Drozdov, Finite Elasticity and Viscoelasticity (1996) and Mechanics of Viscoelastic Solids (1998).

Let $\mathbf{x}(t,X)$ be the flow map. We also denote it by $\varphi_t : \hat{M} \to M$. We will neglect t later in the correspondence table when we have a fixed time t. The reference configuration space $\hat{M}$ is indeed identical to M except they use different coordinate system. Thus, $\partial/\partial X^i$ is a tangent vector on $\hat{M}$, which is realized as $\partial \mathbf{x}/\partial X^i$ in the Euclidean space. The metric of $\hat{M}$ is induced by the imbedded metric in $\mathbb{R}^n$.

Euler		
Name	Vector Calculus	Differential Geometry
basis in tangent space (vectors)	$e_i = \partial \mathbf{x}/\partial x^i$	$\partial/\partial x^i$
metric in tangent space	$(e_i \cdot e_j) = I$	$g_{ij} := \langle \partial/\partial x^i, \partial/\partial x^j \rangle = \delta_{ij}$
basis in cotangent space (co-vectors)	e^i, $e^i \cdot e_j = \delta^i_j$	dx^i, $(dx^i, \partial/\partial x^j) = \delta^i_j$
metric in cotangent space	$g^{ij} = e^i \cdot e^j = \delta^{ij}$	$g^{ij} = \langle dx^i, dx^j \rangle = \delta^{ij}$
contravariant component (vector)	$\mathbf{v} = v^i e_i$	$\mathbf{v} = v^i \partial/\partial x^i$
covariant component (co-vector)	$\eta = \eta_i e^i$	$\eta = \eta_i dx^i$
Music notation	$v^i = g^{ij} v_i$	$\mathbf{v} = \mathbf{v}^\flat = \mathbf{v}^\sharp$
Tensor product	$\mathbf{v}_1 \mathbf{v}_2$	$\mathbf{v}_1 \otimes \mathbf{v}_2$

Lagrange		
Name	Vector Calculus	Differential Geometry
tangent basis	$\bar{g}_\alpha = \partial \mathbf{x}/\partial X^\alpha$	$\partial/\partial X^\alpha$
cotangent basis	$\bar{g}^\alpha = \partial X^\alpha/\partial \mathbf{x}$	dX^α
duality	$\bar{g}^\alpha \cdot \bar{g}_\beta = \delta^\alpha_\beta$	$(dX^\alpha, \partial/\partial X^\beta) = \delta^\alpha_\beta$
deformation gradient	$[\bar{g}_1, \bar{g}_2, \bar{g}_3] = F$	$d\varphi$
metric in tangent space	$(\bar{g}_\alpha \cdot \bar{g}_\beta) = F^T F$	$g_{\alpha\beta} := \langle \partial/\partial X^\alpha, \partial/\partial X^\beta \rangle$
metric in cotangent space	$g^{\alpha\beta} = \bar{g}^\alpha \cdot \bar{g}^\beta$	$g^{\alpha\beta} = \langle dX^\alpha, dX^\beta \rangle$
contravariant component	$\bar{q} = q^\alpha \bar{g}_\alpha$	$\bar{q} = q^\alpha \partial/\partial X^\alpha$
covariant component	$\bar{q} = q_\alpha \bar{g}^\alpha$	$\bar{q} = q_\alpha dX^\alpha$
Music notation	$q^\alpha = g^{\alpha\beta} q_\alpha$	$\bar{q} = \bar{q}^\flat = \bar{q}^\sharp$
Tensor product	$\bar{q}_1 \bar{q}_2$	$\bar{q}_1 \otimes \bar{q}_2$

C.4.2 Coordinate systems and bases

- The configuration space M is in the Euclidean space. We use natural basis $\{e_i\}$ for TM. We also treat $T^*M = TM$ and use $\{e^i\}$ as the basis in T^*M. In the language of differential geometry,
$$e_i = \frac{\partial}{\partial x^i}, \quad e^i = dx^i.$$
- In TM, we can have another frame, the Lagrangian frame:
$$\bar{g}_\alpha := \frac{\partial x^i}{\partial X^\alpha} e_i = F^i_\alpha e_i.$$
In DG,
$$\bar{g}_\alpha = \frac{\partial}{\partial X^\alpha}.$$
The inner product of $\bar{g}_\alpha$ and $\bar{g}_\beta$ is induced by the Euclidean space TM. Thus
$$\bar{g}_\alpha \cdot \bar{g}_\beta := \sum_k F^k_\alpha F^\ell_\beta e_k \cdot e_\ell = \sum_k F^k_\alpha F^k_\beta := g_{\alpha\beta}.$$
- Similarly, in T^*M, the corresponding Lagrangian frame is
$$\bar{g}^\beta = (F^{-1})^\beta_\ell e^\ell.$$
Since $F^i_\beta = \frac{\partial x^i}{\partial X^\beta}$, we get
$$(F^{-1})^\beta_\ell = \frac{\partial X^\beta}{\partial x^\ell}.$$
We have
$$\bar{g}_\alpha \cdot \bar{g}^\beta = \delta^\beta_\alpha$$
and
$$\bar{g}^\alpha \cdot \bar{g}^\beta = (F^{-T}F^{-1})^{\alpha\beta} = \sum_k \frac{\partial X^\alpha}{\partial x^k}\frac{\partial X^\beta}{\partial x^k}.$$
In Differential Geometry,
$$\bar{g}^\alpha = dX^\alpha.$$
- Deformation gradient:
$$\begin{array}{ll} (F)^i_\alpha = F^i_\alpha = \frac{\partial x^i}{\partial X^\alpha} & \quad (F^{-1})^\alpha_i = \frac{\partial X^\alpha}{\partial x^i} \\ (F^T)^\alpha_i = F^i_\alpha = \frac{\partial x^i}{\partial X^\alpha} & \quad (F^{-T})^i_\alpha = (F^{-1})^\alpha_i \end{array}$$
$$(F^TF)_{\alpha\beta} = (F^T)^\alpha_k F^k_\beta = F^k_\alpha F^k_\beta = \bar{g}_\alpha \cdot \bar{g}_\beta.$$
$$(FF^T)^{ij} = F^i_\alpha (F^T)^\alpha_j = F^i_\alpha F^j_\alpha$$

C.4.3 Representation of vectors

- **Euler coordinate** For a vector in $\mathbf{v} \in TM = T^*M$, we can represent it as

$$\mathbf{v} = v^i e_i = v_i e^i.$$

- **Lagrange coordinate** We can also represent $\mathbf{v}$ in Lagrange coordinate system, we call it the pull-back of $\mathbf{v}$ and denote it by $\bar{p}$. It is still the same vector, but in different coordinate system. Thus,

$$\mathbf{v} = v_i dx^i = v_i \frac{\partial x^i}{\partial X^k} dX^k = v_i F^i_k dX^k.$$

or its pull-back (same vector, but represented in Lagrange coordinate system)

$$\bar{p} = p_k \bar{g}^k$$

Thus,

$$p_k = v_i F^i_k.$$

A vector $\bar{p}$ can be represented as

$$\bar{p} = p_k \bar{g}^k = p^k \bar{g}_k.$$

From

$$\bar{g}^i = g^{ij} \bar{g}_j, \quad \bar{g}_i = g_{ij} \bar{g}^j,$$

we get

$$p^i = g^{ij} p_i, \quad p_i = g_{ij} p^j.$$

- Inner product: Suppose the pull-back of $\mathbf{v}$ and $\mathbf{w}$ are $\bar{p}$ and $\bar{q}$, respectively. The inner product of $\mathbf{v}$ and $\mathbf{w}$ is a scalar

$$\mathbf{v} \cdot \mathbf{w} := v_i w^i = v^i w_i = p^i q_i = p_i q^i.$$

We have

$$e_i \cdot e^j = e_i \cdot e_j = e^i \cdot e^j = \delta_i^j$$

$$\bar{g}_i \cdot \bar{g}_j = g_{ij}, \quad \bar{g}^i \cdot \bar{g}^j = g^{ij}, \quad \bar{g}_i \cdot \bar{g}^j = \delta_i^j.$$

C.4.4 Tensor

- The tensor product of $\bar{p}$ and $\bar{q}$ has the representation

$$\bar{p}\bar{q} = p_i q_j \bar{g}^i \bar{g}^j.$$

Note that $\bar{p}\bar{q} \neq \bar{q}\bar{p}$.

- In Eulerian coordinate, a tensor T can be represented as

$$T = T^{ij} e_i e_j = T_{ij} e^i e^j = T^i_j e_i e^j = T_i^j e^i e_j, \quad T_{ij} = T^{ij} = T^i_j = T_i^j.$$

Its pullback Q in the Lagrange coordinate system can be represented as

$$Q = Q_{ij} \bar{g}^i \bar{g}^j = Q^{ij} \bar{g}_i \bar{g}_j = Q^i_j \bar{g}_i \bar{g}^j = Q_i^j \bar{g}^i \bar{g}_j.$$

The transformation of the coefficients is, for example,

$$T^{k\ell} = Q^{ij} F_i^k F_j^\ell$$

obtained by using $\bar{g}_i = F_i^k e_k$.
One can also check that

$$Q_{ij} = Q^{k\ell} g_{ik} g_{j\ell} = Q^k_j g_{ik} = Q_i^k g^{kj}.$$

The transpose of Q the above tensor Q is defined as

$$\begin{aligned} Q^T &= Q_{ji} \bar{g}^i \bar{g}^j = Q^{ji} \bar{g}_i \bar{g}_j = Q_i^j \bar{g}_i \bar{g}^j = Q^i_j \bar{g}^i \bar{g}_j \\ &= Q_{ij} \bar{g}^j \bar{g}^i = Q^{ij} \bar{g}^i \bar{g}^j == Q^i_j \bar{g}_j \bar{g}^i = Q_i^j \bar{g}^j \bar{g}_i. \end{aligned}$$

- The inner product of tensor and vector is

$$Q \cdot \bar{q} = Q_{ij} \bar{g}^i \bar{g}^j \cdot q^k \bar{g}_k = Q_{ik} q^k \bar{g}^i.$$

It can also be represented as

$$Q \cdot \bar{q} = Q_i^j \bar{g}^i \bar{g}_j \cdot q_k \bar{g}^k = Q_i^k q_k \bar{g}^i.$$

One can check that

$$\boxed{Q \cdot \bar{q} = \bar{q} \cdot Q^T \quad \text{and} \quad (P \cdot Q)^T = Q^T \cdot P^T.}$$

For the first one, we have

$$Q \cdot \bar{q} = Q_{ij} \bar{g}^i \bar{g}^j \cdot q^k \bar{g}_k = Q_{ik} q^k \bar{g}^i,$$

$$\bar{q} \cdot Q^T = q^k \bar{g}_k \cdot Q_{ij} \bar{g}_j \bar{g}_i = q^k Q_{ik} \bar{g}_i = Q \cdot \bar{q}.$$

For the second one,

$$P \cdot Q = P_{ij} \bar{g}^i \bar{g}^j \cdot Q^k_\ell \bar{g}_k \bar{g}^\ell = P_{ik} Q^k_\ell \bar{g}^i \bar{g}^\ell.$$

$$Q^T P^T = Q^k_\ell \bar{g}^\ell \bar{g}_k P_{ij} \bar{g}^j \bar{g}^i = Q^k_\ell P_{ik} \bar{g}^\ell \bar{g}^i = (P \cdot Q)^T.$$

One can also define

$$Q^2 := Q \cdot Q, \quad Q^3 := Q \cdot Q^2 = Q^2 \cdot Q, etc.$$

- Convolution
$$P : Q = P_{ij} \bar{g}^i \bar{g}^j Q^{k\ell} \bar{g}_l \bar{g}_\ell := P_{ij} Q^{ij}.$$

- The unit tensor
$$\begin{aligned} I &= e^i e^j = e^i e_j = e_i e^j = e_i e_j \\ &= g_{ij} \bar{g}^i \bar{g}^j = \bar{g}^i \bar{g}_j = \bar{g}_i \bar{g}^j = g^{ij} \bar{g}_i \bar{g}_j \end{aligned}$$

  One can show that for any tensor Q,
$$Q \cdot I = I \cdot Q = Q.$$

- A tensor $Q = Q_{ij} e^i e^j$ is called isotropic if for every rotation R,
$$Q = Q_{ij} (Re^i)(Re^j)$$

  It can be shown that an isotropic 2-tensor has the form $Q = \alpha I$. Similarly, a rank n tensor $Q_{i_1,\ldots,i_n} e^{i_1} \cdots e^{i_n}$ is called isotropic if
$$Q = Q_{i_1,\ldots,i_n} (Re^{i_1}) \cdots (Re^{i_n})$$

  for any rotation R.
  Homework: Show that an isotropic rank n tensor depends only n parameters.

Connections ∇ operator (Connection)

- We define the nabla operator as
$$\nabla := e^i \frac{\partial}{\partial x^i} = \bar{g}^i \frac{\partial}{\partial X^i}.$$

  We can think ∇ is a vector. Its pullback is $\bar{g}^i \frac{\partial}{\partial X^i}$.

- For a function f, its differential

$$
\begin{aligned}
df &= \frac{\partial f}{\partial x^i} dx^i = \nabla f \cdot d\mathbf{x} \\
&= \frac{\partial f}{\partial X^i} dX^i = \frac{\partial f}{\partial X^i}\frac{\partial X^i}{\partial x^j} dx^j = \frac{\partial f}{\partial X^i}\bar{g}^i \cdot d\mathbf{x}
\end{aligned}
$$

Here, we treat $d\mathbf{x}$ as a vector: $d\mathbf{x} = dx^i e_i$. The term ∇f is a vector

$$\nabla f = \frac{\partial f}{\partial x^i} e^i = \frac{\partial f}{\partial X^i}\bar{g}^i.$$

We can change the type of ∇f as

$$\nabla f = \frac{\partial f}{\partial x^i} e^i = \frac{\partial f}{\partial x^i}\delta^{ij} e_j = \frac{\partial f}{\partial x^i} e_i.$$

$$\nabla f = \frac{\partial f}{\partial X^i}\bar{g}^i = \left(\frac{\partial f}{\partial X^i} g^{ij}\right)\bar{g}_j.$$

- For a vector $\mathbf{w} = w^i e_i$ with pull-back $\bar{q} = q^i \bar{g}_i$,

$$\nabla \mathbf{w} = \frac{\partial}{\partial x^i} e^i w_j e^j = \frac{\partial w_j}{\partial x^i} e^i e^j$$

$$d\mathbf{w} = dx^i \frac{\partial w_j}{\partial x^i} e^j = dx^k e_k \cdot \frac{\partial w_j}{\partial x^i} e^i e^j = d\mathbf{x} \cdot \nabla \mathbf{w} = (\nabla \mathbf{w})^T \cdot d\mathbf{x}.$$

- For the pull-back $\bar{q}$ of the vector $\mathbf{w}$, we have

$$\nabla \bar{q} = \bar{g}^i \frac{\partial}{\partial X^i}(q_j \bar{g}^j) = \bar{g}^i \left(\frac{\partial q_j}{\partial X^i}\bar{g}^j + q_k \frac{\partial \bar{g}^k}{\partial X^i}\right),$$

The term $\frac{\partial \bar{g}^k}{\partial X^i}$ is a vector, it can be represented as

$$\frac{\partial \bar{g}^k}{\partial X^i} = -\Gamma^k_{ij}\bar{g}^j.$$

Here, the coefficients Γ^k_{ij} are called the Christoffel symbol of second kind. We denote

$$\nabla_{X^i}\bar{q} := \frac{\partial}{\partial X^i}\bar{q} := \left(\frac{\partial q_j}{\partial X^i} - q_k \Gamma^k_{ij}\right)\bar{g}^j.$$

Thus,

$$\nabla \bar{q} = \bar{g}^i \frac{\partial \bar{q}}{\partial X^i} = \left(\frac{\partial q_j}{\partial X^i} - q_k \Gamma^k_{ij}\right)\bar{g}^i \bar{g}^j.$$

$$d\mathbf{x} = dx^i e_i = dX^j \frac{\partial x^i}{\partial X^j} e_i = dX^j \bar{g}_j.$$

Hence

$$d\mathbf{x} \cdot \nabla \bar{q} = dX^k \bar{g}_k \cdot (\bar{g}_i \frac{\partial \bar{q}}{\partial X^i}) = dX^k \frac{\partial \bar{q}}{\partial X^k} = d\bar{q}$$

We also have

$$d\bar{q} = d\mathbf{x} \cdot \nabla \bar{q} = (\nabla \bar{q})^T \cdot d\mathbf{x}.$$

Similarly, we have

$$\nabla \bar{q} = \bar{g}^i \frac{\partial}{\partial X^i}(q^j \bar{g}_j) = \bar{g}^i \left(\frac{\partial q^j}{\partial X^i} \bar{g}_j + q^k \frac{\partial \bar{g}_k}{\partial X^i} \right),$$

Differentiate $\bar{g}_k \cdot \bar{g}^\ell = \delta_k^\ell$, we get

$$\frac{\partial \bar{g}^k}{\partial X^i} = \Gamma_{ki}^j \bar{g}_j,$$

Thus,

$$\nabla \bar{q} = \left(\frac{\partial q^j}{\partial X^i} + q^k \Gamma_{ki}^j \right) \bar{g}^i \bar{g}_j.$$

- Divergence: for a vector $\mathbf{w}$ and its pull-back $\bar{q}$, the divergence

$$\nabla \cdot \mathbf{w} = e^i \frac{\partial}{\partial x^i} \cdot w^j e_j = \frac{\partial w^i}{\partial x^i}.$$

$$\nabla \cdot \bar{q} = \bar{g}^i \frac{\partial}{\partial X^i} \cdot \left(q^j \bar{g}_j \right) = \frac{\partial q^i}{\partial X^i} + q^\ell \Gamma_{\ell i}^i.$$

For a tensor Q,

$$\nabla \cdot Q = \frac{\partial Q_{ij}}{\partial x^i} e^j.$$

- Properties of ∇:

$$\nabla(f_1 f_2) = (\nabla f_1) f_2 + f_1 (\nabla f_2).$$
$$\nabla(\bar{q}_1 \cdot \bar{q}_2) = (\nabla \bar{q}_1) \cdot \bar{q}_2 + \bar{q}_1 \cdot (\nabla \bar{q}_2).$$
$$\nabla \cdot (Q \cdot \bar{q}) = (\nabla \cdot Q) \cdot \bar{q} + Q : (\nabla q)^T.$$

For a symmetric tensor Q, we have

$$\nabla \cdot (Q \cdot \bar{q}) = (\nabla \cdot Q) \cdot \bar{q} + Q : \varepsilon(\bar{q}), \quad \varepsilon(\bar{q}) := \frac{1}{2} \left(\nabla \bar{q} + (\nabla \bar{q})^T \right).$$

For any tensor P and Q,

$$\nabla \cdot (P \cdot Q) = Q^T \cdot (\nabla \cdot P) + P^T : \nabla Q.$$

C.4.5 Frame invariant Derivatives

Let us consider two observers in our Eulerian space. The first one is fixed. The corresponding coordinate system is denoted by $\mathbf{x}$. The second one moves with translation and rotation. The latter one's coordinate system is denoted by $\mathbf{x}'$. We have

$$\mathbf{x}' = \mathbf{x}'_0(t) + \mathbf{x} \cdot O(t),$$

where $\mathbf{x}'_0$ is the translation and $O(t)$ is the rotation.

The orthonormal bases in these two frames are related by

$$e'_i = e_i \cdot O(t) = O^T(t) \cdot e_i.$$

In Lagrange coordinate system,

$$\bar{g}'_i(t) = \frac{\partial \mathbf{x}'}{\partial X^i} = \frac{\partial \mathbf{x}}{\partial X^i} \cdot O(t) = \bar{g}_i \cdot O(t)$$

and

$$\bar{g}^{i'}(t) = \bar{g}^i \cdot O(t).$$

We are looking for those vectors and tensors that are invariant under this frame change.

Objective (Frame-invariant) tensors

- Objective vector: A vector $\mathbf{v}$ in the old frame becomes a new vector $\mathbf{v}'$ from the observer's point of view. A vector $\mathbf{v}$ is called objective if $\mathbf{v}' = O^T \cdot \mathbf{v}$. Let us present $\mathbf{v}$ and $\mathbf{v}'$ in coordinate system:

  $$\mathbf{v} = v^i e_i, \quad \mathbf{v}' = v^{i'} e'_i$$

  Then objectivity of $\mathbf{v}$ is equivalent to $v^i = v^{i'}$.
  In the Lagrange coordinate system, let $\bar{q}$ be the pull-back of $\mathbf{v}$ and $\bar{q}'$ be the pull-back of $\mathbf{v}'$. The Lagrange frame from the new observer is

  $$\bar{g}'_i = \bar{g}_i \cdot O = O^T \cdot \bar{g}_i.$$

  The objectivity of $\bar{q}$ is

  $$q^{i'} = q^i$$

  which is equivalent to

  $$\bar{q}' = O^T \cdot \bar{q}.$$

- Objective tensor: A tensor T is transformed to T' by the new observer. We want

$$T' \cdot \mathbf{v}' = (T \cdot \mathbf{v})'$$

This means

$$T' \cdot \mathbf{v} \cdot O = O^T \cdot (T \cdot \mathbf{v}).$$

Thus,

$$T' \cdot \mathbf{v} = O^T \cdot T \cdot \mathbf{v} \cdot O^T = O^T \cdot T \cdot O \cdot \mathbf{v}$$

This leads to

$$T' = O^T \cdot T \cdot O.$$

One can show that this is equivalent to $T^{ij'} = T^{ij}$. For Lagrange frame, we have similar result. Suppose Q is the pull-back of T. Then Q is objective if

$$Q' = O^T \cdot Q \cdot O$$

Or equivalently,

$$Q^{ij'} = Q^{ij}.$$

C.4.6 Frame-invariant derivatives

- Characterization of rotation $O(t)$. Since $O(t) \cdot O^T(t) = I$, this leads to

$$\frac{dO}{dt} \cdot O^T + O \cdot \frac{dO^T}{dt} = 0.$$

Let us call $O \cdot \frac{dO^T}{dt}$ by $\Omega(t)$. The above formulae are

$$\frac{dO^T}{dt} = \Omega \cdot O^T, \quad \frac{dO}{dt} = -O \cdot \Omega, \quad \Omega^T = -\Omega.$$

- Let $\mathbf{v} := \frac{\partial \mathbf{x}}{\partial t}$ and $\mathbf{v}' := \frac{\partial \mathbf{x}'}{\partial t}$ be the velocities in the two frames, respectively. We have

$$\nabla' \mathbf{v}' = O^T \cdot \nabla \mathbf{v} \cdot O - \Omega, \quad (\nabla' \mathbf{v}')^T = O^T \cdot \nabla \mathbf{v}^T \cdot O + \Omega.$$

Proof. We give proof in Eulerian coordinate system. You can try to prove it in Lagrangian coordinate system.

$$\mathbf{v}' = \frac{\partial \mathbf{x}'}{\partial t} = \dot{\mathbf{x}}_0 + \mathbf{v} \cdot O - \mathbf{x} \cdot O \cdot \Omega = \dot{\mathbf{x}}_0 + \mathbf{v} \cdot O - \mathbf{x}' \cdot \Omega.$$

We use this to get

$$\begin{aligned}\nabla'\mathbf{v}' &= e^{i'}\frac{\partial}{\partial x^i}\mathbf{v}' = e^{i'}\frac{\partial \mathbf{v}}{\partial x^i}\cdot O - \Omega\\ &= O^T\cdot e^i\frac{\partial \mathbf{v}}{\partial x^i}\cdot O - \Omega = O^T\cdot\nabla\mathbf{v}\cdot O - \Omega.\end{aligned}$$

□

- Define upper-convected derivative of a vector $\bar{q}$ as

$$\bar{q}^{\nabla} := \frac{\partial}{\partial t} - \bar{q}\cdot\nabla\mathbf{v}.$$

Then $\bar{q}^{\nabla}$ is frame invariant, i.e.

$$\bar{q}'^{\nabla} = O^T\cdot\bar{q}^{\nabla}$$

Proof. From $\bar{q}' = O^T\bar{q}$, we get

$$\dot{\bar{q}}' = O^T\cdot\dot{\bar{q}} + \dot{O}^T\cdot\bar{q} = O^T\cdot\dot{\bar{q}} + \Omega\cdot O^T\cdot\bar{q}.$$

$$\begin{aligned}\bar{q}'\cdot\nabla'\mathbf{v}' &= \bar{q}\cdot O\cdot(O^T\cdot\nabla\mathbf{v}\cdot O - \Omega)\\ &= \bar{q}\cdot\nabla\mathbf{v}\cdot O - \bar{q}\cdot O\cdot\Omega\\ &= O^T\cdot\bar{q}\cdot\nabla\mathbf{v} - \Omega^T\cdot O^T\cdot\bar{q}\end{aligned}$$

We get

$$\begin{aligned}\bar{q}'^{\nabla} &= \dot{\bar{q}}' - \bar{q}'\cdot\nabla'\mathbf{v}'\\ &= O^T\cdot(\dot{\bar{q}} - \bar{q}\cdot\nabla\mathbf{v})\end{aligned}$$

In the last step, we have used $\Omega + \Omega^T = 0$. □

- Upper convected derivative of a tensor. Let Q be an objective tensor. Define

$$Q^{\nabla} := \dot{Q} - Q\cdot\nabla\mathbf{v} - \nabla\mathbf{v}^T\cdot Q$$

Then Q^{∇} is also objective. That is

$$Q'^{\nabla} = O^T\cdot Q^{\nabla}\cdot O.$$

Proof. Differentiate $Q' = O^T \cdot Q \cdot O$ in t with fixed X, we get

$$\begin{aligned} \dot{Q}' &= \dot{O}^T \cdot Q \cdot O + O^T \cdot \dot{Q} \cdot O + O^T \cdot Q \cdot \dot{O} \\ &= \Omega \cdot O^T \cdot Q \cdot O + O^T \cdot \dot{Q} \cdot O - O^T \cdot Q \cdot O \cdot \Omega \end{aligned}$$

The term $Q' \cdot \nabla' \mathbf{v}'$ is

$$\begin{aligned} Q' \cdot \nabla' \mathbf{v}' &= O^T \cdot Q \cdot \left(O^T \cdot \nabla \mathbf{v} \cdot O - \Omega\right) \\ \nabla' \mathbf{v}'^T \cdot Q' &= \left(O^T \cdot \nabla \mathbf{v}^T \cdot O + \Omega\right) \end{aligned}$$

Here, we have used $\Omega^T = -\Omega$. Putting the above calculations together, we get

$$\begin{aligned} Q'^{\nabla} &= \dot{Q}' - Q' \cdot \nabla' \mathbf{v}' - \nabla' \mathbf{v}'^T \cdot Q' \\ &= O^T \cdot \left(\dot{Q} - Q \cdot \nabla \mathbf{v} - \nabla \mathbf{v}^T \cdot Q\right) \cdot O \\ &= O^T \cdot Q^{\nabla} \cdot O. \end{aligned}$$

□

- In a similar way, we define lower-convected time derivative as

$$Q^{\Delta} := \dot{Q} + Q \cdot \nabla \mathbf{v} + \nabla \mathbf{v}^T \cdot Q.$$

  It is also objective if Q is objective.

- The upper-convected time derivative for contravariant component. Let $Q = Q^{ij} e_i e_j$. Then

$$Q^{\nabla} = \left(\dot{Q}^{ij} - Q^{kj} \frac{\partial v^i}{\partial x^k} - Q^{ik} \frac{\partial v^j}{\partial x^k}\right) e_i e_j$$

- If I is the identity tensor, then $I^{\nabla} = -\dot{\gamma}$.

$$\begin{aligned} I^{\nabla} &= -\left(\delta^{kj} \frac{\partial v^i}{\partial x^k} + \delta^{ik} \frac{\partial v^j}{\partial x^k}\right) e_i e_j \\ &= -\left(\frac{\partial v^i}{\partial x^j} + \frac{\partial v^j}{\partial x^i}\right) e_i e_j \\ &= -\dot{\gamma}^{ij} e_i e_j \end{aligned}$$

- Let $B = F \cdot F^T$ be the right Cauchy-Green strain tensor. Then $B^{\nabla} = 0$.

Proof. We have

$$\partial_t F = (\nabla \mathbf{v}) \cdot F = 0.$$

Taking transpose, we get

$$\partial_t F^T = F^T \cdot (\nabla \mathbf{v})^T.$$

Thus,

$$\partial_t (F \cdot F^T) = (\partial_t F) \cdot F^T + F \cdot (\partial_t F^T) = (\nabla \mathbf{v}) \cdot (F \cdot F^T) + (F \cdot F^T) \cdot (\nabla \mathbf{v})^T.$$

□

Appendix D

Lie Derivatives

This subsection is mainly from
Albert Chern, Fluid Dynamics with Incompressible Schrödinger Flow, Doctoral Dissertation, California Institute of Technology, 2017.

D.1 Basic notations

Manifolds, tangent space, and cotangent space

- Let M_t be the region occupied by the fluid at time t. We shall call it the configuration space or configuration manifold. The initial manifold M_0 will also be denoted by $\hat{M}$. The coordinate in $\hat{M}$, denoted by X, is called Lagrangian coordinate, or the material coordinate, while the coordinate in M_t, denoted by $\mathbf{x}$, is called the Eulerian coordinate. Below, we shall use M for M_t for some unspecified t and $\hat{M}$ for the initial manifold.

- The tangent vector space of M at a point $\mathbf{x} \in M$ is denoted by $T_{\mathbf{x}}M$. Its dual space is called cotangent space, and is denoted by $T_{\mathbf{x}}^*M$. The sets $TM := \cup_{\mathbf{x}\in M} T_{\mathbf{x}}M$ and $T^*M := \cup_{\mathbf{x}\in M} T_{\mathbf{x}}^*M$ are called the tangent and cotangent bundles of M, respectively.

- The tangent space has a basis $\{e_i | i = 1, ..., n\}$. We shall also denote e_i by ∂_{x^i} or $\frac{\partial}{\partial x^i}$ for reason explained later. Similarly, we shall use ∂_{X^i} or $\frac{\partial}{\partial X^i}$ for the basis in the initial tangent space $T\hat{M}$.

- A vector field is a map $\mathbf{v} : M \to TM$ such that $\mathbf{v}(\mathbf{x}) \in T_{\mathbf{x}}M$. A time-dependent vector field $\mathbf{v}_t$ is a vector field in TM_t, which is also denoted as $\mathbf{v}(t, \mathbf{x})$.

- Given a vector field $\mathbf{v}(t,\mathbf{x})$, its trajectories from an initial position X is $\mathbf{x}(t,X)$ which satisfies
$$\dot{\mathbf{x}} = \mathbf{v}(t,\mathbf{x}), \quad \mathbf{x}(0,X) = X.$$
A flow map $\varphi_t : \hat{M} \to M_t$ is a diffeomorphism with $\varphi_t(X) := \mathbf{x}(t,X)$. The flow map φ_t satisfies
  (i) It is 1-1 and onto;
  (ii) It is Lipschitz continuous, so is its inverse. This means that $\partial\mathbf{x}/\partial X$ is well-defined and bounded except on a low dimensional sub manifold.

  Conversely, given such a flow map φ_t, we can define
$$\mathbf{v}(t,\mathbf{x}) = \partial_t\varphi_t(X), \quad \text{for} \quad \mathbf{x} = \varphi_t(X).$$

- A tangent vector $\mathbf{v}_t := \mathbf{v}(t,\cdot) := v_t^i\partial_{x^i} \in TM_t$. In many situations, we will just write v^i instead v_t^i if the parameter t can be read from the text. That is,
$$\mathbf{v}_t = v^i\partial_{x^i}.$$
Since we will fix t, we will abbreviate $\mathbf{v}_t$ by $\mathbf{v}$ in most of cases.

D.2 Pull-back and Push-forward Operators

Flow maps Let $\hat{M}$ be the initial configuration space (also called the reference space or the material space) and M_t be the configuration space at time t (also called the world space). Both have volume forms, which are $\hat{\mu}$ and μ, respectively. Let $\mathbf{v}(t,\mathbf{x})$ be a velocity field, or a time-dependent vector field on a manifold M. Let $\mathbf{x}(t,X)$ be the solution of the ODE:
$$\dot{\mathbf{x}} = \mathbf{v}(t,\mathbf{x}), \quad \mathbf{x}(0,X) = X$$
We call $\varphi_t(X) := \mathbf{x}(t,X)$ be the flow map generated by $\mathbf{v}$. X is called the Lagrange coordinate, while $\mathbf{x}$ the Eulerian coordinate. The flow map is a mapping from the Lagrangian coordinate to the Eulerian coordinate.

Pullback Functions or differential forms in Eulerian coordinate can be transformed back to the Lagrangian coordinate through the flow map. This is the pull-back operator. This is to pullback a differential form from M_t to $\hat{M}$. Suppose we have an integral, say $\int_C \eta_i dx^i$ on the manifold M_t at time t., we want to pull it back to an integral at $t = 0$ on $\hat{M}$ by the change-of-variable $\mathbf{x} \mapsto X$ through the flow map φ_t. The answer is
$$\int_C \eta_i(t,\mathbf{x})dx^i = \int_{C_0} \eta(t,\mathbf{x}(t,X))\frac{\partial x^i}{\partial X^\alpha}dX^\alpha.$$

Here, $C_0 = \varphi_t^{-1}(C)$. We call

$$\eta(t,\mathbf{x}(t,X))\frac{\partial x^i}{\partial X^\alpha}\,dX^\alpha$$

the pullback of $\eta_i(t,\mathbf{x})dx^i$. Note that the time here is fixed. We merely discuss the pullback the differential forms via the map φ_t with fixed t.

- $f(t,\mathbf{x})$ is pulled back to $\varphi_t^*(f)(t,X) := f(t,\mathbf{x}(t,X))$.
- $\eta = \eta_i\,dx^i$ is pulled back to

$$\varphi_t^*(\eta)(t,X) := \eta_i(t,\mathbf{x}(t,X))\frac{\partial x^i(t,X)}{\partial X^\alpha}dX^\alpha.$$

- The volume form $\mu = dx^1 \wedge \cdots \wedge dx^n$. Its pull back $\varphi_t^*\mu = J\hat{\mu}$, where $J = det(d\varphi_t)$.
- We want to compute the pullback of $\star dx^j$. Suppose $\varphi_t^*(\star dx^j)$ is expressed by $a_j^\alpha(\star dX^\alpha)$, we want to find the coefficient a_j^α. Note that the two stars are different. One is in the space of M the other is in $\hat{M}$. Since $dx^j \wedge \star dx^j = \mu = J\hat{\mu}$ and $dX^\beta \wedge \star dX^\beta = \hat{\mu}$, we get

$$\begin{aligned}
J\hat{\mu}\delta_j^i &= \varphi_t^*\mu\delta_j^i \\
&= \varphi_t^*(dx^i \wedge (\star dx^j)) \\
&= \varphi_t^*(dx^i) \wedge \varphi_t^*(\star dx^j) \\
&= F_\alpha^j dX^\alpha \wedge a_j^\beta(\star dX^\beta) \\
&= F_\alpha^i a_j^\alpha \hat{\mu}.
\end{aligned}$$

  Thus,

$$F_\alpha^i a_j^\alpha = J\delta_j^i.$$

  This leads to

$$a_i^\alpha = J\frac{\partial X^\alpha}{\partial x^i} = J(F^{-1})_i^\alpha, \quad a = JF^{-1},$$

  We obtain

$$\varphi_t^*(\star dx^j) = (JF^{-1})_\alpha^j(\star dX^\alpha) = J\frac{\partial X^\alpha}{\partial x^j}(\star dX^\alpha). \tag{4.1}$$

The general definition of pullback of a differential k-form α by a map φ is

$$\varphi^*(\alpha)(v_1,\ldots,v_k) := \alpha(d\varphi(v_1),\ldots,d\varphi(v_k)). \tag{4.2}$$

It has the following properties.

- $\varphi^*(f) = f \circ \varphi$ for $f \in \Omega^0(M)$
- $\varphi^*(\alpha \wedge \beta) = (\varphi^* \alpha) \wedge (\varphi^* \beta)$.
- $\varphi^*(d\alpha) = d\varphi^*(\alpha)$.
- $\varphi^*(f\alpha) = (\varphi^* f)\varphi^* \alpha$.

Push forward operator φ_{t*} Push forward is to push vector fields in $\hat{M}$ to vector fields in M_t by $d\phi_t$. It is the dual operator of φ_t^*.

- The tangent $\left(\frac{\partial}{\partial X^\alpha}\right)$ on $T\hat{M}$ can be pushed forward to TM_t by

$$\varphi_{t*}\left(\frac{\partial}{\partial X^\alpha}\right) := \frac{\partial x^k}{\partial X^\alpha}\frac{\partial}{\partial x^k}.$$

  Note that

$$\langle \varphi_{t*}\frac{\partial}{\partial X^\alpha} | dx^\ell \rangle = \langle \frac{\partial x^k}{\partial X^\alpha}\frac{\partial}{\partial x^k} | dx^\ell \rangle = \frac{\partial x^\ell}{\partial X^\alpha}$$

  On the other hand,

$$\langle \frac{\partial}{\partial X^\alpha} | \varphi_t^* dx^\ell \rangle = \langle \frac{\partial}{\partial X^\alpha} | \frac{\partial x^\ell}{\partial X^\beta} dX^\beta \rangle = \frac{\partial x^\ell}{\partial X^\alpha}$$

  We get that

$$\langle \varphi_{t*}\frac{\partial}{\partial X^\alpha} | dx^\ell \rangle = \langle \frac{\partial}{\partial X^\alpha} | \varphi_t^* dx^\ell \rangle$$

  for bases in $T\hat{M}$ and T^*M. Thus, φ_{t*} is the dual operator of φ_t^*.

- We can also pull forward a tangent from M_t to $\hat{M}$ by φ_t^{-1}

$$(\varphi_t^{-1})_*\left(\frac{\partial}{\partial x^i}\right) = \frac{\partial X^\alpha}{\partial x^i}\frac{\partial}{\partial X^\alpha} = (F^{-T})^i_\alpha \frac{\partial}{\partial X^\alpha}.$$

D.3 Lie Derivative for Differential Forms

1. **Notations** Let us use the following notations

$$\frac{d}{dt} := d_t := \left(\frac{\partial}{\partial t}\right)_X, \quad \partial_t := \left(\frac{\partial}{\partial t}\right)_{\mathbf{x}}.$$

2. **Motivation:** The Lie derivative is nothing but a generalization of material derivative for differential forms. Let us consider the following example. Let φ_t be the flow map from $\hat{M}$ to M_t. Let us consider the integral

$$\int_{C(t)} \eta_i \, dx^i$$

where $C(t)$ is a closed curve defined by $C(t) = \varphi_t(C(0))$. By changing variable from $\mathbf{x}$ to X, the above integral is

$$\int_{C(0)} \eta_i(t, \mathbf{x}(t,X)) \frac{\partial x^i}{\partial X^\alpha} dX^\alpha.$$

Let us investigate the change of this integral with fixed X:

$$\begin{aligned} &\frac{d}{dt}\int_{C(0)} \eta_i(t,\mathbf{x}(t,X))\frac{\partial x^i}{\partial X^\alpha} dX^\alpha = \int_{C(0)} \frac{d}{dt}\left(\eta_i(t,\mathbf{x}(t,X))\frac{\partial x^i(t,X)}{\partial X^\alpha}\right) dX^\alpha \\ &= \int_{C(0)} \left[(\partial_t + \mathbf{v}\cdot\nabla)\eta_i \frac{\partial x^i}{\partial X^\alpha} + \eta_i \frac{\partial v^i}{\partial X^\alpha}\right] dX^\alpha = \int_{C(t)} (\partial_t + \mathbf{v}\cdot\nabla)\eta_i dx^i + \eta_i \frac{\partial v^i}{\partial x^k} dx^k \\ &=: \int_{C(t)} (\partial_t + \mathscr{L}_{\mathbf{v}_t})\eta \end{aligned}$$

3. The notation $\mathbf{v}_t$ simply stands for a vector field in M_t with t fixed. The Lie derivative $\partial_t + \mathscr{L}_{\mathbf{v}_t}$ for a general differential form α in M_t w.r.t. a vector field $\mathbf{v}_t$ is defined to be the derivative of α with fixed X. That is,

$$\boxed{d_t \varphi_t^*(\alpha) = \varphi_t^*(\partial_t + \mathscr{L}_{\mathbf{v}_t})\alpha.} \tag{4.3}$$

If both α and $\mathbf{v}$ are independent of t, then the Lie derivative $\mathscr{L}_{\mathbf{v}}\alpha$ is defined as

$$\varphi_t^*(\mathscr{L}_{\mathbf{v}}\alpha) := d_t \varphi_t^*(\alpha).$$

We remark that in the time-dependent case, the Lie derivative $\mathscr{L}_{\mathbf{v}_t}$ only involves $v(t,\mathbf{x})$ with t fixed, although we use the flow map φ_t in its definition. Thus, $\mathscr{L}_{\mathbf{v}_t}$ is the Lie derivative of $\mathbf{v}_t$ with t fixed.

4. The Lie derivative $\mathscr{L}_{\mathbf{v}}$ depends only on the differential structure of M and the vector field $\mathbf{v}$. Its concept does not involve with metric nor connection. However, the covariance derivatives involves the concept of connection.

List of Lie derivatives for differential forms

- Lie derivative for scalar function:

$$\begin{aligned} d_t(\varphi_t^* f)(t,X) &= \frac{d}{dt} f(t,\mathbf{x}(t,X)) = \partial_t f + \frac{\partial f}{\partial x^i}\dot{x}^i \\ &= (\partial_t + \mathbf{v}\cdot\nabla) f = (\partial_t + \mathscr{L}_{\mathbf{v}_t}) f. \end{aligned}$$

  Therefore, $\mathscr{L}_{\mathbf{v}_t} f = \mathbf{v}\cdot\nabla f$.

- Lie derivative for dx^i

$$\begin{aligned} \mathscr{L}_{\mathbf{v}}(dx^i) &:= d_t(\varphi_t^*(dx^i))(t,X) \\ &= \frac{d}{dt}\frac{\partial x^i(t,X)}{\partial X^\alpha} dX^\alpha = \frac{\partial v^i}{\partial X^\alpha} dX^\alpha \\ &= \frac{\partial v^i}{\partial X^\alpha}\frac{\partial X^\alpha}{\partial x^k} dx^k = \frac{\partial v^i}{\partial x^k} dx^k. \end{aligned}$$

- For 1-form $\eta = \eta_i dx^i$, we have

$$\begin{aligned} d_t\varphi_t^*(\eta) &= [d_t\varphi_t^*(\eta_i)]\, dx^i + \eta_i \left[d_t\varphi_t^*(dx^i)\right] \\ &= \left(\partial_t \eta_k + v^j \partial_{x^j}\eta_k\right) dx^k + \eta_j \frac{\partial v^j}{\partial x^k} dx^k \\ &= \left(\partial_t \eta + \mathbf{v}\cdot\nabla\eta + \eta\cdot(\nabla\mathbf{v})^T\right)\cdot d\mathbf{x} \\ &= \varphi^*(\partial_t + \mathscr{L}_{\mathbf{v}_t})\eta. \end{aligned}$$

- For volume form $dx^1\wedge\cdots\wedge dx^n$, we have

$$\begin{aligned} d_t\varphi_t^*(dx^1\wedge\cdots\wedge dx^n) &= \sum_i dx^1\wedge\cdots(d_t\varphi_t^*(dx^i))\cdots\wedge dx^n \\ &= \sum_i dx^1\wedge\cdots(\frac{\partial v^i}{\partial x^i} dx^i)\cdots\wedge dx^n \\ &= (\nabla\cdot\mathbf{v})\,(dx^1\wedge\cdots\wedge dx^n) \end{aligned}$$

- For n-form $\rho dx^1\wedge\cdots\wedge dx^n$:

  $$d_t\varphi_t^*\left(\rho dx^1\wedge\cdots\wedge dx^n\right) = (\partial_t\rho + (\nabla\cdot\mathbf{v})\rho)\, dx^1\wedge\cdots\wedge dx^n = (\partial_t + \mathscr{L}_{\mathbf{v}_t})\left(\rho dx^1\wedge\cdots\wedge dx^n\right)$$

- For 2-form

$$\begin{aligned} d_t\varphi_t^*(dx^i\wedge dx^j) &= (d_t\varphi_t^* dx^i)\wedge dx^j + dx^i\wedge(d_t\varphi_t^* dx^j) \\ &= \frac{\partial v^i}{\partial x^k} dx^k\wedge dx^j + dx^i\wedge\left(\frac{\partial v^j}{\partial x^\ell} dx^\ell\right). \end{aligned}$$

- Let
$$\omega = \omega^1 dx^2 \wedge dx^3 + \omega^2 dx^3 \wedge dx^1 + \omega^3 dx^1 \wedge dx^2.$$
We have
$$\begin{aligned}
d_t\varphi_t^*\omega &= (d_t\varphi_t^*\omega^1)dx^2\wedge dx^3 + (d_t\varphi_t^*\omega^2)dx^3\wedge dx^1 + (d_t\varphi_t^*\omega^3)dx^1\wedge dx^2\\
&\quad + \omega^1 d_t\varphi_t^*(dx^2\wedge dx^3) + \omega^2 d_t\varphi_t^*(dx^3\wedge dx^1) + \omega^3 d_t\varphi_t^*(dx^1\wedge dx^2)\\
&= \left[(\partial_t + \mathbf{v}\cdot\nabla)\omega^1 + \omega^1(\frac{\partial v^2}{\partial x^2} + \frac{\partial v^3}{\partial x^3}) - \omega^2\frac{\partial v^1}{\partial x^2} - \omega^3\frac{\partial v^1}{\partial x^3}\right]dx^2\wedge dx^3\\
&\quad + \left[(\partial_t + \mathbf{v}\cdot\nabla)\omega^2 + \omega^2(\frac{\partial v^1}{\partial x^1} + \frac{\partial v^3}{\partial x^3}) - \omega^3\frac{\partial v^2}{\partial x^3} - \omega^1\frac{\partial v^2}{\partial x^1}\right]dx^3\wedge dx^1\\
&\quad + \left[(\partial_t + \mathbf{v}\cdot\nabla)\omega^3 + \omega^3(\frac{\partial v^1}{\partial x^1} + \frac{\partial v^2}{\partial x^2}) - \omega^3\frac{\partial v^3}{\partial x^1} - \omega^1\frac{\partial v^3}{\partial x^2}\right]dx^1\wedge dx^2\\
&= (\partial_t + \mathscr{L}_{\mathbf{v}_t})\omega.
\end{aligned}$$
For each component, we have
$$d_t\omega^i = \partial_t\omega^i + v^k\frac{\partial\omega^i}{\partial x^k} + \omega^i\frac{\partial v^k}{\partial x^k} - \frac{\partial v^i}{\partial x^k}\omega^k$$
In vector calculus, we define $\omega = (\omega^1, \omega^2, \omega^3)^T$. In vector form, it is
$$d_t\omega = \partial_t\omega + \mathbf{v}\cdot\nabla\omega + \omega\nabla\cdot\mathbf{v} - (\nabla\mathbf{v})\omega$$
Alternative, the vorticity ω has another representation
$$\omega = \omega^i(\star dx^i).$$
One can use the Lie derivative for $(\star dx^i)$ to get the same formula.

- Pullback of a flux (an $(n-1)$-form): Let
$$\sigma := \sigma^i_j(\star dx^i)\otimes dx^j$$
The pullback is only applied to the first part of σ. Thus,
$$d_t\varphi_t^*\sigma = (\partial_t + \mathscr{L}_{\mathbf{v}})\left(\sigma^i_j(\star dx^i)\otimes dx^j\right)$$
where
$$\mathscr{L}_{\mathbf{v}}\sigma = \left(v^k\partial_{x^k}\sigma^i_j + \sigma^i_j\frac{\partial v^k}{\partial x^k} - \frac{\partial v^i}{\partial x^k}\sigma^k_j + \sigma^i_\ell\frac{\partial v^\ell}{\partial x^j}\right)(\star dx^i\otimes dx^j)$$

D.4 Lie derivatives for vectors and tensors

The tangent and cotangent spaces are naturally dual to each other. We denote this dual relation by $\langle\cdot|\cdot\rangle$. Thus, $\langle dx^i|\frac{\partial}{\partial x^j}\rangle = \delta^i_j$. The Lie derivative was defined for differential forms, which is in the tensor spaces defined by the cotangent spaces. The Lie derivative for tangent vectors is defined as the dual operator of the Lie derivative for cotangent vectors.

- Lie derivative for $\frac{\partial}{\partial x^i}$:
  - Method 1: Let $\frac{\partial}{\partial x^i}$ be a tangent vector of M_t at $\mathbf{x}$.

$$
\begin{aligned}
\mathscr{L}_{\mathbf{v}}\frac{\partial}{\partial x^i} &:= d_t\left((\varphi_t^{-1})_*(\frac{\partial}{\partial x^i})\right)\\
&= d_t\left(\frac{\partial X^\alpha}{\partial x^i}\frac{\partial}{\partial X^\alpha}\right)\\
&= d_t(F^{-T})^i_\alpha\frac{\partial}{\partial X^\alpha})\\
&= -(F^{-T}\dot{F}^T F^{-T})^i_\alpha\frac{\partial}{\partial X^\alpha}\\
&= -(F^{-T})^i_\beta(\dot{F}^T)^\beta_\ell(F^{-T})^\ell_\alpha\frac{\partial}{\partial X^\alpha}\\
&= -\frac{\partial X^\beta}{\partial x^i}\frac{\partial v^\ell}{\partial X^\beta}\frac{\partial X^\alpha}{\partial x^\ell}\frac{\partial}{\partial X^\alpha}\\
&= -\frac{\partial v^\ell}{\partial x^i}\frac{\partial}{\partial x^\ell}
\end{aligned}
$$

  - Method 2: we use

$$0 = \mathscr{L}_{\mathbf{v}}\langle dx^i|\frac{\partial}{\partial x^j}\rangle = \langle\mathscr{L}_{\mathbf{v}}(dx^i)|\frac{\partial}{\partial x^j}\rangle + \langle dx^i|\mathscr{L}_{\mathbf{v}}\frac{\partial}{\partial x^j}\rangle$$

    to obtain

$$\langle\mathscr{L}_{\mathbf{v}}\frac{\partial}{\partial x^j}|dx^i\rangle = -\langle\frac{\partial}{\partial x^j}|\mathscr{L}_{\mathbf{v}}(dx^i)\rangle = -\langle\frac{\partial}{\partial x^j}|\frac{\partial v^i}{\partial x^k}dx^k\rangle = -\frac{\partial v^i}{\partial x^j}.$$

    Hence,

$$\mathscr{L}_{\mathbf{v}}\frac{\partial}{\partial x^j} = -\frac{\partial v^i}{\partial x^j}\frac{\partial}{\partial x^i}.$$

- Lie derivative for vector field $A = A^i \frac{\partial}{\partial x^i}$.

$$\begin{aligned}\mathscr{L}_{\mathbf{v}} A &= (\mathscr{L}_{\mathbf{v}} A^i)\frac{\partial}{\partial x^i} + A^k \mathscr{L}_{\mathbf{v}}\left(\frac{\partial}{\partial x^k}\right) \\ &= \left(\partial_t A^i + v^k \partial_{x^k} A^i - A^k \frac{\partial v^i}{\partial x^k}\right)\frac{\partial}{\partial x^i}\end{aligned}$$

- The deformation gradient

$$F := F^i_\alpha dX^\alpha \otimes \frac{\partial}{\partial x^i}$$

is a 2-point tensor (see Marsden and Hughes). Its Lie derivative with respective to the second argument $\frac{\partial}{\partial x^i}$ is

$$\partial_t F + \mathscr{L}_{\mathbf{v}} F = \left(\partial_t F^i_\alpha + v^k \partial_{x^k} F^i_\alpha - F^k_\alpha \frac{\partial v^i}{\partial x^k}\right) dX^\alpha \otimes \frac{\partial}{\partial x^i}. \tag{4.4}$$

Thus, the evolution equation for F is

$$(\partial_t + \mathscr{L}_{\mathbf{v}})F = 0.$$

- The inverse deformation gradient

$$(F^{-1}) = (F^{-1})^\alpha_i \frac{\partial}{\partial X^\alpha} \otimes dx^i.$$

is a two-point tensor. Its Lie derivative w.r.t. the second argument is

$$(\partial_t + \mathscr{L}_{\mathbf{v}})(F^{-1}) = \left(\partial_t (F^{-1})^\alpha_i + v^k \partial_{x^k} (F^{-1})^\alpha_i + (F^{-1})^\alpha_k \frac{\partial v^k}{\partial x^i}\right)\frac{\partial}{\partial X^\alpha} \otimes dx^i \tag{4.5}$$

The evolution equation for F^{-1} is

$$(\partial_t + \mathscr{L}_{\mathbf{v}})(F^{-1}) = 0.$$

- Lie derivative for tensor of type $(2,0)$. Let

$$A = A^{ij}\frac{\partial}{\partial x^i} \otimes \frac{\partial}{\partial x^j}.$$

Then the Lie derivative of A is

$$\begin{aligned}(\partial_t + \mathscr{L}_{\mathbf{v}})A &= ((\partial_t + \mathscr{L}_{\mathbf{v}})A^{ij})\frac{\partial}{\partial x^i} \otimes \frac{\partial}{\partial x^j} + A^{kj}\mathscr{L}_{\mathbf{v}}\left(\frac{\partial}{\partial x^k}\right) \otimes \frac{\partial}{\partial x^j} + A^{i\ell}\frac{\partial}{\partial x^i} \otimes \mathscr{L}_{\mathbf{v}}\left(\frac{\partial}{\partial x^\ell}\right) \\ &= \left(\partial_t A^{ij} + v^k \partial_{x^k} A^{ij} - A^{kj}\frac{\partial v^i}{\partial x^k} - A^{i\ell}\frac{\partial v^j}{\partial x^\ell}\right)\frac{\partial}{\partial x^i} \otimes \frac{\partial}{\partial x^j}\end{aligned}$$

This is also known as the upper-convected derivative of the tensor A.

- Lie derivative for tensor of type $(1,1)$. Let

$$B = B^i_j \partial_{x^i} \otimes dx^j.$$

Then the Lie derivative for both argument is

$$\begin{aligned}(\partial_t + \mathscr{L}_{\mathbf{v}})B &= ((\partial_t + \mathscr{L}_{\mathbf{v}})B^i_j)\partial_{x^i} \otimes dx^j + B^k_j \mathscr{L}_{\mathbf{v}}(\partial_{x^k}) \otimes dx^j + B^i_\ell \partial_{x^i} \otimes \mathscr{L}_{\mathbf{v}}\left(dx^\ell\right) \\ &= \left(\partial_t B^i_j + v^k \partial_{x^k} B^i_j - B^k_j \partial_{x^k} v^i + B^i_k \partial_{x^j} v^k\right)\partial_{x^i} \otimes dx^j. \end{aligned} \tag{4.6}$$

D.5 Interior Product and Cartan magic formula

- Extrusion of a set: Let Σ_0 be a k-dimensional submanifold. Define $\Sigma(t)$ by

$$\Sigma(t) := \varphi_t(\Sigma_0)$$

and Extrusion of $\Sigma(t)$ by

$$\Sigma_{\mathbf{v}}(t_1,t_2) := \cup_{t_1 \le t \le t_2} \varphi_t(\Sigma_0)$$

The orientation of $\Sigma_{\mathbf{v}}(t_1,t_2)$ is defined by

$$\partial\Sigma_{\mathbf{v}}(t_1,t_2) = \Sigma(t_2) - \Sigma(t_1) - (\partial\Sigma)_{\mathbf{v}}(t_1,t_2).$$

- Interior product: For a k-form α, define

$$\int_{t_1}^{t_2} \langle i_{\mathbf{v}}\alpha, S\rangle := \langle \alpha, S_{\mathbf{v}}(t_1,t_2)\rangle$$

- When Σ_0 is an n-dimensional submanifold:

$$\boxed{\frac{d}{dt}\int_{\Sigma(t)} f(t,\mathbf{x})\, d^n\mathbf{x} = \int_{\Sigma(t)} \frac{\partial}{\partial t} f(t,\mathbf{x})\, d^n\mathbf{x} + \int_{\partial\Sigma(t)} f(t,\mathbf{x})\mathbf{v}\cdot\mathbf{n}\, d\mathbf{x}} \tag{4.7}$$

This result is called the Reynolds transportation theorem.

- When Σ_0 is a k-dimensional submanifold, α is a k-form.

$$\begin{aligned}\frac{d}{dt}\int_{\Sigma(t)} \alpha &= \int_{\Sigma(t)} \frac{\partial}{\partial t}\alpha + \mathscr{L}_{\mathbf{v}}\alpha \\ &= \int_{\Sigma(t)} \frac{\partial}{\partial t}\alpha + i_{\mathbf{v}} d\alpha + \int_{\partial\Sigma(t)} i_{\mathbf{v}}\alpha \\ &= \int_{\Sigma(t)} \frac{\partial}{\partial t}\alpha + i_{\mathbf{v}} d\alpha + d\, i_{\mathbf{v}}\alpha. \end{aligned}$$

This shows Cartan's magic formula

$$\boxed{\mathscr{L}_{\mathbf{v}} = i_{\mathbf{v}} \circ d + d \circ i_{\mathbf{v}}.}$$