

Fundamentals of Continuum Mechanics

(Draft)

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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 1.1). 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.

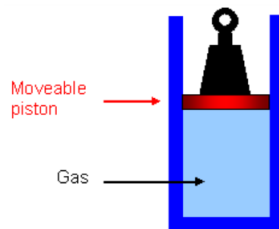


Figure 1.1: Gas in a cylinder with piston. Copied from <http://galileo.phys.virginia.edu/classes/152.mf1i.spring02/Boyle.htm>

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 Fig:CarnotThermoplane.

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.

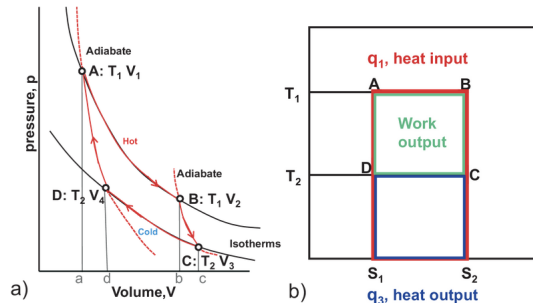


Figure 1.2: Carnot cycle on the thermodynamic plane. The left figure represents the p - V plane, while the right figure represents the T - S plane. Image source: https://www.tf.uni-kiel.de/matwis/amat/td_kin_i/kap_1/backbone/r_se31.html

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):

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

A practical unit is the calorie:

$$1 \text{ cal} = 4.1858J.$$

- **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

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

- 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 $dW = -pdV$. 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 $-Fdx$ is the work done by the piston on the gas particles in the cylinder. The first law of thermodynamics gives

$$\boxed{dU = -pdV} \quad (1.2)$$

along an adiabatic process.

Existence of the entropy function We will now demonstrate that the relationship $U = U(p, V)$ and equation (1.3) 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. We plug $U = U(p, V)$ into (1.3) to get

$$U_p dp + (U_V + p)dV = 0. \quad (1.3)$$

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

$$\frac{dp}{dV} = -\frac{U_V(p, V) + p}{U_p(p, V)}. \quad (1.4)$$

Note that from (1.1), the right-hand side of (1.4) is always less than 0 in the region $(p > 0, V > 0)$. Thus, (1.4) is always solvable in this region.

¹Lionello 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 (1.3) (or (1.4)) if

$$(dp, dV) \perp (U_p, U_V + p)$$

along this curve. A function $\sigma(p, V)$ is called an integral of (1.4) if its level set ($\sigma(p, V) = \text{constant}$) is an integral curve of (1.4). The solutions of (1.4) 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 (1.3) is termed an *entropy function* of the system.

3. The level set of σ satisfies

$$d\sigma = 0 \Leftrightarrow (dp, dV) \perp (\sigma_p, \sigma_V)$$

as well as the ODE

$$(\sigma_p, \sigma_V) \parallel (U_p, U_V + p).$$

Thus, there exists a function $\mu(p, V) \neq 0$ (referred to as the integration factor) such that

$$(\sigma_p, \sigma_V) = \mu(U_p, U_V + p).$$

Equivalently,

$$d\sigma = \sigma_p dp + \sigma_V dV = \mu \cdot (U_p dp + (U_V + p)dV) = \mu \cdot (dU + pdV). \quad (1.5)$$

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 $\bar{\mu} := v(\sigma)\mu$, where $v(\sigma)$ is an arbitrary chosen function. In fact, by multiplying (1.5) by $v(\sigma)$:

$$v(\sigma)d\sigma = v(\sigma)\mu \cdot (dU + pdV),$$

we see that $\bar{\sigma}$ with $d\bar{\sigma} = v(\sigma)d\sigma$ 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:

$$dU = \tau d\sigma - pdV, \quad (1.6)$$

where $\tau = 1/\mu = U_\sigma$.

2. **Interpretation of the Formula:** 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 \mathcal{S}_1 and \mathcal{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 ($\mathcal{S}_1 \sim \mathcal{S}_2$).
- **The zeroth law of thermodynamics:**

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

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

- **Ideal gas thermometer** The ideal gas is postulated to satisfy $pV = \text{constant}$ 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 \mathcal{S} into a heat bed filled with ideal gases, we measure its temperature. The empirical temperature of the heat bed represents the temperature of \mathcal{S} . Thus, each state of $\mathcal{S}(p, V)$ 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:

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

Absolute temperature T and the entropy S Let us revisit the solution of the Pfaffin equation (1.3). 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 \mathcal{S} into two subsystems \mathcal{S}_1 and \mathcal{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, $\mathcal{S} = (\sigma, \theta)$, $\mathcal{S}_1 = (\sigma_1, \theta)$, $\mathcal{S}_2 = (\sigma_2, \theta)$, and by adding heat to \mathcal{S} without doing work, equation (1.6) gives:

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

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

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

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

are independent of θ .

5. This implies the existence of functions $T(\theta)$, $v_1(\sigma_1)$, $v_2(\sigma_2)$, $v(\sigma)$ such that

$$\begin{aligned} \tau_1(\theta, \sigma_1) &= T(\theta)v_1(\sigma_1), \\ \tau_2(\theta, \sigma_2) &= T(\theta)v_2(\sigma_2), \\ \tau(\theta, \sigma) &= T(\theta)v(\sigma). \end{aligned}$$

Equation (1.8) becomes

$$Tv(\sigma)d\sigma = Tv_1(\sigma_1)d\sigma_1 + Tv_2(\sigma_2)d\sigma_2. \quad (1.9)$$

6. If we define

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

then (1.9) implies

$$dS = dS_1 + dS_2. \quad (1.10)$$

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

$$T > 0.$$

Choosing the integration factor $\mu := 1/T$ implies that the corresponding entropy function has the property (1.10). If \mathcal{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

$$S = \sum_{i=1}^m S_i. \quad (1.11)$$

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

$$\boxed{dU = TdS - pdV}. \quad (1.12)$$

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

$$U = U(S, V). \quad (1.13)$$

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 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 constitutive equations of states: kinetic and caloric, govern these variables, deriving from either measurements or statistical mechanics.. Here, we illustrate a specific example of a gas thermodynamic system, known as 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 $8.314462618 \text{ J} \cdot \text{K}^{-1} \cdot \text{mol}^{-1}$, see Gas Constant, Wiki. Under a mild assumption (stated below), the ideal gas law and Gibbs's relation imply that U is solely a function of T .

- **Theorem:** *Under a mild assumption (1.16) below, the ideal gas law and Gibbs's relation imply that U is only a function of T .* ³

Derivation:

²Courant and Friedrichs, Supersonic Flows and Shock Waves

³This derivation is referred to in Courant-Friedrichs' book.

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:

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

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 $h: \mathbb{R}^+ \rightarrow \mathbb{R}$ 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

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

Next, from

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

we see that T is a function of ϕ . We shall make an assumption that this function is invertible. That is, the derivative

$$(h'(\phi)\phi)' > 0 \text{ for } \phi > 0. \quad (1.16)$$

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.

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:

$$\begin{cases} pV = RT \\ U = c_v T \\ dU = TdS - pdV \end{cases}.$$

2. Plugging the two constitutive relations

$$pV = RT \text{ and } U = c_v T \quad (1.17)$$

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

$$\begin{aligned} dU &= TdS - pdV \\ \frac{c_v}{R}d(pV) &= \frac{pV}{R}dS - pdV \\ c_v \frac{d(pV)}{pV} &= dS - R \frac{dV}{V} \\ dS &= d \ln((pV)^{c_v}) + d \ln(V^R) \\ &= d \ln(p^{c_v} \cdot V^{c_v+R}) \\ S - S_0 &= \ln(p^{c_v} \cdot V^{c_v+R}) \\ e^{S-S_0} &= (pV^{(c_v+R)/c_v})^{c_v} \\ e^{(S-S_0)/c_v} &= pV^{(c_v+R)/c_v}. \end{aligned}$$

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

$$\begin{cases} p = A(S)V^{-\gamma} \\ T = \frac{A(S)}{R}V^{-\gamma+1} \\ U = \frac{c_v A(S)}{R}V^{-\gamma+1}. \end{cases} \quad (1.18)$$

- **The specific heat capacities** The physical meaning of c_v and $c_v + R$ can be described as follows: Define $dQ = TdS$ to be the heat added to the system. Then $dQ = dU + pdV$. 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:

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

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.

- **The physical meaning of $\gamma := c_p/c_v$**

1. The parameter γ is the ratio between c_p and c_v :

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

For monatomic gases, $\gamma = 5/3$ from statistical mechanics. In general,

$$1 < \gamma \leq \frac{5}{3}.$$

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.

2. For ideal gases, the heat capacity ratio γ can be related to the degree of freedom f of a molecule:

$$\gamma = \frac{f+2}{f}.$$

For monatomic gas, $f = 3$ and the corresponding $\gamma = 5/3$. For diatomic gas, $f = 3 + 2$ (\mathbb{R}^3 for translation and S^2 for rotation⁴), the corresponding $\gamma = 7/5 =$

1.4. For further discussion about γ , we refer to wiki: Heat Capacity Ratio.

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) :

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

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

- 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.

⁴The vibrational degree of freedom is not involved except at high temperatures.

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:

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

and noting

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

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

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

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

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

through both

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

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:**

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

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 $f : \mathbb{R} \rightarrow \mathbb{R}$. The differential

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

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

$$x \mapsto y = f'(x). \tag{1.19}$$

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 (1.19). 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 $f^*(y)$:

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

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

- **Lemma.** f^* is convex. Further, 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 a convex function of (S, V) .

- 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:

$$\left(\frac{\partial T}{\partial V} \right)_S = - \left(\frac{\partial p}{\partial S} \right)_V = \frac{\partial^2 U}{\partial S \partial V} \quad (1.20)$$

$$\left(\frac{\partial T}{\partial p} \right)_S = \left(\frac{\partial V}{\partial S} \right)_p = \frac{\partial^2 H}{\partial S \partial p} \quad (1.21)$$

$$\left(\frac{\partial S}{\partial V} \right)_T = \left(\frac{\partial p}{\partial T} \right)_V = - \frac{\partial^2 \Psi}{\partial T \partial V} \quad (1.22)$$

$$- \left(\frac{\partial S}{\partial p} \right)_T = \left(\frac{\partial V}{\partial T} \right)_p = \frac{\partial^2 G}{\partial T \partial p}. \quad (1.23)$$

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

$$c_v = \left(\frac{dQ}{dT} \right)_V = T \left(\frac{\partial S}{\partial T} \right)_V = -T \left(\frac{\partial^2 \Psi}{\partial T^2} \right)_V, \quad (1.24)$$

$$c_p = \left(\frac{dQ}{dT} \right)_p = T \left(\frac{\partial S}{\partial T} \right)_p = -T \left(\frac{\partial^2 G}{\partial T^2} \right)_p. \quad (1.25)$$

Compression rate The isentropic/isothermal compressibility rate are defined as

$$\kappa_S := -\frac{1}{V} \left(\frac{\partial V}{\partial p} \right)_S = -\frac{1}{V} \left(\frac{\partial^2 H}{\partial p^2} \right)_S, \quad (1.26)$$

$$\kappa_T := -\frac{1}{V} \left(\frac{\partial V}{\partial p} \right)_T = -\frac{1}{V} \left(\frac{\partial^2 G}{\partial p^2} \right)_T. \quad (1.27)$$

Expansion rate: The expansion rate is defined as

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

Proposition 1.1. *The heat capacities and compressibility satisfy*

$$\kappa_T(c_p - c_v) = TV\alpha_p^2$$

$$c_p(\kappa_T - \kappa_S) = TV\alpha_p^2,$$

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

$$\begin{aligned} \kappa_T(c_p - c_v) &= -\frac{T}{V} \left(\frac{\partial V}{\partial p}\right)_T \left(\frac{\partial S}{\partial V}\right)_T \left(\frac{\partial V}{\partial T}\right)_p \\ &= -\frac{T}{V} \left(\frac{\partial S}{\partial p}\right)_T \left(\frac{\partial V}{\partial T}\right)_p && \because \text{chain rule} \\ &= +\frac{T}{V} \left(\frac{\partial V}{\partial T}\right)_p \left(\frac{\partial V}{\partial T}\right)_p && \because (1.23) \\ &= TV \left(\frac{1}{V} \left(\frac{\partial V}{\partial T}\right)_p\right)^2 \\ &= TV \alpha_p^2 \end{aligned}$$

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

$$\begin{aligned}
 c_p(\kappa_T - \kappa_S) &= -\frac{T}{V} \left(\frac{\partial S}{\partial T} \right)_p \left(\frac{\partial V}{\partial S} \right)_p \left(\frac{\partial S}{\partial p} \right)_T \\
 &= -\frac{T}{V} \left(\frac{\partial V}{\partial T} \right)_p \left(\frac{\partial S}{\partial p} \right)_T \quad \because \text{chain rule} \\
 &= \frac{T}{V} \left(\frac{\partial S}{\partial p} \right)_T \left(\frac{\partial S}{\partial p} \right)_T \quad \because (1.23) \\
 &= \frac{T}{V} \left(\frac{\partial V}{\partial T} \right)_p^2 \\
 &= TV \left(\frac{1}{V} \left(\frac{\partial V}{\partial T} \right)_p \right)^2 \\
 &= TV \alpha_p^2.
 \end{aligned}$$

□

Theorem 1.1. *The following statements hold.*

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

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

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

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

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

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

□

Definition 1.1. A gas system is called *thermodynamic stable* if U is a convex function of (S, V) .

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

Corollary 1.1. Assuming thermodynamic stability, then

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

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 $\gamma > 1$.

Historial remarks

- The axiomatic approach in this chapter is mainly due to Gibbs and Carathéodory.
- Historical Note of Thermodynamics, see <https://www.wolframscience.com/reference/notes/1019b>

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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 \mathbf{v} , and flow velocity \mathbf{v} in its vicinity, the mass flux is defined as $\rho \mathbf{v} \cdot (-\mathbf{v})$.¹ Here, $-\mathbf{v}$ 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:

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

The conservation of mass is expressed as

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

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*:

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

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 $(\rho \mathbf{v})[\mathbf{v} \cdot (-\mathbf{v})]$,

¹The 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 $(\mathbf{v}\Delta t \cdot \mathbf{v})dA$. The mass in this parallelogram is $\rho(\mathbf{v}\Delta t \cdot \mathbf{v})dA$. Thus the mass flows into Ω through dA per unit time, per unit area is $\rho \mathbf{v} \cdot (-\mathbf{v})$.

(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

$$\mathbf{t} = \boldsymbol{\sigma} \cdot \mathbf{v},$$

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

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

This holds for arbitrary domain Ω . Thus, we obtain³

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

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

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

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

$$\boldsymbol{\sigma} = -pI,$$

where p is the pressure and I is the 3×3 identity matrix. The minus sign means that the surface force $\boldsymbol{\sigma} \cdot \mathbf{v} = -p\mathbf{v}$ 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 $\boldsymbol{\sigma} = -pI$, the momentum equation now reads

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

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

³The notation $\mathbf{v} \mathbf{v}$ stands for a tensor: $\mathbf{v} \mathbf{v} = (v^i v^j)$, and $\nabla \cdot (\rho \mathbf{v} \mathbf{v})$ stands for a vector whose i th 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 boundary $\partial\Omega$, which is $\rho E \mathbf{v} \cdot (-\mathbf{v})$ ($= -\rho E v^i v^i$),
- (b) the work done by the stress from boundary, which is $\mathbf{v} \cdot \boldsymbol{\sigma} \cdot \mathbf{v}$ ($= v^i \sigma_{ij} v^j$),
- (c) the work done by the body force in Ω , which is $\mathbf{v} \cdot \mathbf{f}$ ($= v^i f^i$).

The conservation of energy reads

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

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

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

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

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

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

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

This is equivalent to the following Neumann boundary condition:

$$\boxed{\mathbf{v} \cdot \mathbf{v} = 0 \text{ on } \partial M.} \quad (2.5)$$

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

2.1.3 General conservation laws in Eulerian coordinate

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

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

where

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

Here, \mathcal{F} is an $m \times 3$ matrix. It can be expressed as $\mathcal{F} = (\mathcal{F}_1, \mathcal{F}_2, \mathcal{F}_3)$. $\nabla_{\mathbf{x}} \cdot \mathcal{F} := \partial_{x_i} \mathcal{F}_i$. In the last equation, we add a new term \mathbf{q} , called the *heat flux* in the energy equation for generality. It will be needed in the case of heat conduction in a later chapter. By using the divergence theorem, the above equation can be expressed in the following integral form:

$$\int_{\Omega} \partial_t \mathcal{U} d\mathbf{x} + \int_{\partial\Omega} \mathcal{F} \cdot \mathbf{v} dS_t = \int_{\Omega} \mathcal{R} d\mathbf{x}. \quad (2.7)$$

where $\Omega \subset M_t$ is an arbitrary subdomain and \mathbf{v} is its outer normal.

2.2 Equations of Inviscid Fluid Flows in Lagrangian Coordinates

2.2.1 Flow maps and velocity fields

Lagrangian coordinate and Eulerian coordinates Let us recall that we have a continuum object occupying a region \hat{M} initially and evolving to $M_t \subset \mathbb{R}^3$ at time t . We refer to M_t as the observer's domain and \hat{M} as the reference domain.

Flow map and velocity field

- **Fluid parcel:** The fluid in a small box dX centered at X is called a fluid parcel at X .
- **Flow map:** The mapping $\varphi_t : \hat{M} \rightarrow M_t$ which maps

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

is called a *flow map*. Its trajectory is $\mathbf{x}(\cdot, X)$ is the trajectory of the fluid parcel. Its time derivative $\dot{\mathbf{x}}(t, X)$ is the parcel velocity denoted it by \mathbf{v} . In the Lagrangian coordinate system,

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

In observer's coordinate, we still 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:

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

Therefore, **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

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

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

$$\begin{aligned} - (F^T)_i^\alpha &:= F_\alpha^i = \frac{\partial x^i}{\partial X^\alpha} \\ - (F^{-1})_i^\alpha &:= \frac{\partial X^\alpha}{\partial x^i}, \quad \because (F \cdot F^{-1})_j^i = F_\alpha^i (F^{-1})_j^\alpha = \delta_j^i. \\ - (F^{-T})_\alpha^i &:= (F^{-1})_i^\alpha = \frac{\partial X^\alpha}{\partial x^i}. \end{aligned}$$

- 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*

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

where \mathbf{v} is the outer normal on $\partial\Omega(t)$.

Proof. We have

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

and

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

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 $\mathbf{v}dS_t$ on ∂M_t and $\mathbf{n}dS_0$ on $\partial\hat{M}$ satisfy the following transformation formula*

$$\boxed{\mathbf{v}dS_t = JF^{-T} \mathbf{n}dS_0,} \quad (2.10)$$

where \mathbf{v} 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

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

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

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

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

$$\begin{aligned} \mathbf{v}dS_t &= d\mathbf{x}_1 \times d\mathbf{x}_2 \\ &= FdX_1 \times FdX_2. \end{aligned}$$

Multiplying both sides by F^T gives

$$F^T \cdot \mathbf{v}dS_t = F^T \cdot FdX_1 \times FdX_2.$$

In coordinate form, it reads

$$\begin{aligned} F_\gamma^i \mathbf{v}^i dS_t &= F_\gamma^i \left(\varepsilon_{ijk} F_\alpha^j dX_1^\alpha F_\beta^k dX_2^\beta \right) \\ &= \varepsilon_{ijk} F_\gamma^i F_\alpha^j F_\beta^k dX_1^\alpha dX_2^\beta \\ &= J \varepsilon_{\gamma\alpha\beta} dX_1^\alpha dX_2^\beta \\ &= J n^\gamma dS_0 \end{aligned}$$

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

$$\varepsilon_{ijk} F_1^i F_2^j F_3^k = \det(F) = J.$$

Thus, we get

$$F^T \cdot \mathbf{v}dS_t = ((F^T)_i^\gamma \mathbf{v}^i dS_t = F_\gamma^i \mathbf{v}^i dS_t = J n^\gamma dS_0 = \mathbf{J} \mathbf{n} dS_0.$$

□

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

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

Choosing the arbitrary domain $\Omega(t) := \varphi_t(\Omega_0)$ for some fixed $\Omega_0 \subset \hat{M}$, and using (2.9), we obtain

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

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

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This leads to the conservation laws becoming

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

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

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

Here, we have used

$$\mathbf{v} dS_t = JF^{-T} \cdot \mathbf{n} dS_0.$$

Thus, the system of conservation laws in the Lagrange frame of reference becomes

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

where

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

Since $\rho J = \rho_0$ (see (2.17) in the next section), we get

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

The stress term is transformed to

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

where the tensor

$$\boxed{P := J\boldsymbol{\sigma}F^{-T}} \quad (2.14)$$

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

$$\boxed{P_\alpha^i = J\sigma_j^i (F^{-T})_\alpha^j = J\sigma_j^i (F^{-1})_j^\alpha = J\sigma_j^i \frac{\partial X^\alpha}{\partial x^j}}$$

The work done by the stress is

$$\mathbf{v} \cdot \boldsymbol{\sigma} \cdot \mathbf{v} dS_t = \mathbf{v} \cdot P \cdot \mathbf{n} dS_0.$$

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

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

Thus,

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

or

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

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 $\left. \frac{d}{dt} \right|_X$ as $\frac{d}{dt}$ or simply use the dot notation.

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*

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

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:

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

where $\dot{F} := \frac{dF}{dt}$.

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

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

Then

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

This follows from the Lemma below.

Lemma 2.1. (i) Let A be an $n \times n$ matrix, and $J := \det A$. It holds that

$$\frac{\partial J}{\partial a_{ij}} = J(A^{-T})_{ij}. \quad (2.16)$$

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

$$\frac{d}{d\varepsilon} \det(A) = \text{tr}(A^{-T} \dot{A}) \det(A)$$

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

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

where $\text{cof} A := (A_{ij})$, 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,

$$\begin{aligned} \dot{J} &= \frac{\partial J}{\partial a_{ij}} \frac{da_{ij}}{d\varepsilon} = A_{ij} \dot{a}_{ij} \\ &= J(A^{-T})_{ij} \dot{a}_{ij} = J \text{tr}(A^{-T} \dot{A}) \end{aligned}$$

□

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,

$$\boxed{\rho(t, \mathbf{x}(t, X))J(t, X) = \rho_0(X) \quad \text{or equivalently} \quad \frac{d}{dt}(\rho J) = 0.} \quad (2.17)$$

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 (2.17). The corresponding rate-of-change of density is

$$\boxed{\frac{d}{dt}\rho + \rho \nabla \cdot \mathbf{v} = 0.} \quad (2.18)$$

This means that

$$\nabla \cdot \mathbf{v} = -\frac{\dot{\rho}}{\rho} = \frac{\dot{V}}{V} = \frac{\dot{J}}{J} \quad (2.19)$$

is the relative rate of change of specific volume.

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

$$\frac{\partial \mathbf{v}}{\partial t} + \mathbf{v} \cdot \nabla \mathbf{v} = -\frac{\nabla p}{\rho}. \quad (2.20)$$

$$\boxed{\frac{d\mathbf{v}}{dt} = -\frac{\nabla p}{\rho}}. \quad (2.21)$$

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 (2.21) by \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

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

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:

$$\frac{dU}{dt} + \frac{p}{\rho} \nabla \cdot \mathbf{v} = 0. \quad (2.22)$$

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

$$\boxed{\frac{dS}{dt} = 0}. \quad (2.23)$$

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

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

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 Fluid Dynamic Equations on Differential Manifolds

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 include:

- 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 is the following surface integral without the integral sign:

$$\int_{\Sigma} \omega_1 dx^2 \wedge dx^3 + \omega_2 dx^3 \wedge dx^1 + \omega_3 dx^1 \wedge dx^2 = \int_{\Sigma} \boldsymbol{\omega} \cdot \mathbf{v} dS.$$

where $\boldsymbol{\omega} = (\omega_1, \omega_2, \omega_3)$ is a vector, \mathbf{v} 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 3-D manifold M , we define $\Omega^4(M) = \{0\}$.

To give you some intuition of differential forms, we have the following lemma.

Lemma 2.2. *Given a surface S in \mathbb{R}^3 , the normal surface element vdS can be expressed as*

$$vdS = (dx^2 \wedge dx^3, dx^3 \wedge dx^1, dx^1 \wedge dx^2).$$

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

Proof. Let us parametrize the surface by $u = (u^1, u^2)$ locally. That is, the surface S is locally given by $\mathbf{x}(u)$. 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

$$\left(\frac{\partial \mathbf{x}}{\partial u^1} du^1 \right) \times \left(\frac{\partial \mathbf{x}}{\partial u^2} du^2 \right) = \frac{\frac{\partial \mathbf{x}}{\partial u^1} \times \frac{\partial \mathbf{x}}{\partial u^2}}{\left\| \frac{\partial \mathbf{x}}{\partial u^1} \times \frac{\partial \mathbf{x}}{\partial u^2} \right\|} \left\| \frac{\partial \mathbf{x}}{\partial u^1} \times \frac{\partial \mathbf{x}}{\partial u^2} \right\| du^1 \wedge du^2 = vdS.$$

On the other hand, from

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

we get

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

where

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

and we have used

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

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

Exterior Derivatives:

- The exterior derivative d is defined as $d : \Omega^k(M) \rightarrow \Omega^{k+1}(M), k = 0, \dots, 3$. satisfying

- d is linear;
- For $k = 0$, define $df := f_{x^i} dx^i$.
- For $\omega = w_I(x) dx^I$, define $d(w_I(x) dx^I) := dw_I(x) \wedge dx^I$.

- Examples:

- For 0-form: $df = f_{x^1} dx^1 + f_{x^2} dx^2 + f_{x^3} dx^3$.
- For 1-form:

$$\begin{aligned} d(A_1 dx^1 + A_2 dx^2 + A_3 dx^3) &= (A_{1,x^2} dx^2 + A_{1,x^3} dx^3) \wedge dx^1 \\ &\quad + (A_{2,x^1} dx^1 + A_{2,x^3} dx^3) \wedge dx^2 + (A_{3,x^1} dx^1 + A_{3,x^2} dx^2) \wedge dx^3 \\ &= (A_{3,x^2} - A_{2,x^3}) dx^2 \wedge dx^3 + (A_{1,x^3} - A_{3,x^1}) dx^3 \wedge dx^1 + (A_{2,x^1} - A_{1,x^2}) dx^1 \wedge dx^2. \end{aligned}$$

- For 2-form:

$$d(B_1 dx^2 \wedge dx^3 + B_2 dx^3 \wedge dx^1 + B_3 dx^1 \wedge dx^2) = (B_{1,x^1} + B_{2,x^2} + B_{3,x^3}) dx^1 \wedge dx^2 \wedge dx^3.$$

- 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} .
- 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 its connection with ρ is 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

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

Then ρ and ρ_0 are related through

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

That is,

$$\rho_0 = J\rho. \tag{2.24}$$

- The specific volume is defined to be

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

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 only use exterior derivative, which is a differential structure.
- 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.

$$d_t(\rho \mu_t) = 0.$$

- The flow is adiabatic .

$$d_t S = 0.$$

- 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

$$\dot{v}_i dx^i = d_t(v_i dx^i) - v_i dv_i = -\frac{1}{\rho} dp,$$

$$d_t \eta = \varphi_t^* \left(\frac{1}{2} d|\mathbf{v}|^2 - \frac{1}{\rho} dp \right). \quad (2.25)$$

Fluid Dynamic Equation in Eulerian coordinates

- The Lie derivative $\partial_t + \mathcal{L}_v$ in the Eulerian coordinate is defined to be

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

- We can rewrite the above equations in terms of the Lie derivatives in the Eulerian coordinate system:

$$\begin{cases} (\partial_t + \mathcal{L}_v)(\rho\mu_t) = 0, \\ (\partial_t + \mathcal{L}_v)S = 0, \\ (\partial_t\eta + \mathcal{L}_v\eta) = \frac{1}{2}d|\mathbf{v}|^2 - \frac{1}{\rho}dp. \end{cases} \quad (2.26)$$

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

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

The equation of motion for viscous fluid flow is

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

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

$$d_t\omega = \varphi_t^* (-dV \wedge dp + d(V \star d\tau)). \quad (2.27)$$

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

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

With this notation, we have

- Euler equation:

$$\partial_t\eta + \mathcal{L}_v\eta = \frac{1}{2}d|\mathbf{v}|^2 - \frac{1}{\rho}dp.$$

– Navier-Stokes equation

$$\partial_t \eta + \mathcal{L}_v \eta = \frac{1}{2} d|\mathbf{v}|^2 - \frac{1}{\rho} dp + \frac{1}{\rho} \star d\tau.$$

– Viscous vorticity equation

$$\partial_t \omega + \mathcal{L}_v \omega = -dV \wedge dp + d(V \star d\tau).$$

For details, see appendix.

Chapter 3

Properties of Inviscid Fluid Flows

In the previous 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 law and circulation theory. A fundamental assumption underlies our discussion: the degenerate thermo relation.

3.1 Degenerate thermo relation

Certain fluid flows satisfy $\nabla V \times \nabla p = 0$, indicating that the level sets of velocity potential 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's important to note that this condition doesn't imply constancy for temperature T or entropy S .
- **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.

3.2 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 function Φ such that:

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

A classic example of such a force is gravitational force.

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

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

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

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

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

we obtain

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

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

$$\boxed{\partial_t \mathbf{v} + \boldsymbol{\omega} \times \mathbf{v} + \nabla \left(\frac{1}{2} |\mathbf{v}|^2 + h + \Phi \right) = 0.} \quad (3.3)$$

In the case of steady flows, the equation becomes:

$$\boldsymbol{\omega} \times \mathbf{v} + \nabla \left(\frac{1}{2} |\mathbf{v}|^2 + h + \Phi \right) = 0. \quad (3.4)$$

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

$$\mathbf{v} \cdot \nabla \left(\frac{1}{2} |\mathbf{v}|^2 + h + \Phi \right) = 0.$$

This implies that the directional derivative of $\frac{1}{2} |\mathbf{v}|^2 + h + \Phi$ in the direction \mathbf{v} is zero, indicating that this quantity remains constant along the integral curve of \mathbf{v} , which is the streamline. \square

Remarks

1. Formula (3.3) indicates that the acceleration is attributed to:
 - (i) a rotation ($\boldsymbol{\omega} \times \mathbf{v}$), where $\dot{\mathbf{v}} = -\boldsymbol{\omega} \times \mathbf{v}$ represents a rotation of \mathbf{v} .
 - (ii) a conservative force $\nabla(|\mathbf{v}|^2/2 + h + \Phi)$.
2. For steady barotropic flows, the equation becomes:

$$\boldsymbol{\omega} \times \mathbf{v} + \nabla \mathcal{H} = 0. \quad (3.5)$$

We observe that \mathcal{H} remains constant along the integral curve of \mathbf{v} . Similarly, applying the same procedure, we derive:

$$\boldsymbol{\omega} \cdot \nabla \mathcal{H} = 0.$$

This implies that \mathcal{H} also remains constant along the integral of $\boldsymbol{\omega}$, referred to as the vortex filament.

3. In the case of $\boldsymbol{\omega} \equiv 0$, such a flow is termed an irrotational flow. Subsequently, we will discover in the next subsection that if the flow is irrotational, it will remain irrotational for all later times. For steady, irrotational, and barotropic flows, we have $\nabla \mathcal{H} \equiv 0$. Consequently, we obtain:

$$\mathcal{H} = \text{constant}$$

in every simply connected subdomain of the flow region.

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.

3. Pitot tube

- The Pitot tube utilizes Bernoulli's law to measure wind speed, employing the equation:

$$\frac{1}{2}v^2 + \frac{p_a}{\rho} = \frac{p_1}{\rho}.$$

This yields the wind speed equation:

$$v = \sqrt{\frac{2(p_1 - p_a)}{\rho}} = \sqrt{\frac{2\rho_m g h}{\rho}},$$

where ρ_m is the density of mercury, and ρ is the density of gas.

3.3 Circulation Theory

Vorticity and circulation play theory important roles in fluid dynamics. It 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,

$$\int_C \mathbf{v} \cdot \mathbf{t} ds = \int_{\Sigma} \nabla \times \mathbf{v} \cdot \mathbf{v} dS \quad (3.6)$$

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

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

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

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

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

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 $X(s)$.

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

□

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*

$$\frac{d}{dt} \int_{\Sigma(t)} \boldsymbol{\omega} \cdot \mathbf{v} dS_t = 0.$$

Proof. From Stokes theorem,

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

□

Corollary 3.3. *For fluid flows with degenerate thermo relation and under conservative field, if $\boldsymbol{\omega} \equiv 0$ initially, then it stays $\boldsymbol{\omega}(t) \equiv 0$ for all later time.*

Remarks

- A vortex filament (or line) C is an integral curve of the vorticity field $\boldsymbol{\omega}$. 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.

3.3.1 Vorticity Equation in Eulerian coordinate

1. In this subsection, 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:

$$\boxed{\partial_t \boldsymbol{\omega} + \mathbf{v} \cdot \nabla \boldsymbol{\omega} - (\boldsymbol{\omega} \cdot \nabla) \mathbf{v} + \boldsymbol{\omega} (\nabla \cdot \mathbf{v}) = \nabla p \times \nabla V.} \quad (3.8)$$

Here, we have used the identities from vector calculus

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

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

$$\nabla \times (V\nabla p) = \nabla V \times \nabla p + V\nabla \times (\nabla p) = \nabla V \times \nabla p.$$

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

$$\boxed{\partial_t \boldsymbol{\omega} + \mathbf{v} \cdot \nabla \boldsymbol{\omega} - (\boldsymbol{\omega} \cdot \nabla) \mathbf{v} + \boldsymbol{\omega} (\nabla \cdot \mathbf{v}) = \nabla T \times \nabla S.} \quad (3.9)$$

2. 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 .
3. For fluid flows with degenerate thermo relation and under conservative force field, the thermo area element degenerate. The vorticity equation becomes

$$\boxed{\partial_t \boldsymbol{\omega} + \mathbf{v} \cdot \nabla \boldsymbol{\omega} - (\boldsymbol{\omega} \cdot \nabla) \mathbf{v} + \boldsymbol{\omega} (\nabla \cdot \mathbf{v}) = 0.} \quad (3.10)$$

This gives the circulation theorem.

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

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

3.3.2 Vorticity equation in Lagrangian coordinate

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

$$\boldsymbol{\omega} = \boldsymbol{\omega} \cdot \mathbf{v} dS = \boldsymbol{\omega}_1 dx^2 \wedge dx^3 + \boldsymbol{\omega}_2 dx^3 \wedge dx^1 + \boldsymbol{\omega}_3 dx^1 \wedge dx^2$$

and treat it as a function in (t, X) (denoted by $\varphi_t^* \boldsymbol{\omega}$), then the left-hand-side of (3.8) is the material derivative of the vorticity 2-form, while the right-hand side is the area

element of the thermo plane (either use (p, V) or (S, T) as the thermo coordinate system.) Thus, the vorticity equation states that the rate-of-change of the vorticity 2-form is the area element of the thermo plane. We shall come back to this in the section of geometric perspective of fluid mechanics in later section.

2. Let us denote the pull-back of ω by

$$\begin{aligned}\varphi_t^* \omega(t, X) &:= \omega_1(t, \mathbf{x}(t, X)) dx^2(t, X) \wedge dx^3(t, X) \\ &\quad + \omega^2(t, \mathbf{x}(t, X)) dx^3(t, X) \wedge dx^1(t, X) \\ &\quad + \omega^3(t, \mathbf{x}(t, X)) dx^1(t, X) \wedge dx^2(t, X)\end{aligned}$$

Which is still ω but expressed in (t, X) coordinate instead (t, \mathbf{x}) coordinate. Let d_t be the abbreviation of d/dt , which is the partial derivative in t with fixed X , i.e. the material derivative.

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

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

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

Thus, we get

$$\boxed{d_t \omega = \varphi_t^* (dp \wedge dV)}. \quad (3.11)$$

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

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

With this notation, we have

$$\boxed{\partial_t \omega + \mathcal{L}_v \omega = dp \wedge dV = dT \wedge dS}. \quad (3.12)$$

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

3.3.3 Deformation of ω/ρ

For compressible flows, Helmholtz derived the following advection equation for ω/ρ to replace ω .

$$\begin{aligned}
 \frac{d}{dt} \left(\frac{\omega}{\rho} \right) &= \frac{1}{\rho} \frac{d\omega}{dt} - \frac{1}{\rho^2} \frac{d\rho}{dt} \omega \\
 &= \frac{1}{\rho} ((\omega \cdot \nabla) \mathbf{v} - \omega \nabla \cdot \mathbf{v}) + \frac{1}{\rho^3} \nabla \rho \times \nabla p + \frac{\omega}{\rho} \nabla \cdot \mathbf{v} \\
 &= \left(\frac{\omega}{\rho} \cdot \nabla \right) \mathbf{v} + \frac{1}{\rho^3} \nabla \rho \times \nabla p.
 \end{aligned} \tag{3.13}$$

The first term on the right-hand side can be expressed as $(\nabla \mathbf{v})(\omega/\rho)$. 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 second term on the right-hand side is called the buoyancy effect.

In the case of thermo degeneracy, from (3.13), we have the following theorem.

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

$$\frac{d}{dt} \left(\frac{\omega}{\rho} \right) = \left(\frac{\omega}{\rho} \cdot \nabla \right) \mathbf{v}. \tag{3.14}$$

and

$$\boxed{\frac{\omega}{\rho}(t) = \frac{\omega}{\rho}(0) \frac{\partial \mathbf{x}(t, X)}{\partial X}}. \tag{3.15}$$

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

Proof. 1. Formulae (3.14) and (3.15) are equivalent because of the following arguments. Assuming (3.15), we differentiate it in t to get

$$\begin{aligned}
 \frac{d}{dt} \left(\frac{\omega}{\rho} \right) &= \frac{d}{dt} \frac{\partial \mathbf{x}(t, X)}{\partial X} \cdot \frac{\omega}{\rho}(0) \\
 &= \dot{F} \cdot \frac{\omega}{\rho}(0) \\
 &= (\nabla \mathbf{v}) \cdot F \cdot \frac{\omega}{\rho}(0) \\
 &= (\nabla \mathbf{v}) \cdot \frac{\omega}{\rho}(t).
 \end{aligned}$$

2. Formula (3.15) is equivalent to

$$\frac{\boldsymbol{\omega}}{\rho}(t) \frac{\partial X}{\partial \mathbf{x}}(t) = \frac{\boldsymbol{\omega}}{\rho}(0)I,$$

or

$$\frac{d}{dt} \left(\frac{\boldsymbol{\omega}}{\rho} \frac{\partial X}{\partial \mathbf{x}} \right) = 0. \quad (3.16)$$

To show this, we use Lagrange coordinate

$$\frac{d}{dt} \left(\frac{\boldsymbol{\omega}}{\rho} \right) = \left(\frac{\boldsymbol{\omega}}{\rho} \cdot \nabla \right) \mathbf{v} = \frac{\boldsymbol{\omega}}{\rho} \frac{\partial X}{\partial \mathbf{x}} \frac{\partial \mathbf{v}}{\partial X}$$

We differentiate the identity

$$\frac{\partial X}{\partial \mathbf{x}} \frac{\partial \mathbf{x}}{\partial X} = I$$

in t to get

$$\frac{d}{dt} \left(\frac{\partial X}{\partial \mathbf{x}} \right) \frac{\partial \mathbf{x}}{\partial X} + \frac{\partial X}{\partial \mathbf{x}} \frac{\partial \mathbf{v}}{\partial X} = 0.$$

Plug this into the above equation, we get

$$\frac{d}{dt} \left(\frac{\boldsymbol{\omega}}{\rho} \right) + \frac{\boldsymbol{\omega}}{\rho} \frac{d}{dt} \left(\frac{\partial X}{\partial \mathbf{x}} \right) \left(\frac{\partial \mathbf{x}}{\partial X} \right) = 0.$$

or

$$\frac{d}{dt} \left(\frac{\boldsymbol{\omega}}{\rho} \right) \left(\frac{\partial X}{\partial \mathbf{x}} \right) + \frac{\boldsymbol{\omega}}{\rho} \frac{d}{dt} \left(\frac{\partial X}{\partial \mathbf{x}} \right) = 0.$$

This is

$$\frac{d}{dt} \left(\frac{\boldsymbol{\omega}}{\rho} \frac{\partial X}{\partial \mathbf{x}} \right) = 0. \quad (3.17)$$

We integrate it to obtain

□

Remarks

- An equivalent form is

$$\boldsymbol{\omega}^i(t) = \frac{1}{J} F_{\alpha}^i \boldsymbol{\omega}_0^{\alpha}.$$

- The push forward of the vorticity two form is

$$\star_t \boldsymbol{\omega}(t) = F \star_0 \boldsymbol{\omega}_0.$$

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

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

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

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

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

This shows that the vortex filament stays as a vortex filament. It flows with the fluid.

Chapter 4

Variational Principles for Fluid Flows

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

- (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 variational principle in Lagrangian coordinate.
- (1809) Poisson introduced Poisson bracket.
- (1833) Hamilton formulated Hamilton mechanics based on Lagrange mechanics

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

4.1 Lagrange Variational Approach

Lagrange (1788) derived Euler equation based on variation principle in Lagrange coordinate. Mimic to the variational approach in classical mechanics, we shall take variation of 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 Lagrange coordinate to be

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

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

- 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 a constant along a particle path. Therefore, $W = \rho_0(X)U(S, V)$ is a function of $\det(F)$ along a parcel path.

We will derive equation of motion in Lagrange coordinate without the body force. We first work for compressible fluid flows. Next we work out for incompressible fluid flows.

4.1.1 Variation of action w.r.t. flow maps for compressible flows

We shall study the variation of 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 call

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

the variation of the flow map $\mathbf{x}(\cdot, \cdot)$. We write the variation of \mathbf{x} by $\delta \mathbf{x}$. The variation of a functional $I[\mathbf{x}]$ in the direction of $\delta \mathbf{x}$ means that

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

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

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

Since, for small ε , $\mathbf{x}^\varepsilon(t, \cdot)$ are flow maps, its variation

$$\delta \mathbf{x}(t, X) = \lim_{\varepsilon \rightarrow 0} \frac{\mathbf{x}^\varepsilon - \mathbf{x}_0}{\varepsilon}$$

is an infinitesimal variation of position, thus, can be called a pseudo-velocity.

We shall choose those variations $\delta \mathbf{x}$ which satisfy $\delta \mathbf{x}(t, X) = 0$ for $t = t_0$ and $t = t_1$ so that we can take integration by part for t without appearance of boundary terms.

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

Here, we have chosen those variations satisfying

$$\int_{\Omega_0} W'(F) \delta \mathbf{x} \cdot \mathbf{n} dS_0 = 0 \quad (4.1)$$

on the boundary of Ω_0 so that no boundary terms show up in the integration-by-part in the above integration. This leads to the following Euler-Lagrange equation

$$\boxed{\rho_0(X) \ddot{\mathbf{x}}(t, X) = \nabla_X \cdot P \left(\frac{\partial \mathbf{x}}{\partial X} \right)}. \quad (4.2)$$

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

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

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

Equation of motion in Lagrangian coordinate Let us express this equation of motion in terms of \mathbf{v} and thermo variables in Lagrangian coordinate. First, the Euler-Lagrange equation (4.2) 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

$$\begin{aligned} P = W'(F) &= \frac{\partial(\rho_0(X)U(S_0(X), V))}{\partial F} = \rho_0 \frac{\partial U}{\partial V} \frac{\partial V}{\partial F} \\ &= -\rho_0 p \frac{\partial V}{\partial F} = -p \frac{\partial(\rho_0 V)}{\partial F} = p \frac{\partial J}{\partial F} = -p J F^{-T}. \end{aligned}$$

Here, we have used $V = 1/\rho$, $\rho J = \rho_0$ and $\partial \det(F)/\partial F = J F^{-T}$, which is (2.16). Thus, the equation of motion is

$$\begin{cases} \rho_0 \dot{\mathbf{v}} = \nabla_X \cdot P(F) \\ \dot{F} = \frac{\partial \mathbf{v}(t, X)}{\partial X} \end{cases} \quad (4.3)$$

where

$$P = -p J F^{-T}. \quad (4.4)$$

The thermo 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 (4.3), (4.4) is closed with unknowns $\mathbf{v}(t, X)$ and $F(t, X)$.

The above derivation shows that if $\mathbf{x}(t, X)$ satisfies PDE (4.2), then its derivatives $(\mathbf{v}(t, X), F(t, X))$ satisfies PDE (4.3). 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 *compatibility conditions*

$$\frac{\partial F_\alpha^i}{\partial X^\beta} = \frac{\partial F_\beta^i}{\partial X^\alpha} \quad (4.5)$$

and

$$\dot{F}_\alpha^i = \frac{\partial v^i}{\partial X^\alpha}. \quad (4.6)$$

The second one is already appeared in our equation (4.3). So (4.5) is an addition condition. It is also called *integrability condition* for F .

Conversely, if a pair of functions $(\mathbf{v}(t, X), F(t, X))$ satisfies PDE (4.3), 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 (4.2)? Certainly there is no guarantee that F satisfies (4.5). However, if F satisfies (4.5) at $t = 0$, we claim that F satisfies (4.5) for all later time. This is because

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

If \mathbf{v} and F satisfy the compatibility conditions (4.5), (4.6), 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 coordinate The equation of motion in Eulerian coordinate is simpler. From (2.14) and (4.4), the Cauchy stress for fluids is

$$\boldsymbol{\sigma} = J^{-1} W'(F) F^T = -J^{-1} p J F^{-T} F^T = -p I.$$

Using the Euler-Lagrange transformation formula, we obtain

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

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

$$\rho(t, \mathbf{x}(t, X)) J(t, X) = \rho_0(X), \quad S(t, \mathbf{x}(t, X)) = S_0(X). \quad (4.7)$$

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

$$\begin{aligned} \partial_t \rho + \nabla_{\mathbf{x}}(\rho \mathbf{v}) &= 0, \\ \partial_t S + \mathbf{v} \cdot \nabla_{\mathbf{x}} S &= 0. \end{aligned}$$

They are obtained by differentiating (4.7) in t .

Boundary conditions In the above derivation of the Euler-Lagrange equation (4.2), we require the boundary condition (4.1) for $\delta \mathbf{x}$. Express this in component form reads

$$P_{\alpha}^i n^{\alpha} \delta x^i dS_0 = 0 \quad (4.8)$$

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, $P = -p J F^{-T}$. This gives

$$0 = p \delta \mathbf{x} \cdot J F^{-T} \mathbf{n} dS_0 = p \delta \mathbf{x} \cdot \mathbf{v} dS_t.$$

Thus, a natural boundary condition is

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

The condition

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

implies $\delta \mathbf{x} \cdot \mathbf{v} = 0$ on $\partial\Omega_t$. This is called the natural boundary condition.

4.1.2 Variation of action w.r.t. flow maps for incompressible flows

A flow map $\mathbf{x}(t, X)$ is called incompressible if

$$J(t, X) := \det \left(\frac{\partial \mathbf{x}}{\partial X}(t, X) \right) = 1.$$

This means its volume is unchanged. 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.

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

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

The Piola stress

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

Next, the variation

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

where

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

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

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

Thus, we obtain the constraint-flow equation

$$\rho_0 \dot{\mathbf{x}} = -\nabla_X \cdot (p F^{-T}), \quad \det = 1, \quad F := \frac{\partial \mathbf{x}}{\partial X}$$

for the unknown $\mathbf{x}(t, X)$ and $p(t, X)$. Here, the boundary terms appeared in the integration-by-part is

$$\int_{t_0}^{t_1} \int_{\partial \hat{M}} \delta \mathbf{x} \cdot (p F^{-T}) \cdot \mathbf{n} dS_0 dt.$$

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:

$$\begin{cases} \rho_0 \dot{\mathbf{v}} &= -\nabla_X \cdot (p F^{-T}) \\ \dot{F} &= \frac{\partial \mathbf{v}(t, X)}{\partial X} \\ \nabla \cdot \mathbf{v} &= 0 \end{cases}$$

The unknowns are (F, \mathbf{v}, p) . The constraint $\det F = 1$ is a consequence of the $\nabla \cdot \mathbf{v} = 0$ and $F(0) = I$.

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 (ρ, \mathbf{v}, p) .

Incompressibility

- When the density of each fluid parcel is unchanged during its motion, such fluid is called incompressible. That is

$$\boxed{\frac{d\rho}{dt} = 0.} \quad (4.9)$$

- Incompressibility is equivalent to

$$\boxed{\nabla \cdot \mathbf{v} = 0.} \quad (4.10)$$

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

$$\boxed{J(t, X) := \det F = 1.} \quad (4.11)$$

where $F = \frac{\partial x^i}{\partial X^j}$ is the deformation gradient. This follows from

$$\left(\frac{d}{dt}(\rho J) = 0, \frac{d}{dt}\rho = 0 \right) \Rightarrow \frac{d}{dt}J = 0.$$

Since $J(0, X) = 1$, we get $J(t, X) = 1$ for all t .

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

$$\boxed{\rho \frac{d\mathbf{v}}{dt} + \nabla p = \mathbf{f}.} \quad (4.12)$$

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

Remark For incompressible flows, there is only one thermo variable. Thus, we cannot include the energy equation. The role of pressure p is a Lagrange multiplier from the constraint $\det F = 1$. We shall come back to explain in detail in the chapter of variation approach.

Boundary Conditions We impose the boundary condition

$$\mathbf{v} \cdot \mathbf{n} = 0, \quad \mathbf{x} \in \partial D. \quad (4.13)$$

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 w such that $w'(\rho) = p'(\rho)/\rho$. Then the barotropic flow equation becomes

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

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 approach's 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).
3. P.J. Morrison, Hamiltonian Fluid Mechanics, in Encyclopedia of Mathematical Physics, vol. 2, (Elsevier, Amsterdam, 2006)
4. J. Serrin, Mathematical Principles of Classical Fluid Mechanic (1959)
5. Beris and Edwards, Thermodynamics of Flowing Systems (1994).

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

1. Configuration space and space of Vector fields

- Configuration space: Let

$$\mathcal{Q} := \{\mathbf{q} : M \rightarrow M \text{ diffeomorphism}\}$$

the collection of flow maps. \mathcal{Q} is called a configuration space. A flow map $\mathbf{x}(t, X)$ is treated as a map $[t_0, t_1] \rightarrow \mathcal{Q}$ and is considered as a trajectory on \mathcal{Q} .

- Space of vector fields: Let

$$\mathcal{V} := \{\mathbf{v} : M \rightarrow \mathbb{R}^3 \text{ continuous}\}$$

A velocity field $\mathbf{v}(t, \mathbf{x})$ is treated as a map $[t_0, t_1] \rightarrow \mathcal{V}$, and is considered as a trajectory on \mathcal{V} .

- The flow map $\mathbf{x}(\cdot, \cdot)$ and velocity field $\mathbf{v}(\cdot, \cdot)$ are related by

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

The space \mathcal{V} can be embedded into the tangent bundle of \mathcal{Q} .¹

2. **Perturbation of flow map by a vector field \mathbf{w} .** Given a flow map $\mathbf{x}(t, X)$, or equivalently, a vector field \mathbf{v} , we want to perturb it in an arbitrary direction $\mathbf{w}(t, \mathbf{x})$. For this, we consider a family of flow maps $\mathbf{x}^s(t, X)$ such that the vector field \mathbf{w} is obtained by

$$\mathbf{w}(t, \mathbf{x}) = (\partial_s)_X \mathbf{x}^s(t, X), \quad \text{with} \quad \mathbf{x} = \mathbf{x}^s(t, X).$$

The perturbation perturbs the flow map $\mathbf{x}(t, X)$ in direction \mathbf{w} by a parameter s at $s = 0$. Thus, given \mathbf{w} , we can construct such a family of flow maps $\mathbf{x}^s(t, X)$ such that $(\partial_s)_X \mathbf{x}^s(t, X) = \mathbf{w}(t, \mathbf{x}(t, X))$. Conversely, given a family of flow maps $\mathbf{x}^s(t, X)$, its infinitesimal generator is a vector field \mathbf{w} . The role of s is very similar to time t in the flow maps $\mathbf{x}^s(t, \cdot)$. Thus, we call \mathbf{w} a pseudo-velocity.

¹Assuming uniqueness of ODEs for velocity fields

3. **Dynamically accessible variations** The perturbation \mathbf{w} induces variations on \mathbf{v} , ρ and S as the follows:

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

with $\mathbf{x} = \mathbf{x}(t, X)$ fixed, where $\frac{\partial}{\partial s}$ is evaluated at $s = 0$. Note that

$$(\partial_s)_X = (\partial_s)_{\mathbf{x}} + \mathbf{w} \cdot \nabla_{\mathbf{x}}, \quad (\partial_t)_X = (\partial_t)_{\mathbf{x}} + \mathbf{v} \cdot \nabla_{\mathbf{x}}. \quad (4.14)$$

We have the following lemma.

Lemma 4.3. $\delta\mathbf{v}$ satisfies

$$\delta\mathbf{v} + \mathbf{w} \cdot \nabla\mathbf{v} = \partial_t\mathbf{w} + \mathbf{v} \cdot \nabla\mathbf{w}. \quad (4.15)$$

Proof. We use

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

The LHS gives

$$(\partial_s)_X (\partial_t)_X \mathbf{x}^s(t, X) = (\partial_s)_X \mathbf{v}(t, \mathbf{x}^s(t, X)) = (\partial_s)_{\mathbf{x}} \mathbf{v} + (\partial_{\mathbf{x}}) \mathbf{v} (\partial_s)_X \mathbf{x}^s = \delta\mathbf{v} + \mathbf{w} \cdot \nabla_{\mathbf{x}} \mathbf{v}$$

The RHS is

$$(\partial_t)_X (\partial_s)_X \mathbf{x}^s(t, X) = (\partial_t)_X \mathbf{w} = \partial_t\mathbf{w} + \mathbf{v} \cdot \nabla\mathbf{w}.$$

We get

$$\delta\mathbf{v} + \mathbf{w} \cdot \nabla\mathbf{v} = \partial_t\mathbf{w} + \mathbf{v} \cdot \nabla\mathbf{w}.$$

□

Lemma 4.4. If ρ and S satisfy

$$\rho(t, \mathbf{x}^s(t, X)) J^s(t, X) = \rho_0(X) \quad (4.16)$$

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

then the corresponding $\delta\rho$ and δS satisfy

$$\delta\rho + \nabla \cdot (\rho\mathbf{w}) = 0, \quad (4.18)$$

$$\delta S + \mathbf{w} \cdot \nabla_{\mathbf{x}} S = 0. \quad (4.19)$$

Proof. We have

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

we get

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

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

$$\delta J = (\nabla \cdot \mathbf{w})J.$$

Differentiating (4.16) in s , using (4.14), we get

$$(\partial_s)_X (\rho(t, \mathbf{x}^s(t, X)) J^s(t, X)) = 0$$

$$(\delta \rho + \mathbf{w} \cdot \nabla \rho) J + \rho (\nabla \cdot \mathbf{w}) J = 0.$$

This gives (4.18). Similarly, differentiating (4.17) in s , we get (4.19). \square

Remark The above $\delta \mathbf{v}$, $\delta \rho$ and δS satisfying (4.18) (4.19) are called *dynamically accessible variations* in the direction \mathbf{w} .

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

$$\mathcal{S}[\rho, \mathbf{v}, S] := \int_{t_0}^{t_1} \int_{\Omega} \left(\frac{1}{2} \rho |\mathbf{v}|^2 - \rho U(\rho, S) \right) d\mathbf{x} dt. \quad (4.20)$$

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

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

The variations $\delta \rho$, δS and $\delta \mathbf{v}$ are induced by \mathbf{w} . We now express them in terms of \mathbf{w} :

$$\begin{aligned} \delta \mathcal{S} &= \int_{t_0}^{t_1} \int_{\Omega} \left(\frac{1}{2} |\mathbf{v}|^2 - U - \frac{p}{\rho} \right) (-\nabla \cdot (\rho \mathbf{w})) + \rho T (\nabla S \cdot \mathbf{w}) + \rho \mathbf{v} (\mathbf{w}_t + \mathbf{v} \cdot \nabla \mathbf{w} - \nabla \mathbf{v} \cdot \mathbf{w}) d\mathbf{x} dt \\ &= \int_{t_0}^{t_1} \int_{\Omega} [-(\rho \mathbf{v})_t - \nabla \cdot (\rho \mathbf{v} \mathbf{v}) - \nabla p] \cdot \mathbf{w} - \rho [\nabla U - \frac{p}{\rho^2} \nabla \rho - T \nabla S] \cdot \mathbf{w} d\mathbf{x} dt \end{aligned} \quad (4.21)$$

Here, we have performed integration by part and used $\mathbf{w} \cdot \mathbf{v} = 0$ 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 approach's (constrained variation)

Herivel-Lin treat the equations for thermo 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 $\delta I[\rho, S, \mathbf{v}]$. However, it was found by C.C. Lin that there is another constraint, the **relabelling symmetry** (invariant), which is crucial in the representation of velocity and the vorticity. Let $X(t, \mathbf{x})$ be the inversion of $\mathbf{x}(t, X)$. Then $X(t, \mathbf{x})$ (which is φ_t^{-1}) satisfies

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

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

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

²These 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.

Taking the variation of the action w.r.t. the Lagrange multipliers (φ, η, γ) lead to the constraints. The variations of the action w.r.t. ρ, S, X and \mathbf{v} are listed below.

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

These give

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

where $\dot{\varphi} := (\partial_t + v^j \partial_j) \varphi$. Let us write $\mathbf{v} = \nabla \varphi + \eta \nabla S + \gamma \cdot \nabla X = \sum_k \xi_k \nabla \eta_k$. Applying the material derivative to \mathbf{v} to get

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

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.

4.2.3 Clebsch representation and relabeling symmetry

1. The representation

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

is called a Clebsch representation for \mathbf{v} . It has been shown that the corresponding flow has zero helicity:

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

The helicity is a conservative quantity. Thus, such Clebsch representation of \mathbf{v} can only represent flows with zero helicity, see [Graham and Henyey, 2000].

2. For general velocity field, we need more terms in the Clebsch representation. The Darboux theorem states that for any 1-form $\eta := v_i dx^i$, there exists functions ξ_i, η_i , $i = 1, \dots, k$, such that

$$\eta = \sum_{i=1}^k \xi_i d\eta_i.$$

In this representation, we can always choose $\xi_1 = 1$ by integrating $\xi_1 \partial_{x_3} \eta_1(x_1, x_2, x_3)$ in x_3 direction and reset ξ_2, \dots, ξ_k . The number k depends on the *rank* of \mathbf{v} , which we consult with the original Darboux theorem. An extension of Darboux theorem is the Carathéodory–Jacobi–Lie theorem which allows us to prescribe ξ_1, \dots, ξ_r and extend them to ξ_{r+1}, \dots, ξ_k and η_1, \dots, η_k . Thus, we can always represent the velocity \mathbf{v} as

$$\mathbf{v} = \nabla\varphi + \eta\nabla S + \sum_{i=1}^k \xi_i \nabla\eta_i, \quad (4.22)$$

called a generalized Clebsch representation. The η_i terms comes from the *relabeling* of the material coordinates. Given any initial velocity field \mathbf{v}_0 , we can always find such Clebsch representation for \mathbf{v}_0 . The dynamics of the Clebsch variables are

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

$$\dot{\xi}_i = 0, \quad \dot{\eta}_i = 0, \quad i = 1, \dots, k.$$

We have seen that the corresponding \mathbf{v}_t satisfies the Euler equation. Thus, any solution of the Euler equations can be represented by a generalized Clebsch representation and the corresponding dynamics.

3. By taking *curl* of (4.22), we get

$$\omega = \nabla\eta \times \nabla S + \sum_{i=1}^k \nabla\xi_i \times \nabla\eta_i. \quad (4.23)$$

The Lie derivative in time of ω gives

$$\dot{\omega} = \nabla\dot{\eta} \times \nabla S + \nabla\eta \times \nabla\dot{S} + \sum_{i=1}^k \left(\nabla\dot{\xi}_i \times \nabla\eta_i + \nabla\xi_i \times \nabla\dot{\eta}_i \right) = \nabla T \times \nabla S.$$

The formula shows that the relabeling does not affect $\dot{\omega}$ because they advect along the flow. 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. The term η_i comes from the relabeling of the initial mass. The appearance η_i and its conjugate ξ_i allows us to construct any initial vorticity field:

$$\omega(0) = \sum_{i=1}^k (\nabla\xi_i \times \nabla\eta_i)(0).$$

Thus, the relabeling, which corresponds to a perturbation of flow path, induces an invariant, the vorticity. “*The vorticity laws arise from the particle-relabeling symmetry*”, quoted from Salmon.³

In general, the vorticity laws holds on the level set of entropy function.

³Rick Salmon, *Hamiltonian Fluid Mechanics* (1998). In fact, Salmon derives the vorticity equation (in Lagrangian coordinate) via variation of action with respect to the material variable \mathbf{a} (where $d\mathbf{a} = \rho_0(X) dX$).

Chapter 5

Hamiltonian Fluid Mechanics

5.1 Hamiltonian Fluid Dynamics in Lagrangian coordinate

5.1.1 Hamilton's dynamics in Lagrangian coordinate

Let us define the configuration space

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

Define

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

We assume: on the target space \mathbb{R}^3 , there is a natural volume measure $d\mathbf{x}$, while in the domain 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 $S_0 : \Omega \rightarrow \mathbb{R}$ and an internal energy $e(V, S_0)$. 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 $\mathcal{L} : \mathcal{M} \rightarrow \mathbb{R}$ is defined by

$$\mathcal{L}[\mathbf{x}, \mathbf{v}] := \int_{\Omega_0} L\left(\mathbf{x}, \frac{\partial \mathbf{x}}{\partial X}, \mathbf{v}\right) dX$$

A path is a trajectory on \mathcal{M} . That is $(\mathbf{x}, \mathbf{v}) : [t_0, t_1] \rightarrow \mathcal{M}$. Associate with a path $(\mathbf{x}(\cdot), \mathbf{v}(\cdot))$ we define the action to be

$$\mathcal{S}[\mathbf{x}] := \int_{t_0}^{t_1} \mathcal{L}[\mathbf{x}(t), \dot{\mathbf{x}}(t)] dt.$$

The Euler-Lagrange equation is governed by $\delta\mathcal{S}/\delta\mathbf{x} = 0$, which is

$$\frac{d}{dt} \frac{\delta\mathcal{L}}{\delta\mathbf{v}} + \frac{\delta\mathcal{L}}{\delta\mathbf{x}} = 0.$$

Here,

$$\begin{aligned} \frac{\delta\mathcal{L}}{\delta\mathbf{v}}[\mathbf{x}, \dot{\mathbf{x}}] &= \rho_0 \dot{\mathbf{x}} \\ \frac{\delta\mathcal{L}}{\delta\mathbf{x}}[\mathbf{x}, \dot{\mathbf{x}}] &= \nabla_X \cdot (pJF^{-T}), \end{aligned}$$

with

$$\begin{aligned} F &:= \frac{\partial\mathbf{x}}{\partial X}, \quad J = \det(F), \\ p &:= \frac{\partial U}{\partial V}, \quad V = \frac{J}{\rho_0}. \end{aligned}$$

Variations $\delta\mathbf{x}, \delta\mathbf{v}$ are 1-forms on \mathcal{M} , while $\delta\mathcal{L}/\delta\mathbf{x}$ and $\delta\mathcal{L}/\delta\mathbf{v}$ are tangent vectors on \mathcal{M} . Thus,

$$\left(\frac{\delta\mathcal{L}}{\delta\mathbf{v}}, \frac{\delta\mathcal{L}}{\delta\mathbf{x}} \right) \in \mathcal{TM}.$$

The Hamiltonian \mathcal{H} is defined on $\mathcal{T}^*\mathcal{Q}$ by

$$\mathcal{H}[\mathbf{x}, \mathbf{p}] := \langle \mathbf{p}, \mathbf{v} \rangle - \mathcal{L}[\mathbf{x}, \mathbf{v}]$$

with \mathbf{v} obtained from the relation:

$$\mathbf{p} = \delta\mathcal{L}/\delta\mathbf{v}[\mathbf{x}, \mathbf{v}]. \quad (5.1)$$

This relation gives $\mathbf{v} = \mathbf{p}/\rho_0$. Thus,

$$\boxed{\mathcal{H}[\mathbf{x}, \mathbf{p}] = \int_{\Omega_0} H(\mathbf{x}, \frac{\partial\mathbf{x}}{\partial X}, \mathbf{p}) dX := \int_{\Omega_0} \frac{|\mathbf{p}|^2}{2\rho_0} + \rho_0 U(\rho_0/J, S_0) dX.} \quad (5.2)$$

The variations $(\frac{\delta\mathcal{H}}{\delta\mathbf{x}}, \frac{\delta\mathcal{H}}{\delta\mathbf{p}})$ is considered as a vector field on $\mathcal{T}^*\mathcal{Q}$. The Hamilton's equation of motion is

$$\begin{cases} \dot{\mathbf{x}} = \frac{\delta\mathcal{H}}{\delta\mathbf{p}} \\ \dot{\mathbf{p}} = -\frac{\delta\mathcal{H}}{\delta\mathbf{x}} \end{cases} \quad (5.3)$$

where

$$\frac{\delta \mathcal{H}}{\delta \mathbf{p}} = \frac{\mathbf{p}}{\rho_0}$$

$$\begin{aligned} \delta \mathcal{H} &= \int_{\Omega_0} \rho_0 \frac{\partial U}{\partial V} \frac{\partial V}{\partial F} \delta \left(\frac{\partial \mathbf{x}}{\partial X} \right) dX \\ &= \int_{\Omega_0} \nabla_X \cdot (p J F^{-T}) \cdot \delta \mathbf{x}. \end{aligned}$$

This gives

$$\frac{\delta \mathcal{H}}{\delta \mathbf{x}} = \nabla_X \cdot (p J F^{-T}).$$

Thus, $\dot{\mathbf{p}} = \frac{\delta \mathcal{H}}{\delta \mathbf{x}}$ is the Euler equation in Lagrangian coordinate.

5.1.2 Poisson Bracket in Lagrange variables

1. Given two functionals \mathcal{F} and \mathcal{G} on $\mathcal{T}^*\Omega$, we define their Poisson bracket by

$$\boxed{\{\mathcal{F}, \mathcal{G}\} := \int_{\Omega_0} \frac{\delta \mathcal{F}}{\delta \mathbf{x}} \cdot \frac{\delta \mathcal{G}}{\delta \mathbf{p}} - \frac{\delta \mathcal{G}}{\delta \mathbf{x}} \cdot \frac{\delta \mathcal{F}}{\delta \mathbf{p}} dX} \quad (5.4)$$

The Poisson bracket $\{\cdot, \cdot\}$ is bilinear and satisfies

- non-degenerate: if $\{\mathcal{F}, \mathcal{G}\} = 0$ for all \mathcal{G} , then $\mathcal{F} = \text{const.}$,
- antisymmetry: $\{\mathcal{F}, \mathcal{G}\} = -\{\mathcal{G}, \mathcal{F}\}$,
- Jacobi identity:

$$\{\{\mathcal{E}, \mathcal{F}\}, \mathcal{G}\} + \{\{\mathcal{F}, \mathcal{G}\}, \mathcal{E}\} + \{\{\mathcal{G}, \mathcal{E}\}, \mathcal{F}\} = 0.$$

2. The Hamilton equation of motion is equivalent to

$$\frac{d\mathcal{F}[\mathbf{x}(t), \mathbf{p}(t)]}{dt} = \{\mathcal{F}, \mathcal{H}\} \quad (5.5)$$

for any $\mathcal{F} : \mathcal{T}^*\Omega \rightarrow \mathbb{R}$. To see this, we choose $\mathcal{F} = x^i \delta(X - X')$. 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 momentum equation at X' when we choose $f = p^i \delta(X - X')$. This shows (5.5) \Rightarrow (5.3). Conversely, given a Hamiltonian flow $(\mathbf{x}(t), \mathbf{p}(t))$ satisfying (5.3) and for any $f : \mathcal{T}^*\mathcal{Q} \rightarrow \mathbb{R}$, we have

$$\begin{aligned} \frac{d}{dt} f[\mathbf{x}(t), \mathbf{p}(t)] &= \frac{\delta f}{\delta \mathbf{x}} \cdot \dot{\mathbf{x}}(t) + \frac{\delta f}{\delta \mathbf{p}} \cdot \dot{\mathbf{p}}(t) \\ &= \frac{\delta f}{\delta \mathbf{x}} \cdot \frac{\delta \mathcal{H}}{\delta \mathbf{p}} - \frac{\delta f}{\delta \mathbf{p}} \cdot \frac{\delta \mathcal{H}}{\delta \mathbf{x}} \\ &= \{f, \mathcal{H}\}. \end{aligned}$$

This shows (5.3) \Rightarrow (5.5).

5.2 Hamilton Fluid Mechanics in Eulerian coordinate

5.2.1 Non-canonical transformation

1. Change-of-variables from Lagrangian variables to Eulerian variables.

The Eulerian variables are $\rho, \mathbf{m} := \rho \mathbf{v}$ and $\mathfrak{s} := \rho S$. The space spanned by the Eulerian variables $(\rho, \mathbf{m}, \mathfrak{s})$ has 5 free variables, whereas the space of the Lagrangian variables (\mathbf{q}, \mathbf{p}) has 6 free variables.

The mapping

$$\Phi : (\mathbf{q}, \mathbf{p}) \mapsto (\rho, \mathfrak{s}, \mathbf{m})$$

can be found as

$$\begin{aligned} \rho(\mathbf{x}) &= \int_{\Omega_0} \rho_0(X) \delta(\mathbf{x} - \mathbf{q}(X)) dX \\ \mathfrak{s}(\mathbf{x}) &= \int_{\Omega_0} \mathfrak{s}_0(X) \delta(\mathbf{x} - \mathbf{q}(X)) dX \\ \mathbf{m}(\mathbf{x}) &= \int_{\Omega_0} \mathbf{p}(X) \delta(\mathbf{x} - \mathbf{q}(X)) dX \end{aligned} \tag{5.6}$$

The derivation of these formulae is the follows. 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

$$\begin{aligned} \int_{\Omega_0} \rho_0(X) \delta(\mathbf{x} - \mathbf{q}(X)) dX &= \int_{\Omega_0} \rho(\mathbf{q}(X))J(X) \delta(\mathbf{x} - \mathbf{q}(X)) dX \\ &= \int_{\Omega} \rho(\mathbf{y}) \delta(\mathbf{x} - \mathbf{y}) d\mathbf{y} = \rho(\mathbf{x}). \end{aligned}$$

The proofs for \mathfrak{s} and \mathbf{m} are similar. These formulae only hold for conservative quantities.

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 $\tilde{\mathcal{F}}$ defined in $(\rho, \mathfrak{s}, \mathbf{m})$, it induces a functional \mathcal{F} defined on (\mathbf{q}, \mathbf{p}) by function composition:

$$\mathcal{F}[\mathbf{q}, \mathbf{p}] = \tilde{\mathcal{F}}[\Phi(\mathbf{q}, \mathbf{p})].$$

Its variation can be represented as

$$\begin{aligned}\delta\mathcal{F} &= \int_{\Omega_0} \left(\frac{\delta\mathcal{F}}{\delta\mathbf{q}} \delta\mathbf{q} + \frac{\delta\mathcal{F}}{\delta\mathbf{p}} \delta\mathbf{p} \right) dX \\ &= \int_{\Omega} \left(\frac{\delta\tilde{\mathcal{F}}}{\delta\rho} \delta\rho + \frac{\delta\tilde{\mathcal{F}}}{\delta\mathfrak{s}} \delta\mathfrak{s} + \frac{\delta\tilde{\mathcal{F}}}{\delta\mathbf{m}} \delta\mathbf{m} \right) d\mathbf{x}.\end{aligned}$$

In this expression, $\frac{\delta \bar{\mathcal{F}}}{\delta \rho}$ is a function of $(\rho, \mathbf{m}, \mathfrak{s})$, hence a function of \mathbf{x} .

$$\begin{aligned} \frac{\delta \bar{\mathcal{F}}}{\delta \mathbf{q}}(X) &= \int_{\Omega} \left(\frac{\delta \bar{\mathcal{F}}}{\delta \rho} \frac{\delta \rho}{\delta \mathbf{q}} + \frac{\delta \bar{\mathcal{F}}}{\delta \mathfrak{s}} \frac{\delta \mathfrak{s}}{\delta \mathbf{q}} + \frac{\delta \bar{\mathcal{F}}}{\delta \mathbf{m}} \frac{\delta \mathbf{m}}{\delta \mathbf{q}} \right) d\mathbf{x} \\ &= - \int_{\Omega} \left(\rho_0(X) \frac{\delta \bar{\mathcal{F}}}{\delta \rho} + \mathfrak{s}_0(X) \frac{\delta \bar{\mathcal{F}}}{\delta \mathfrak{s}} + \mathbf{p}(X) \cdot \frac{\delta \bar{\mathcal{F}}}{\delta \mathbf{m}} \right) \nabla_{\mathbf{x}} \delta(\mathbf{x} - \mathbf{q}(X)) d\mathbf{x} \\ &= \int_{\Omega} \left(\rho_0 \nabla_{\mathbf{x}} \frac{\delta \bar{\mathcal{F}}}{\delta \rho} + \mathfrak{s}_0 \nabla_{\mathbf{x}} \frac{\delta \bar{\mathcal{F}}}{\delta \mathfrak{s}} + \mathbf{p} \cdot \nabla_{\mathbf{x}} \frac{\delta \bar{\mathcal{F}}}{\delta \mathbf{m}} \right) \delta(\mathbf{x} - \mathbf{q}(X)) d\mathbf{x} \\ \frac{\delta \bar{\mathcal{F}}}{\delta \mathbf{p}}(X) &= \int_{\Omega} \frac{\delta \bar{\mathcal{F}}}{\delta \mathbf{m}} \delta(\mathbf{x} - \mathbf{q}(X)) d\mathbf{x} = \frac{\delta \bar{\mathcal{F}}}{\delta \mathbf{m}} \Big|_{\mathbf{x}=\mathbf{q}(X)}. \end{aligned}$$

5.2.2 Poisson bracket in Eulerian conservative variables

- Lie-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 $\Phi : (\mathbf{q}, \mathbf{p}) \mapsto (\rho, \mathfrak{s}, \mathbf{m})$. That is,

$$\{\bar{\mathcal{F}}, \bar{\mathcal{G}}\} := \{\bar{\mathcal{F}} \circ \Phi, \bar{\mathcal{G}} \circ \Phi\}$$

where $\bar{\mathcal{F}}, \bar{\mathcal{G}}$ are two functionals defined in Eulerian variables $(\rho, \mathfrak{s}, \mathbf{m})$. Let us call $\bar{\mathcal{F}} \circ \Phi = \mathcal{F}, \bar{\mathcal{G}} \circ \Phi = \mathcal{G}$. We have

$$\begin{aligned} \{\bar{\mathcal{F}}, \bar{\mathcal{G}}\} &= \{\mathcal{F}, \mathcal{G}\} \\ &= \int_{M_0} \left(\frac{\delta \mathcal{F}}{\delta \mathbf{q}} \cdot \frac{\delta \mathcal{G}}{\delta \mathbf{p}} - \frac{\delta \mathcal{G}}{\delta \mathbf{q}} \cdot \frac{\delta \mathcal{F}}{\delta \mathbf{p}} \right) dX \\ &= \int_{M_0} \int_M \delta(\mathbf{x} - \mathbf{q}(X)) \left(\rho_0 \nabla_{\mathbf{x}} \frac{\delta \bar{\mathcal{F}}}{\delta \rho} + \mathfrak{s}_0 \nabla_{\mathbf{x}} \frac{\delta \bar{\mathcal{F}}}{\delta \mathfrak{s}} + \mathbf{p} \cdot \nabla_{\mathbf{x}} \frac{\delta \bar{\mathcal{F}}}{\delta \mathbf{m}} \right) \cdot \frac{\delta \bar{\mathcal{G}}}{\delta \mathbf{m}} \\ &\quad - \delta(\mathbf{x} - \mathbf{q}(X)) \left(\rho_0 \nabla_{\mathbf{x}} \frac{\delta \bar{\mathcal{G}}}{\delta \rho} + \mathfrak{s}_0 \nabla_{\mathbf{x}} \frac{\delta \bar{\mathcal{G}}}{\delta \mathfrak{s}} + \mathbf{p} \cdot \nabla_{\mathbf{x}} \frac{\delta \bar{\mathcal{G}}}{\delta \mathbf{m}} \right) \cdot \frac{\delta \bar{\mathcal{F}}}{\delta \mathbf{m}} d\mathbf{x} dX \end{aligned}$$

We use (5.6) and a lemma below to get the Poisson bracket formula

$$\begin{aligned} \{\bar{\mathcal{F}}, \bar{\mathcal{G}}\} &= \int_M \left(\rho \nabla_{\mathbf{x}} \frac{\delta \bar{\mathcal{F}}}{\delta \rho} + \mathfrak{s} \nabla_{\mathbf{x}} \frac{\delta \bar{\mathcal{F}}}{\delta \mathfrak{s}} + \mathbf{m} \cdot \nabla_{\mathbf{x}} \frac{\delta \bar{\mathcal{F}}}{\delta \mathbf{m}} \right) \cdot \frac{\delta \bar{\mathcal{G}}}{\delta \mathbf{m}} \\ &\quad - \left(\rho \nabla_{\mathbf{x}} \frac{\delta \bar{\mathcal{G}}}{\delta \rho} + \mathfrak{s} \nabla_{\mathbf{x}} \frac{\delta \bar{\mathcal{G}}}{\delta \mathfrak{s}} + \mathbf{m} \cdot \nabla_{\mathbf{x}} \frac{\delta \bar{\mathcal{G}}}{\delta \mathbf{m}} \right) \cdot \frac{\delta \bar{\mathcal{F}}}{\delta \mathbf{m}} d\mathbf{x}. \end{aligned}$$

Here,

$$\left(\mathbf{m} \cdot \nabla_{\mathbf{x}} \frac{\partial \bar{G}}{\partial \mathbf{m}} \right) \cdot \frac{\partial \bar{F}}{\partial \mathbf{m}} := m_i \left(\frac{\partial}{\partial x^j} \frac{\delta \bar{\mathcal{G}}}{\delta m_i} \right) \frac{\delta \bar{\mathcal{F}}}{\delta m_j}.$$

2. If the functionals $\bar{\mathcal{F}}, \bar{\mathcal{G}}$ are expressed as

$$\bar{\mathcal{F}}[\rho, \mathfrak{s}, \mathbf{m}] = \int \bar{F}(\rho(\mathbf{x}), \mathfrak{s}(\mathbf{x}), \mathbf{m}(\mathbf{x})) d\mathbf{x}, \quad \bar{\mathcal{G}}[\rho, \mathfrak{s}, \mathbf{m}] = \int \bar{G}(\rho(\mathbf{x}), \mathfrak{s}(\mathbf{x}), \mathbf{m}(\mathbf{x})) d\mathbf{x},$$

then the above functional variation is

$$\frac{\delta \bar{\mathcal{F}}}{\delta \rho} = \frac{\partial \bar{F}}{\partial \rho}, \dots$$

Thus, the above Poisson bracket has the following expression

$$\begin{aligned} \{\bar{\mathcal{F}}, \bar{\mathcal{G}}\} &= \int_M \left(\rho \nabla_{\mathbf{x}} \frac{\partial \bar{F}}{\partial \rho} + \mathfrak{s} \nabla_{\mathbf{x}} \frac{\partial \bar{F}}{\partial \mathfrak{s}} + \mathbf{m} \cdot \nabla_{\mathbf{x}} \frac{\partial \bar{F}}{\partial \mathbf{m}} \right) \cdot \frac{\partial \bar{G}}{\partial \mathbf{m}} \\ &\quad - \left(\rho \nabla_{\mathbf{x}} \frac{\partial \bar{G}}{\partial \rho} + \mathfrak{s} \nabla_{\mathbf{x}} \frac{\partial \bar{G}}{\partial \mathfrak{s}} + \mathbf{m} \cdot \nabla_{\mathbf{x}} \frac{\partial \bar{G}}{\partial \mathbf{m}} \right) \cdot \frac{\partial \bar{F}}{\partial \mathbf{m}} d\mathbf{x}, \end{aligned}$$

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 $(\rho, \mathfrak{s}, \mathbf{m})$. Such Poisson bracket is called a Lie-Poisson bracket.

The lemma is

$$\int_{M_0} \int_M \delta(\mathbf{x} - \mathbf{q}(X)) \rho_0(X) \phi(\mathbf{x}) \psi(\mathbf{q}(X)) d\mathbf{x} dX = \int_M \rho(\mathbf{x}) \phi(\mathbf{x}) \psi(\mathbf{x}) d\mathbf{x}.$$

1

3. The Poisson bracket $\{\cdot, \cdot\}$ is bilinear and satisfies

- antisymmetry: $\{\bar{\mathcal{F}}, \bar{\mathcal{G}}\} = -\{\bar{\mathcal{G}}, \bar{\mathcal{F}}\}$,
- Jacobi identity:

$$\{\{\bar{\mathcal{E}}, \bar{\mathcal{F}}\}, \bar{\mathcal{G}}\} + \{\{\bar{\mathcal{F}}, \bar{\mathcal{G}}\}, \bar{\mathcal{E}}\} + \{\{\bar{\mathcal{G}}, \bar{\mathcal{E}}\}, \bar{\mathcal{F}}\} = 0.$$

¹Let $\mathbf{y} = \mathbf{q}(X)$. Then the above integral is

$$\begin{aligned} &\int_{\Omega} \int_{\Omega} \delta(\mathbf{x} - \mathbf{y}) \rho_0(\mathbf{q}^{-1}(\mathbf{y})) \phi(\mathbf{x}) \psi(\mathbf{y}) d\mathbf{x} J^{-1}(\mathbf{q}^{-1}(\mathbf{y})) d\mathbf{y} \\ &= \int_{\Omega} \int_{\Omega} \delta(\mathbf{x} - \mathbf{y}) \rho(\mathbf{y}) \phi(\mathbf{x}) \psi(\mathbf{y}) d\mathbf{x} d\mathbf{y} = \int_{\Omega} \rho(\mathbf{x}) \phi(\mathbf{x}) \psi(\mathbf{x}) d\mathbf{x}. \end{aligned}$$

4. **Hamiltonian dynamics** The Hamiltonian $H[\mathbf{q}, \mathbf{p}]$ can be expressed in terms of $(\rho, \mathfrak{s}, \mathbf{m})$ as

$$\begin{aligned}\bar{\mathcal{H}}[\rho, \mathfrak{s}, \mathbf{m}] &= \mathcal{H}[\mathbf{q}, \mathbf{p}] \\ &= \int_{\Omega} \frac{|\mathbf{m}|^2}{2\rho} + \rho U\left(\rho, \frac{\mathfrak{s}}{\rho}\right) d\mathbf{x} \\ &= \int_{\Omega} H(\rho, \mathfrak{s}, \mathbf{m}) d\mathbf{x}\end{aligned}$$

From this expression, we get

$$\begin{aligned}\frac{\delta \mathcal{H}}{\delta \rho} &= \frac{\partial H}{\partial \rho} = -\frac{|\mathbf{v}|^2}{2} + U + \frac{p}{\rho} - TS \\ \frac{\delta \mathcal{H}}{\delta \mathfrak{s}} &= \frac{\partial H}{\partial \mathfrak{s}} = T \\ \frac{\delta \mathcal{H}}{\delta \mathbf{m}} &= \frac{\partial H}{\partial \mathbf{m}} = \mathbf{v}.\end{aligned}$$

By taking

$$\rho(\mathbf{x}') = f[\rho, \mathfrak{s}, \mathbf{m}] = \int \rho(\mathbf{x}) \delta(\mathbf{x}' - \mathbf{x}) d\mathbf{x}$$

we get

$$\{\rho(\mathbf{x}'), \mathcal{H}\} = \{f, \mathcal{H}\} = \int \rho(\mathbf{x}) \nabla_{\mathbf{x}} \delta(\mathbf{x}' - \mathbf{x}) \cdot \mathbf{v} d\mathbf{x} = -\nabla_{\mathbf{x}'} \cdot (\rho \mathbf{v})(\mathbf{x}').$$

Similarly, we get

$$\{\mathfrak{s}(\mathbf{x}'), \mathcal{H}\} = \int \mathfrak{s}(\mathbf{x}) \nabla_{\mathbf{x}} \delta(\mathbf{x}' - \mathbf{x}) \cdot \mathbf{v} d\mathbf{x} = -\nabla_{\mathbf{x}'} \cdot (\mathfrak{s} \mathbf{v}).$$

$$\begin{aligned}\{\mathbf{m}(\mathbf{x}'), \mathcal{H}\} &= \int \mathbf{m} \cdot \nabla_{\mathbf{x}} \delta(\mathbf{x} - \mathbf{x}') \cdot \mathbf{v} \\ &\quad - \left(\rho \nabla_{\mathbf{x}} \left(-\frac{|\mathbf{v}|^2}{2} + e + \frac{p}{\rho} - TS \right) + \mathfrak{s} \nabla_{\mathbf{x}} T + \mathbf{m} \cdot \nabla_{\mathbf{x}} \mathbf{v} \right) \delta(\mathbf{x} - \mathbf{x}') d\mathbf{x} \\ &= -\nabla_{\mathbf{x}'} \cdot (\mathbf{v} \mathbf{m}) - \rho \nabla_{\mathbf{x}} \left(-\frac{|\mathbf{v}|^2}{2} + U + \frac{p}{\rho} - TS \right) - \mathfrak{s} \nabla_{\mathbf{x}} T \\ &= -\nabla_{\mathbf{x}'} \cdot (\mathbf{v} \mathbf{m}) - \nabla p.\end{aligned}$$

Thus, we get the equation of the Hamiltonian flow

$$\begin{aligned}\dot{\rho} &= \{\rho, \mathcal{H}\} \\ \dot{\mathfrak{s}} &= \{\mathfrak{s}, \mathcal{H}\} \\ \dot{\mathbf{m}} &= \{\mathbf{m}, \mathcal{H}\}\end{aligned}$$

is the Eulerian coordinates.

5.2.3 Poisson bracket in terms of (ρ, S, \mathbf{v})

1. We change variables $(\rho, \mathfrak{s}, \mathbf{m})$ to (ρ, S, \mathbf{v}) by $S = \mathfrak{s}/\rho$ and $\mathbf{v} = \mathbf{m}/\rho$. We get

$$\begin{aligned}\frac{\partial}{\partial \rho} \Big|_{(\mathfrak{s}, \mathbf{m})} &= \frac{\partial}{\partial \rho} \Big|_{(S, \mathbf{v})} - \frac{S}{\rho} \frac{\partial}{\partial S} - \frac{\mathbf{v}}{\rho} \cdot \frac{\partial}{\partial \mathbf{v}} \\ \frac{\partial}{\partial \mathfrak{s}} &= \frac{1}{\rho} \frac{\partial}{\partial S} \\ \frac{\partial}{\partial \mathbf{m}} &= \frac{1}{\rho} \frac{\partial}{\partial \mathbf{v}}.\end{aligned}$$

Plug this into the Poisson bracket

$$\begin{aligned}\{\mathcal{F}, \mathcal{G}\} &= \int_{\Omega} \left(\rho \nabla_{\mathbf{x}} \frac{\delta \mathcal{F}}{\delta \rho} + \mathfrak{s} \nabla_{\mathbf{x}} \frac{\delta \mathcal{F}}{\delta \mathfrak{s}} + \mathbf{m} \cdot \nabla_{\mathbf{x}} \frac{\delta \mathcal{F}}{\delta \mathbf{m}} \right) \cdot \frac{\delta \mathcal{G}}{\delta \mathbf{m}} \\ &\quad - \left(\rho \nabla_{\mathbf{x}} \frac{\delta \mathcal{G}}{\delta \rho} + \mathfrak{s} \nabla_{\mathbf{x}} \frac{\delta \mathcal{G}}{\delta \mathfrak{s}} + \mathbf{m} \cdot \nabla_{\mathbf{x}} \frac{\delta \mathcal{G}}{\delta \mathbf{m}} \right) \cdot \frac{\delta \mathcal{F}}{\delta \mathbf{m}} dx.\end{aligned}$$

Note that $\frac{\delta \mathcal{F}}{\delta \mathbf{m}} = \frac{\partial F}{\partial \mathbf{m}}$. We have

$$\begin{aligned}&\left[\rho \nabla_{\mathbf{x}} \left(\partial_{\rho} - \frac{\mathbf{v}}{\rho} \cdot \partial_{\mathbf{v}} - \frac{S}{\rho} \partial_S \right) F + \rho S \nabla_{\mathbf{x}} \left(\frac{1}{\rho} \partial_S F \right) + \rho \mathbf{v} \cdot \nabla_{\mathbf{x}} \left(\frac{1}{\rho} \partial_{\mathbf{v}} F \right) \right] \cdot \frac{1}{\rho} \partial_{\mathbf{v}} G \\ &- \left[\rho \nabla_{\mathbf{x}} \left(\partial_{\rho} - \frac{\mathbf{v}}{\rho} \cdot \partial_{\mathbf{v}} - \frac{S}{\rho} \partial_S \right) G + \rho S \nabla_{\mathbf{x}} \left(\frac{1}{\rho} \partial_S G \right) + \rho \mathbf{v} \cdot \nabla_{\mathbf{x}} \left(\frac{1}{\rho} \partial_{\mathbf{v}} G \right) \right] \cdot \frac{1}{\rho} \partial_{\mathbf{v}} F\end{aligned}$$

We get that

$$\begin{aligned}\{\mathcal{F}, \mathcal{G}\} &= \int_{\Omega} \left[(\nabla_{\mathbf{x}} \partial_{\rho} F) \cdot \partial_{\mathbf{v}} G - (\nabla_{\mathbf{x}} \partial_{\rho} G) \cdot \partial_{\mathbf{v}} F \right. \\ &\quad \left. - \frac{\nabla_{\mathbf{x}} S}{\rho} \cdot (\partial_S F \partial_{\mathbf{v}} G - \partial_S G \partial_{\mathbf{v}} F) \right. \\ &\quad \left. + \frac{1}{\rho} (\partial_{x^i} v^j - \partial_{x^j} v^i) \partial_{v^i} F \partial_{v^j} G \right] dx\end{aligned}$$

The last term can also be expressed as

$$-\frac{1}{\rho} \partial_{x^j} v^i (\partial_{v^i} F \partial_{v^j} G - \partial_{v^i} G \partial_{v^j} F) = -\frac{\nabla_{\mathbf{x}} \times \mathbf{v}}{\rho} \cdot \frac{\partial F}{\partial \mathbf{v}} \times \frac{\partial G}{\partial \mathbf{v}}.$$

Thus, the Poisson bracket is

$$\begin{aligned} \{\mathcal{F}, \mathcal{G}\} = \int_{\Omega} \left[(\nabla_{\mathbf{x}} \partial_{\rho} F) \cdot \partial_{\mathbf{v}} G - (\nabla_{\mathbf{x}} \partial_{\rho} G) \cdot \partial_{\mathbf{v}} F \right. \\ \left. - \frac{\nabla_{\mathbf{x}} S}{\rho} \cdot (\partial_S F \partial_{\mathbf{v}} G - \partial_S G \partial_{\mathbf{v}} F) \right. \\ \left. - \frac{\nabla_{\mathbf{x}} \times \mathbf{v}}{\rho} \cdot \frac{\partial F}{\partial \mathbf{v}} \times \frac{\partial G}{\partial \mathbf{v}} \right] d\mathbf{x}. \end{aligned}$$

2. The Poisson bracket $\{\mathcal{F}, \mathcal{G}\}$ satisfies

- Antisymmetry: $\{\mathcal{F}, \mathcal{G}\} = -\{\mathcal{G}, \mathcal{F}\}$
- Jacobi identity:

$$\{\{\mathcal{E}, \mathcal{F}\}, \mathcal{G}\} + \{\{\mathcal{F}, \mathcal{G}\}, \mathcal{E}\} + \{\{\mathcal{G}, \mathcal{E}\}, \mathcal{F}\} = 0.$$

3. With $H = \frac{1}{2}\rho|\mathbf{v}|^2 + \rho U(\rho, S)$ and $\mathcal{H} = \int H d\mathbf{x}$, we get

$$\frac{\delta \mathcal{H}}{\delta \rho} = \frac{1}{2}|\mathbf{v}|^2 + U + \frac{p}{\rho}, \quad \frac{\delta \mathcal{H}}{\delta S} = \rho T, \quad \frac{\delta \mathcal{H}}{\delta \mathbf{v}} = \rho \mathbf{v}.$$

Thus,

$$\{\rho(\cdot - \mathbf{x}'), \mathcal{H}\} = \int (\nabla_{\mathbf{x}} \delta(\mathbf{x} - \mathbf{x}')) \cdot (\rho \mathbf{v}) d\mathbf{x} = -\nabla_{\mathbf{x}} \cdot (\rho \mathbf{v})(\mathbf{x}').$$

$$\{S(\cdot - \mathbf{x}'), \mathcal{H}\} = \int -\frac{\nabla_{\mathbf{x}} S}{\rho} \cdot (\delta(\mathbf{x} - \mathbf{x}')(\rho \mathbf{v})) d\mathbf{x} = -\mathbf{v} \cdot \nabla_{\mathbf{x}} S(\mathbf{x}')$$

$$\begin{aligned} \{\mathbf{v}(\cdot - \mathbf{x}'), \mathcal{H}\} &= \int -(\nabla_{\mathbf{x}} \partial_{\rho} H) \cdot \delta(\mathbf{x} - \mathbf{x}') I + \frac{\nabla_{\mathbf{x}} S}{\rho} \partial_S H \delta(\mathbf{x} - \mathbf{x}') \\ &\quad + \frac{1}{\rho} (\partial_{x^i} v^j - \partial_{x^j} v^i) \delta(\mathbf{x} - \mathbf{x}') \rho v^i d\mathbf{x} \\ &= -\nabla_{\mathbf{x}} \left(\frac{1}{2}|\mathbf{v}|^2 + U + \frac{p}{\rho} \right) + \frac{\nabla_{\mathbf{x}} S}{\rho} (\rho T) + (\partial_{x^i} v^j - \partial_{x^j} v^i) v^j \\ &= -v^j \partial_{x^j} v^i - \frac{1}{\rho} \partial_{x^i} p = -\mathbf{v} \cdot \nabla_{\mathbf{x}} \mathbf{v} - \frac{\nabla_{\mathbf{x}} p}{\rho} \end{aligned}$$

These are summarized as

$$\begin{aligned} \partial_t \rho &= \{\rho, \mathcal{H}\} = -\nabla_{\mathbf{x}} \cdot (\rho \mathbf{v}) \\ \partial_t S &= \{S, \mathcal{H}\} = -\mathbf{v} \cdot \nabla_{\mathbf{x}} S \\ \partial_t \mathbf{v} &= \{\mathbf{v}, \mathcal{H}\} = -\mathbf{v} \cdot \nabla_{\mathbf{x}} \mathbf{v} - \frac{\nabla_{\mathbf{x}} p}{\rho}, \end{aligned}$$

which are the Euler equations.

Homework For Burgers equation $u_t + uu_x = 0$, the corresponding Poisson bracket and the Hamiltonian are

$$\{\bar{\mathcal{F}}, \bar{\mathcal{G}}\} = \int_{\mathbb{R}} u \left\{ \left[\frac{\partial \bar{\mathcal{F}}}{\partial u} \right]_x \frac{\partial \bar{\mathcal{G}}}{\partial u} - \left[\frac{\partial \bar{\mathcal{G}}}{\partial u} \right]_x \frac{\partial \bar{\mathcal{F}}}{\partial u} \right\} dx$$

$$H(u) = \frac{1}{2}u^2.$$

5.2.4 Casimir and Conservation of Helicity

1. **Casimirs** There are 5 Eulerian variables whereas there are 6 Lagrangian variables. The symplectic 2-form in terms of Eulerian variables is expected to be singular. A function $\mathcal{C}(\rho, S, \mathbf{v})$ is called a Casimir invariant of the Euler system if

$$\{\mathcal{C}, \mathcal{F}\} = 0 \text{ for all function } \mathcal{F}(\rho, S, \mathbf{v}).$$

From the Poisson bracket formula, this gives the following equations for \mathcal{C} :

$$\begin{aligned} \nabla \cdot \frac{\delta \mathcal{C}}{\delta \mathbf{v}} &= 0, \\ \frac{1}{\rho} \nabla S \cdot \frac{\delta \mathcal{C}}{\delta \mathbf{v}} &= 0, \\ \nabla \frac{\delta \mathcal{C}}{\delta \rho} + \frac{\nabla \times \mathbf{v}}{\rho} \times \frac{\delta \mathcal{C}}{\delta \mathbf{v}} - \frac{\nabla S}{\rho} \frac{\delta \mathcal{C}}{\delta S} &= 0. \end{aligned}$$

2. **Helicity.** Let us suppose \mathcal{C} depends only on \mathbf{v} . Let $\mathbf{w} = \frac{\delta \mathcal{C}}{\delta \mathbf{v}}$. Then \mathbf{w} satisfies

$$\nabla \cdot \mathbf{w} = 0, \quad (\nabla \times \mathbf{v}) \times \mathbf{w} = 0.$$

These two imply $\mathbf{w} = \text{Const.} \nabla \times \mathbf{v}$ for some constant *Const.* The helicity

$$\mathcal{C}(\mathbf{v}) = \int \mathbf{v} \cdot \nabla \times \mathbf{v} d\mathbf{x}$$

satisfies $\delta \mathcal{C} / \delta \mathbf{v} = 2 \nabla \times \mathbf{v}$.

3. Let

$$q = \frac{\nabla \times \mathbf{v}}{\rho} \cdot \nabla S$$

be the potential vorticity. Then

$$\mathcal{C} := \int \rho f(q) d\mathbf{x}$$

is a Casimir for any function f .

4. Suppose \mathcal{E} only depends on the thermo variables, that is,

$$\mathcal{E}(\rho, S) = \int C(\rho, S) d\mathbf{x}.$$

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 \mathcal{E} is

$$\mathcal{E}(\rho, S) = \int \rho f(S) d\mathbf{x}.$$

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Chapter 6

Mathematical Theory of Fluid Dynamics

6.1 Dimensional Analysis

The incompressible Navier-Stokes equation is

$$\rho(\partial_t \mathbf{v} + \mathbf{v} \cdot \nabla \mathbf{v}) = -\nabla p + \mu \Delta \mathbf{v} + \mathbf{f}, \quad \nabla \cdot \mathbf{v} = 0.$$

Let us assume $\rho = \text{constant}$. Thus, ρ and μ are the parameters. There are 7 dimension quantities: $[t], [x], [\mathbf{v}], [p], [f], [\rho], [\mu]$. The equation should have equal dimensions for each terms. These give 4 relations. Therefore, there are only three independent fundamental dimensions. Let us choose them to be

$$[x] = L, \quad [t] = T, \quad [\mathbf{v}] = U.$$

Comparing $\mu \Delta \mathbf{v}$ and ∇p gives

$$[p] = \mu \frac{U}{L}.$$

Comparing $\mu \Delta \mathbf{v}$ and \mathbf{f} gives

$$[f] = \frac{L^2}{\mu U}.$$

Comparing $\mu \Delta \mathbf{v}$ and the convection term $\rho \mathbf{v} \nabla \mathbf{v}$, we get

$$\rho \frac{U^2}{L} = \mu \frac{U}{L}.$$

Finally, comparing $\mu \Delta \mathbf{v}$ and the inertial term $\rho \partial_t \mathbf{v}$, we get

$$\rho \frac{U}{T} = \mu \frac{U}{L}$$

Define dimensionless variables

$$\mathbf{x}^* = x/L, \quad \mathbf{v}^* = \mathbf{v}/U, \quad t^* = t/T, \quad p^* = p \frac{L}{\mu U}, \quad \mathbf{f}^* = \mathbf{f} \frac{L^2}{\mu U}.$$

Incompressible Navier-Stokes equations read

$$Re (St \partial_{t^*} \mathbf{v}^* + \mathbf{v}^* \cdot \nabla^* \mathbf{v}^*) = -\nabla^* p^* + \Delta^* \mathbf{v}^* + \mathbf{f}^* \quad (6.1)$$

$$\nabla^* \cdot \mathbf{v}^* = 0. \quad (6.2)$$

where

$$Re = \frac{\rho U L}{\mu}, \quad St = \frac{L}{UT}. \quad (6.3)$$

are the Reynolds 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: $\nabla \cdot \mathbf{v} = 0$ and $\nabla \times \mathbf{v} = 0$.
- Stokes flows: the convection term is neglected.

6.2 Potential flows

In the previous subsection, we see that for barotropic flows, if $\omega \equiv 0$ initially, then $\omega \equiv 0$ in all later time. In this case, we call such flows irrotational. That is,

$$\nabla \times \mathbf{v} \equiv 0.$$

If the domain is simply connected, then we can find a scalar function ϕ such that

$$\mathbf{v} = \nabla \phi$$

Such a function is called the velocity potential. If, in addition, the flow is incompressible, i.e.

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

then we have

$$\Delta \phi = 0. \quad (6.4)$$

We call such incompressible and irrotational flow a *potential flow*. On the boundary, we should apply slip boundary condition, i.e.

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

6.2.1 Two-dimensional potential flows

- A single vortex, pair of vortices (same sign, opposite sign)
- Vortex dynamics
- von Karman vortex street
- Flow passes a cylinder
- Vortex patches

6.2.2 Three-dimensional potential flows

- Shear flows, flow instability
- Vortex ring, leap frog motion of a pair of vortex rings
- Dynamics of vortex filament

6.3 One dimensional compressible flows

6.3.1 Riemann problems for hyperbolic conservation laws

Elementary Waves We consider the following systems of PDEs:

$$u_t + f(u)_x = 0, \quad (6.5)$$

$$u = \begin{pmatrix} u_1 \\ u_2 \\ \vdots \\ u_n \end{pmatrix}, \quad f: \mathbb{R}^n \rightarrow \mathbb{R}^n.$$

The system (6.5) is called *hyperbolic* if the $n \times n$ matrix $f'(u)$ can be diagonalized with real eigenvalues $\lambda_1(u) \leq \lambda_2(u) \leq \dots \leq \lambda_n(u)$ for all u under consideration. The system is called strictly hyperbolic if $\lambda_1(u) < \lambda_2(u) < \dots < \lambda_n(u)$ for all u . Let us denote corresponding left/right eigenvectors by $\ell_i(u)/r_i(u)$, respectively. Let us normalize them by requiring

$$\|r_i(u)\| \equiv 1, \quad \ell_i(u) \cdot r_j(u) \equiv \delta_{ij}.$$

It is important to notice that the system is Galilean invariant, meaning that the equation is unchanged under the transformation:

$$t \rightarrow \lambda t, \quad x \rightarrow \lambda x, \quad \forall \lambda > 0.$$

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 (6.5) and yield

$$\begin{aligned} u' \cdot \left(-\frac{x}{t^2}\right) + f'(u)u' \cdot \frac{1}{t} &= 0 \\ \implies f'(u)u' &= \frac{x}{t}u'. \end{aligned}$$

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 6.3. *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

$$R_i^+(u_0) = \{u \in R_i(u_0) \mid \lambda_i(u) \geq \lambda_i(u_0)\}.$$

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*.

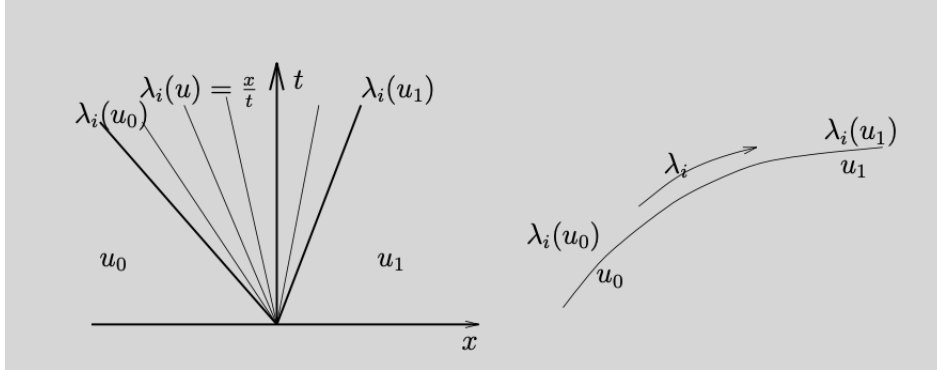


Figure 6.1: (Left) The rarefaction wave. (Right) The integral curve of $u' = r_i(u)$.

Shock Waves The shock wave is expressed by:

$$u\left(\frac{x}{t}\right) = \begin{cases} u_0 & \text{for } \frac{x}{t} < \sigma \\ u_1 & \text{for } \frac{x}{t} > \sigma, \end{cases}$$

where σ is the shock speed. Here, (u_0, u_1, σ) need to satisfy the jump condition:

$$f(u_1) - f(u_0) = \sigma(u_1 - u_0). \quad (6.6)$$

Lemma 6.5. (Local structure of shock curves)

1. The solution of (6.6) for (u, σ) consists of n algebraic curves passing through u_0 locally, named them by $S_i(u_0), i = 1, \dots, n$.
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. $\sigma_i(u_0, u) \rightarrow \lambda_i(u_0)$ as $u \rightarrow u_0$, 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

$$\begin{aligned} f(u) - f(u_0) &= \left[\int_0^1 f'(u_0 + t(u - u_0)) dt \right] (u - u_0) \\ &= \tilde{A}(u_0, u)(u - u_0) \\ &= \sigma(u - u_0). \end{aligned}$$

$\therefore u \in S(u_0) \iff (u - u_0)$ is an eigenvector of $\tilde{A}(u_0, u)$.

Assuming $A(u) = f'(u)$ has real and distinct eigenvalues $\lambda_1(u) < \dots < \lambda_n(u)$, then, from perturbation theory (or implicit function theorem), for $u \sim u_0$, $\tilde{A}(u_0, u)$ also has real and distinct eigenvalues $\tilde{\lambda}_1(u_0, u) < \dots < \tilde{\lambda}_n(u_0, u)$, 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 $u \rightarrow u_0$ respectively. We normalize these 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:

$$\tilde{\ell}_k(u_0, u)(u - u_0) = 0, \quad k = 1, \dots, n, k \neq i,$$

Thus we define

$$S_i(u_0) = \{u \mid \tilde{\ell}_k(u_0, u)(u - u_0) = 0, k = 1, \dots, n, k \neq i\}.$$

We claim that this is a smooth curve passing through u_0 . Choose coordinate system $r_1(u_0), \dots, r_n(u_0)$. Differential this 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, $(\partial/\partial r_j \tilde{\ell}_k)$ is a full rank matrix. By implicit function theorem, $S_i(u_0)$ is a smooth curve passing through u_0 . Since any $u \in S_i(u_0)$ must satisfy $\tilde{\ell}_k(u_0, u)(u - u_0) = 0$ for $k = 1, \dots, n, k \neq i$ 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 find 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 $u \rightarrow u_0$

$$\begin{aligned} f'(u_0)S_i'(u_0) &= \sigma_i'(u_0, u_0)S_i'(u_0) \\ \implies S_i'(u_0) &= r_i(u_0) \text{ and } \sigma_i(u_0, u_0) = \lambda_i(u_0). \end{aligned}$$

Now we Consider 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

$$(f'' r_i, r_i) + f' S''_i = 2\sigma'_i r_i + \sigma_i S''_i.$$

On the other hand, we take derivative of $f'(u)r_i(u) = \lambda_i(u)r_i(u)$ along $R_i(u_0)$, then evaluate at $u = u_0$ to get

$$(f'' r_i, r_i) + f'(\nabla r_i \cdot r_i) = \lambda'_i r_i + \lambda_i \nabla r_i \cdot r_i,$$

where $\nabla r_i \cdot r_i = R''_i$. Comparing these two equations, 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

$$\alpha_k = 0 \quad \forall k \neq i \text{ and } \lambda'_i = 2\sigma'_i \text{ at } u_0.$$

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

$$(u_0, u_1) = \begin{cases} u_0 & \text{for } \frac{x}{t} < \sigma_i(u_0, u_1) \\ u_1 & \text{for } \frac{x}{t} > \sigma_i(u_0, u_1) \end{cases}$$

$$u_0 \quad \mathfrak{R}_i^+ \quad \mathfrak{R}_i \\ \mathfrak{S}_i$$

(u_0, u_1) is a weak solution.

We propose the following entropy condition: (Lax entropy condition)

$$\lambda_i(u_0) > \sigma_i(u_0, u_1) > \lambda_i(u_1). \quad (6.7)$$

If the i -th characteristic field is genuinely nonlinear, then for $u_1 \in S_i^-(u_0)$, and $u_1 \sim u_0$, (6.7) 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

$$(u_0, u_1) = \begin{cases} u_0 & \frac{x}{t} < \sigma_i(u_0, u_1) \\ u_1 & \frac{x}{t} > \sigma_i(u_0, u_1) \end{cases}$$

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 6.5. (Lax) For strictly hyperbolic system (6.5), 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 $u_0 = u_L, \dots, u_n = u_R$ such that (u_{i-1}, u_i) is an i -wave.

Proof. Given $(\alpha_1, \dots, \alpha_n) \in \mathbb{R}^n$, define u_i inductively $u_i \in T_i(u_{i-1})$, and the arclength of (u_{i-1}, u_i) on $T_i = \alpha_i$.

$$u_i = f(u_0, \alpha_1, \dots, \alpha_i)$$

We want to find $\alpha_1, \dots, \alpha_n$ such that

$$u_R = f(u_L, \alpha_1, \dots, \alpha_n).$$

First $u_L = f(u_L, 0, \dots, 0)$, as $u_R = u_L, (\alpha_1, \dots, \alpha_n) = (0, \dots, 0)$ is a solution. When $u_R \sim u_L$ and $\{r_i(u_0)\}$ are independent,

$$\left. \frac{\partial}{\partial \alpha_i} \right|_{\alpha=0} f(u_L, 0, \dots, 0) = r_i(u_0) \text{ and } f \in C^2$$

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

6.3.2 Riemann Problem for Gas Dynamics

This subsection is 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

$$\begin{bmatrix} \rho \\ u \\ S \end{bmatrix}_t + \begin{bmatrix} u & \rho & 0 \\ \frac{c^2}{\rho} & u & \frac{P_S}{\rho} \\ 0 & 0 & u \end{bmatrix} \begin{bmatrix} \rho \\ u \\ S \end{bmatrix}_x = 0$$

t
 2-wave n -wave
 1-wave u_1 u_2 u_{n-1}
 $u_0 = u_L$ $u_n = u_R$

x

Here, $P(\rho, S) = A(S)\rho^\gamma$, $\gamma > 1$, and $c^2 = \left. \frac{\partial P}{\partial \rho} \right|_S$. This system is hyperbolic. The eigenvalues and eigenvectors are

$$\begin{aligned} \lambda_1 &= u - c, & \lambda_2 &= u, & \lambda_3 &= u + c, \\ r_1 &= \begin{bmatrix} \rho \\ -c \\ 0 \end{bmatrix}, & r_2 &= \begin{bmatrix} -P_S \\ 0 \\ c^2 \end{bmatrix}, & r_3 &= \begin{bmatrix} \rho \\ c \\ 0 \end{bmatrix}, \\ \ell_1 &= [c, -\rho, \frac{P_S}{c}], & \ell_2 &= [0, 0, 1], & \ell_3 &= [c, \rho, \frac{P_S}{c}]. \end{aligned}$$

Note that

$$\begin{aligned} \nabla \lambda_1 \cdot r_1 &= \frac{1}{c} \left(\frac{1}{2} \rho P_{\rho\rho} + c^2 \right) > 0, \\ \nabla \lambda_3 \cdot r_3 &= \frac{1}{c} \left(\frac{1}{2} \rho P_{\rho\rho} + c^2 \right) > 0, \\ \nabla \lambda_2 \cdot r_2 &\equiv 0. \end{aligned}$$

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

$$\begin{aligned} &\begin{cases} (d\rho, du, dS) \cdot (0, 0, 1) = 0 \\ (d\rho, du, dS) \cdot (c, \rho, \frac{P_S}{c}) = 0. \end{cases} \\ \implies &\begin{cases} dS = 0 \\ cd\rho + \rho du + \frac{P_S}{c} dS = 0 \end{cases} \end{aligned}$$

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,

$$\begin{aligned} \ell - \ell_0 &= \frac{2}{\gamma-1} \left(\sqrt{\gamma P \left(\frac{P_0}{P} \right)^{1/\gamma} \rho_0^{-1}} - \sqrt{\frac{\gamma P_0}{\rho_0}} \right) \\ &= \frac{2\sqrt{\gamma}}{\gamma-1} \rho_0^{-\frac{1}{2}} P_0^{\frac{1}{2\gamma}} (P^{\frac{\gamma-1}{2\gamma}} - P_0^{\frac{\gamma-1}{2\gamma}}) := \psi_0(P). \end{aligned}$$

$$\therefore \mathfrak{R}_1 : u = u_0 - \psi_0(P)$$

$$\mathfrak{R}_3 : u = u_0 + \psi_0(P).$$

The contact discontinuity On \mathfrak{R}_2 , $(d\rho, du, dS) \perp \ell_1, \ell_3$, which gives

$$\begin{aligned} \implies & \begin{cases} c^2 d\rho + c\rho du + P_S dS = 0 \\ c^2 d\rho - c\rho du + P_S dS = 0 \end{cases} \\ \implies & \begin{cases} dP + c\rho du = 0 \\ dP - c\rho du = 0 \end{cases} \end{aligned}$$

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. You can check the jump conditions for the 2-characteristic field. Which gives $\rho_0(u_0 - \sigma) = \rho(u - \sigma) = 0$ because $u_0 = u = \sigma$, and $P = P_*$. (see the paragraph of shock curves below.)

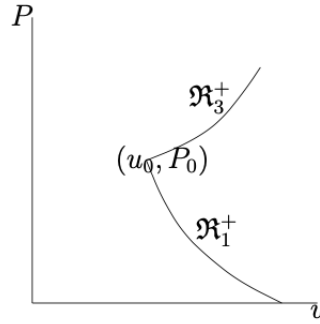


Figure 6.2: The integral curve of the rarefaction curves \mathfrak{R}_1 and \mathfrak{R}_3 on the u - P plane. Here (u_0, P_0) is a left state. For any point (u_1, P_1) on \mathfrak{R}_1^+ , $((u_0, P_0), (u_1, P_1))$ forms a 1-rarefaction wave. Note that the entropy $S = S_0$ along a rarefaction curve.

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 have expressions of \mathfrak{S}_1 (resp. \mathfrak{S}_3) on the u - P plane.

Let $v := u - \sigma$. The jump conditions give

$$\begin{cases} [\rho v] = 0 \\ [\rho v^2 + P] = 0 \\ [(\frac{1}{2}\rho v^2 + \rho e + P)v] = 0. \end{cases}$$

Let

$$m := \rho v.$$

From the first jump condition, we have

$$m = m_0.$$

The second jump condition is

$$\rho_0 v_0^2 + P_0 = \rho v^2 + P \implies m v_0 + P_0 = m v + P.$$

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 $m \neq 0$.¹

$$\therefore m^2 = -\frac{P - P_0}{V - V_0}, \quad v - v_0 = -\frac{P - P_0}{m}$$

¹The case $m = 0$ corresponds to the contact discontinuity.

These give

$$(u - u_0)^2 = (v - v_0)^2 = -(P - P_0)(V - V_0). \quad (6.8)$$

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

$$\frac{1}{2}v_0^2 + e_0 + P_0 V_0 = \frac{1}{2}v^2 + e + PV.$$

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

$$H(P, V) := e - e_0 + \frac{P + P_0}{2}(V - V_0) = 0$$

Using $e = \frac{PV}{\gamma - 1}$, we get

$$\frac{PV}{\gamma - 1} - \frac{P_0 V_0}{\gamma - 1} + \left(\frac{P + P_0}{2}\right)(V - V_0) = 0.$$

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:

$$\mathfrak{S}_1: \quad u = u_0 - \phi_0(P)$$

$$\mathfrak{S}_3: \quad u = u_0 + \phi_0(P)$$

$$\phi_0(P) = (P - P_0) \sqrt{\frac{\frac{2}{\gamma + 1} V_0}{P + \frac{\gamma - 1}{\gamma + 1} P_0}} = \frac{(P - P_0)}{Z_0},$$

$$Z_0 = \sqrt{\frac{P_0}{V_0}} \Phi\left(\frac{P}{P_0}\right), \quad \Phi(w) = \sqrt{\frac{\gamma + 1}{2} w + \frac{\gamma - 1}{2}}.$$

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

$$\begin{aligned}\mathfrak{R}_1^+(\ell) &= u_0 - \psi_0(P) \text{ for } P < P_0 \\ \mathfrak{S}_1^-(\ell) &= u_0 - \phi_0(P) \text{ for } P > P_0\end{aligned}$$

and the admissible rarefaction curves and shock curves for the right state (r) as

$$\begin{aligned}\mathfrak{R}_3^-(r) &= u_0 + \psi_0(P) \text{ for } P < P_0 \\ \mathfrak{S}_3^+(r) &= u_0 + \phi_0(P) \text{ for } P > P_0.\end{aligned}$$

The admissible wave curves are defined to be

$$\begin{aligned}T_1^{(\ell)} &:= \mathfrak{R}_1^+(\ell) \cup \mathfrak{S}_1^-(\ell) \\ T_3^{(r)} &:= \mathfrak{R}_3^-(r) \cup \mathfrak{S}_3^+(r).\end{aligned}$$

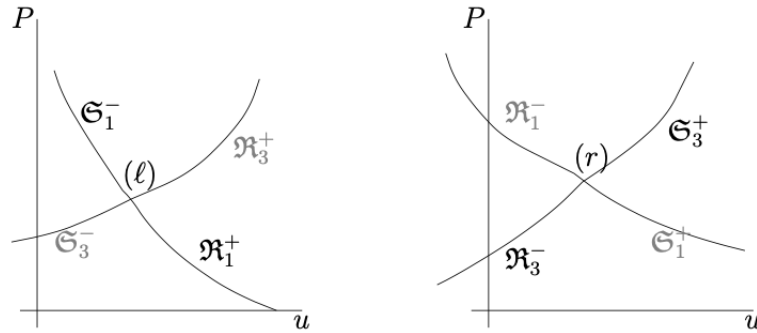


Figure 6.3: The admissible rarefaction curves and shock curves on the u - P plane with left/right states.

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:

$$\begin{aligned}1\text{-wave} &: ((\rho_L, P_L, u_L), (\rho_I, P_I, u_I)), \\ 2\text{-wave} &: ((\rho_I, P_I, u_I), (\rho_{II}, P_{II}, u_{II})), \\ 3\text{-wave} &: ((\rho_{II}, P_{II}, u_{II}), (\rho_R, P_R, u_R)).\end{aligned}$$

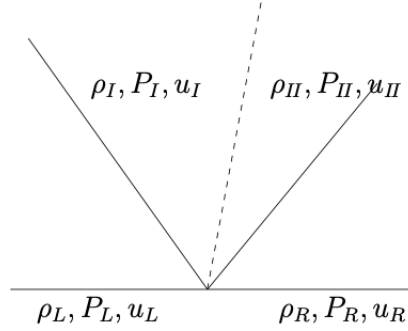


Figure 6.4: The three elementary waves with the left state (ρ_L, P_L, u_L) and the right state (ρ_R, P_R, u_R) . The states (ρ_I, P_I, u_I) and $(\rho_{II}, P_{II}, u_{II})$ are called the mid states, which forms a contact discontinuity.

Recall that the second wave is a contact discontinuity, on which $[u] = 0$, $[P] = 0$. Thus, we have

$$\begin{aligned} u_I &= u_{II} = u_*, \\ P_I &= P_{II} = P_*. \end{aligned}$$

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 a 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

$$\begin{cases} -Z_L(u_* - u_L) = P_* - P_L \\ Z_R(u_* - u_R) = P_* - P_R, \end{cases} \quad (6.9)$$

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 (6.9) 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.

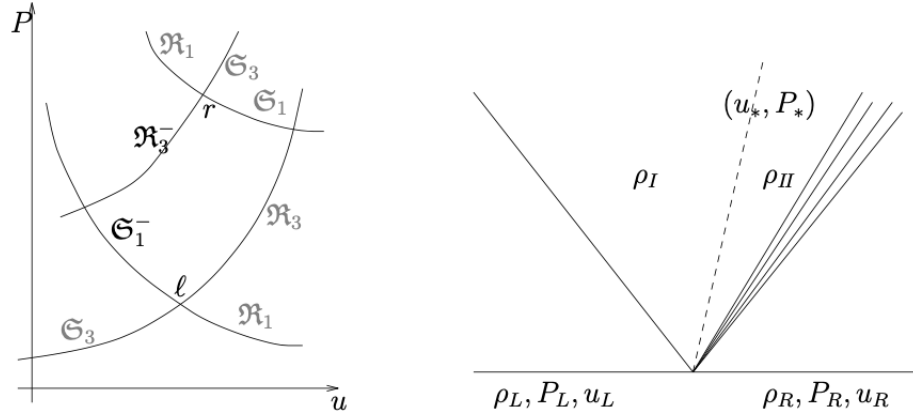


Figure 6.5: This is a solution of the Riemann problem with $p_L < p_R$. In this case, from the left state (ℓ) , we follow \mathfrak{S}_1^- ; and from the right state (r) , we follow \mathfrak{R}_3^- . Their intersection gives the mid state (u_*, P_*) .

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 := $c_L \left(\frac{p_R}{p_L} - 1 \right) \sqrt{\frac{2}{\gamma((\gamma-1) + (\gamma+1)\frac{p_R}{p_L})}}$,
- $du := u_R - u_L$.

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) $(p_R < p_L) \ \& \ (-\text{shk} < du < \text{shk}) \Rightarrow R_1 + S_3$

$$(4) (P_R < P_L) \ \& \ (du \leq -\text{raref}) \ \text{or} \ (p_R \geq P_L) \ \& \ (du < -\text{shk}) \Rightarrow S_1 + S_3.$$

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.

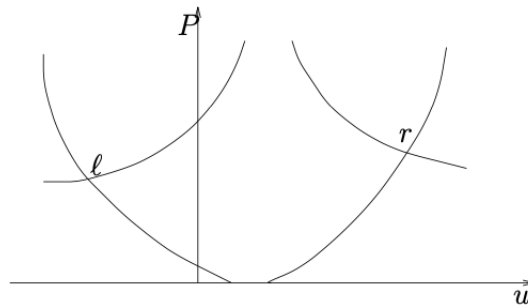


Figure 6.6: The vacuum state appears when $P_* < 0$.

Chapter 7

Viscous Fluids

7.1 Viscosity

7.1.1 Stress

The stress is a surface force. It is comprised with a hydrostatic part $-p\mathbf{I}$ and a deviatoric part τ . The hydrostatic force is due to random collisions of particles. It exists even when the macroscopic velocity $\mathbf{v} = 0$. The deviatoric stress consists of a restoration force and a resistance force in response to the fluid motions. The restoration part is called the elastic stress, while the resistance part, the *viscous stress*. In fluids, we do not have the elastic stress.

Consider a small piece of surface centered at \mathbf{x} with area dA and (outer) normal \mathbf{v} . Suppose this surface is exerted a force $\mathbf{t}dA$ from its neighboring particles. Cauchy postulates the following principles to characterize the stress:

- Cauchy stress principle: The stress is assumed to be a function of the Euler coordinate \mathbf{x} and the normal of the surface \mathbf{v} .
- Conservation of linear momentum: This leads to that there exists a tensor $\sigma(\mathbf{x})$ such that

$$\mathbf{t} = \sigma(\mathbf{x}) \cdot \mathbf{v}, \quad \text{or} \quad t_i = \sigma_{ij}v^j. \quad (7.1)$$

- Principle of angular momentum: There is no internal torque and thus the macroscopic angular momentum is conserved. This leads to

$$\sigma(\mathbf{x}) \text{ is symmetric.} \quad (7.2)$$

The proofs of these principles will be given in later chapter. In fluids, such stress is comprised with a hydrostatic part $-p\mathbf{I}$ and a viscous part τ :

$$\sigma = -p\mathbf{I} + \tau. \quad (7.3)$$

The first term is due to direct impact of particles to the surface. It is a thermodynamic force. It exists even when the velocity is zero or a constant. We assume the fluid is isotropic (i.e. a property that has the same value in all directions). Then this thermodynamic stress is $-p\mathbf{I}$. The second term τ is called the *viscous stress tensor*. It is due to the resistance of fluids to the fluid motions. It occurs when different fluid parcels move at different velocities. Thus, τ depends on $\nabla\mathbf{v}$, or maybe, $\nabla\nabla\mathbf{v}, \dots$, etc. We note that $\tau = 0$ when \mathbf{v} is a constant. The hypothesis of *Newtonian fluids* is that τ as a linear function of $\nabla\mathbf{v}$.

7.1.2 Rate-of-Strain

The term $\nabla\mathbf{v}$ measures the rate of material deformation and is called rate-of-deformation. We can decompose $\nabla\mathbf{v}$ into two parts:

$$2\nabla\mathbf{v} = (\nabla\mathbf{v} + (\nabla\mathbf{v})^T) + (\nabla\mathbf{v} - (\nabla\mathbf{v})^T) = \dot{\gamma} + \omega. \quad (7.4)$$

Here, $\dot{\gamma}$ is called rate-of-strain tensor and ω the vorticity tensor.

Examples Let us see two examples of $\nabla\mathbf{v}$ to understand how fluid responds to this deformation rate.

- **Rigid-body rotation** *We do not observe any resistance force in a rigid-body rotation of fluids* The rotation can be expressed as

$$\mathbf{v} = \boldsymbol{\alpha} \times \mathbf{x}, \quad \boldsymbol{\alpha} = (\alpha_1, \alpha_2, \alpha_3)^T \text{ is the rotation vector.}$$

This implies that

$$\nabla\mathbf{v} = \begin{bmatrix} 0 & -\alpha_3 & \alpha_2 \\ \alpha_3 & 0 & -\alpha_1 \\ -\alpha_2 & \alpha_1 & 0 \end{bmatrix},$$

which is an antisymmetric matrix, i.e.

$$\nabla\mathbf{v} + (\nabla\mathbf{v})^T = 0.$$

For this rotational flow, we find the corresponding $\tau = 0$ from experiment. 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

$$v_1 = \dot{\gamma}_{21}x_2, \quad v_2 = 0, \quad v_3 = 0. \quad (7.5)$$

Here, $\dot{\gamma}_{21}$ is the shear rate. We assume it is a constant. This flow is an inviscid, incompressible fluid flow.

It is found experimentally for a wide class of fluids and over a wide range of shear rate that the pressure p is independent of $\dot{\gamma}_{21}$ and

$$\tau_{21} = \mu \dot{\gamma}_{21}$$

for some constant μ . Such ratio μ is called the shear viscosity.

7.1.3 The stress and strain-rate relation for Newtonian fluids

Assumptions of isotropic Newtonian fluids

- The viscous stress tensor τ is linear in strain rate $\nabla \mathbf{v}$,
- τ is isotropic
- τ is symmetric

From the assumption that τ is *linear* w.r.t. $\nabla \mathbf{v}$, we can write

$$\tau_{ij} = a_{ijkl} \frac{\partial v^k}{\partial x^l}$$

for some constants (a_{ijkl}) . From τ being isotropic, i.e. this rank 4 tensor (a_{ijkl}) is *isotropic* (i.e. a property that has identical value in all directions), then it can be shown that

$$a_{ijkl} = \alpha \delta_{ij} \delta_{kl} + \beta \delta_{ik} \delta_{jl} + \gamma \delta_{il} \delta_{jk} \quad (7.6)$$

for some constants α, β, γ .¹ From τ being *symmetric*, we get that a_{ijkl} is symmetric in i, j . This leads to $\beta = \gamma$. That is,

$$a_{ijkl} = \alpha \delta_{ij} \delta_{kl} + \beta (\delta_{ik} \delta_{jl} + \delta_{il} \delta_{jk}). \quad (7.7)$$

¹This 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 $e'_i = R_i^k e_k$ and R_i^k 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 $e'_i = R_i^k e_k$ and R_i^k is a rotation matrix.

Lemma 7.6. (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 .

Hence

$$\begin{aligned}
 \tau_{ij} &= a_{ijkl} \frac{\partial v^k}{\partial x^l} \\
 &= [\alpha \delta_{ij} \delta_{kl} + \beta (\delta_{ik} \delta_{jl} + \delta_{il} \delta_{jk})] \frac{\partial v^k}{\partial x^l} \\
 &= \beta \left(\frac{\partial v^i}{\partial x^j} + \frac{\partial v^j}{\partial x^i} \right) + \alpha \delta_{ij} \frac{\partial v^k}{\partial x^k} \\
 &= \beta \dot{\gamma}_{ij} + \alpha \delta_{ij} \dot{\gamma}_{kk}
 \end{aligned}$$

We write it as

$$\boldsymbol{\tau} = \beta \dot{\boldsymbol{\gamma}} + \alpha \text{tr}(\dot{\boldsymbol{\gamma}}) \mathbf{I}.$$

Let us define the strain rate

$$D = \frac{1}{2} (\nabla \mathbf{v} + (\nabla \mathbf{v})^T), \quad (7.8)$$

the rate of shear strain and rate of bulk strain by

$$D_s := D - \frac{1}{3} \text{Tr}(D) \mathbf{I}, \quad D_b = \frac{1}{3} \text{Tr}(D).$$

We can express $\boldsymbol{\tau}$ in terms of D_s and D_b by

$$\boxed{\boldsymbol{\tau} = 2\eta D_s(\mathbf{v}) + 2\zeta D_b(\mathbf{v})}. \quad (7.9)$$

The coefficient η is called the shear viscosity, while ζ the bulk viscosity. They satisfy

$$\eta > 0, \quad \zeta > 0. \quad (7.10)$$

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 .

Momentum equation The viscous force is

$$\begin{aligned}
 \nabla \cdot \boldsymbol{\tau} &= \nabla \cdot \left[\eta \left(\nabla \mathbf{v} + (\nabla \mathbf{v})^T - \frac{2}{3} \nabla \cdot \mathbf{v} \mathbf{I} \right) + \zeta \nabla \cdot \mathbf{v} \mathbf{I} \right] \\
 &= \eta \nabla^2 \mathbf{v} + \left(\zeta + \frac{\eta}{3} \right) \nabla (\nabla \cdot \mathbf{v}).
 \end{aligned}$$

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

$$\rho (\partial_t \mathbf{v} + \mathbf{v} \nabla \mathbf{v}) + \nabla p = \eta \nabla^2 \mathbf{v} + \left(\zeta + \frac{\eta}{3} \right) \nabla (\nabla \cdot \mathbf{v}). \quad (7.11)$$

Vorticity equation for compressible viscous flows From (3.2), the momentum equation can also expressed as

$$\rho \left(\mathbf{v}_t + \boldsymbol{\omega} \times \mathbf{v} + \nabla \left(\frac{1}{2} |\mathbf{v}|^2 \right) \right) + \nabla p = \nabla \cdot \boldsymbol{\tau}, \quad (7.12)$$

By taking *curl* on this equation, assuming **incompressibility**, we obtain the vorticity equation for incompressible viscous flows:

$$\partial_t \boldsymbol{\omega} + \mathbf{v} \cdot \nabla \boldsymbol{\omega} - (\boldsymbol{\omega} \cdot \nabla) \mathbf{v} + \boldsymbol{\omega} (\nabla \cdot \mathbf{v}) = \eta \Delta \boldsymbol{\omega}. \quad (7.13)$$

Note that the bulk viscosity does not effect the diffusion of the vortices.

Boundary condition For a fixed boundary, a natural boundary for viscous flow is

$$\mathbf{v} = 0 \quad \text{on boundary.}$$

7.2 Heat conduction and Energy equation

The energy equation involves the rate-of-work done by the surface force and body force, which are $\boldsymbol{\sigma} \cdot \mathbf{v}$ 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

$$\mathbf{q} = -\kappa \nabla T, \quad (7.14)$$

where κ is a positive parameter, called heat conductivity. Formula (7.14) is called the Fourier law.

With the above two sources of rate-of-energy, the new energy equation becomes

$$\frac{\partial(\rho E)}{\partial t} + \nabla \cdot (\rho E \mathbf{v} - \boldsymbol{\sigma} \mathbf{v} + \mathbf{q}) = \mathbf{f} \cdot \mathbf{v}, \quad \boldsymbol{\sigma} = -pI + \boldsymbol{\tau}. \quad (7.15)$$

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

$$\begin{cases} T(\mathbf{x}) = T_d(\mathbf{x}) & \mathbf{x} \in \Gamma_d \\ \nabla T \cdot \mathbf{v}(\mathbf{x}) = g(\mathbf{x}) & \mathbf{x} \in \Gamma_n. \end{cases}$$

7.3 Energy dissipation and entropy production

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:

$$\begin{aligned} \mathbf{v} \cdot [\rho(\mathbf{v}_t + \mathbf{v} \cdot \nabla \mathbf{v})] &= \partial_t \left(\frac{1}{2} \rho |\mathbf{v}|^2 \right) + \nabla \cdot (\rho \mathbf{v}) \frac{|\mathbf{v}|^2}{2} + \mathbf{v} \cdot (\rho \mathbf{v} \cdot \nabla \mathbf{v}) \\ &= \partial_t \left(\frac{1}{2} \rho |\mathbf{v}|^2 \right) + \partial_j (\rho v^j) \frac{v^i v^i}{2} + v^i \rho v^j \partial_j v^i \\ &= \partial_t \left(\frac{1}{2} \rho |\mathbf{v}|^2 \right) + \nabla \cdot \left(\frac{1}{2} \rho |\mathbf{v}|^2 \mathbf{v} \right). \end{aligned}$$

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:

$$\begin{aligned} \mathbf{v} \cdot (\nabla \cdot \boldsymbol{\tau}) &= \nabla \cdot (\mathbf{v} \cdot \boldsymbol{\tau}) - \nabla \mathbf{v} : \boldsymbol{\tau} \\ &= \nabla \cdot (\mathbf{v} \cdot \boldsymbol{\tau}) - \frac{1}{2} (\nabla \mathbf{v} + (\nabla \mathbf{v})^T) : \boldsymbol{\tau} \quad \because \boldsymbol{\tau} \text{ is symmetric} \\ &= \nabla \cdot (\mathbf{v} \cdot \boldsymbol{\tau}) - \boldsymbol{\tau} : D \end{aligned}$$

Recall that

$$\boldsymbol{\tau} = 2\eta D_s + 2\zeta D_b, \quad D = D_s + D_b$$

and note that $D_s : D_b = 0$, we get

$$\boldsymbol{\tau} : D = 2\eta |D_s|^2 + 2\zeta |D_b|^2. \quad (7.16)$$

Finally, we get the following equation for the kinetic energy:

$$\partial_t (\rho E_k) + \nabla \cdot [(\rho E_k \mathbf{I} + p \mathbf{I} - \boldsymbol{\tau}) \cdot \mathbf{v}] - p \nabla \cdot \mathbf{v} = -\boldsymbol{\tau} : D.$$

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.

Increase of entropy First, we subtract the kinetic energy from the energy equation

$$\partial_t(\rho E) + \text{div}[(\rho E + p)\mathbf{v}] = \nabla \cdot (\boldsymbol{\tau} \cdot \mathbf{v} - \mathbf{q}).$$

to get an equation for internal energy:

$$\partial_t(\rho U) + \nabla \cdot (\rho U \mathbf{v}) = -p \nabla \cdot \mathbf{v} - \nabla \cdot \mathbf{q} + \boldsymbol{\tau} : D.$$

- 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;
- $\boldsymbol{\tau} : D$ is the heat source generated from viscosity.

From continuity equation, the above equation can also be expressed as

$$\rho \frac{dU}{dt} = -p \nabla \cdot \mathbf{v} - \nabla \cdot \mathbf{q} + \boldsymbol{\tau} : D. \quad (7.17)$$

From the first law of thermodynamics

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

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

$$\rho T \frac{dS}{dt} = -\nabla \cdot \mathbf{q} + \boldsymbol{\tau} : D.$$

or

$$\rho \frac{dS}{dt} = -\frac{\nabla \cdot \mathbf{q}}{T} + \frac{1}{T} \boldsymbol{\tau} : D,$$

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

$$\frac{d}{dt}(\rho S) + \nabla \cdot \left(\frac{\mathbf{q}}{T}\right) = -\frac{1}{T^2} \mathbf{q} \cdot \nabla T + \frac{1}{T} \boldsymbol{\tau} : D.$$

$$\boxed{\partial_t(\rho S) + \nabla \cdot (\mathbf{v} \rho S) + \nabla \cdot \left(\frac{\mathbf{q}}{T}\right) = -\frac{1}{T^2} \mathbf{q} \cdot \nabla T + \frac{1}{T} \boldsymbol{\tau} : D.} \quad (7.18)$$

The integral form is

$$\boxed{\frac{d}{dt} \int_{\Omega(t)} \rho S d\mathbf{x} + \int_{\partial\Omega(t)} \frac{\mathbf{q} \cdot \mathbf{n}}{T} dS = \int_{\Omega(t)} \left(-\frac{1}{T^2} \mathbf{q} \cdot \nabla T + \frac{1}{T} \boldsymbol{\tau} : D\right) d\mathbf{x}} \quad (7.19)$$

- The terms $\frac{1}{T} \boldsymbol{\tau} : D > 0$;
- 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

$$\frac{d}{dt} \int_{\Omega(t)} \rho S d\mathbf{x} + \int_{\partial\Omega(t)} \frac{\mathbf{q} \cdot \mathbf{n}}{T} dS - \int_{\Omega(t)} \frac{\rho r}{T} d\mathbf{x} \geq 0, \quad (7.20)$$

where r is the heat source, \mathbf{q} the heat flux. This is called the *Clausius-Duhem inequality*. Comparing (7.19) and (7.20), and use (7.16), we see the heat source in gas system is

$$\rho r = \kappa \frac{|\nabla T|^2}{T^2} + \frac{2}{T} (\eta |D_s|^2 + \zeta |D_b|^2).$$

Thus, the second law of thermodynamics, expressed as (7.20) if and only if

$$\kappa \geq 0, \quad \eta \geq 0, \quad \zeta \geq 0. \quad (7.21)$$

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 $\tau_N := \boldsymbol{\tau} \cdot \mathbf{v}$. 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

$$\frac{d}{dt} \int_{\Omega} s d\mathbf{x} > 0.$$

7.4 Viscous Flows**7.4.1 Stokes Flows****Shear flows**

- Poiseuille flow (Laminar flow in a tube)
- Cavity flow

7.4.2 Bifurcation of fluid flows

- Flow passes a cylinder
- Flow separation
- Taylor-Couette flow
- Rayleigh-Bénard Flow

Part II

Elasticity

Chapter 8

Kinematics of Elasticity

Solid mechanics includes elasticity, plasticity, viscoelasticity, visco-plasticity, liquid crystal, etc. ¹ 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.

¹The references of this chapter include

- 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.

8.1 Deformation and Strain

8.1.1 Flow maps and Deformation gradient

Flow maps and velocity fields Let us imagine an elastic material deforms from a domain \hat{M} at time 0 to M_t at time t . The domain M_t is a manifold, called the configuration space or the observer's space. The initial region \hat{M} is called the reference space or the material space. We denote such a deformation or flow map by ²

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

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 . ³ 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 $\mathbf{v} : \cup_{t \geq 0} \{t\} \times M_t \rightarrow \mathbb{R}^3$, 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

$$F(t, X) := \nabla_X \mathbf{x}(t, X) = \frac{\partial \mathbf{x}}{\partial X}(t, X) \quad (8.1)$$

is called the *deformation gradient*. ⁴ It is clear that $F(0, X) = I$. Its component expression is

$$dx^i = F_\alpha^i dX^\alpha := \frac{\partial x^i}{\partial X^\alpha} dX^\alpha.$$

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.

²In 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.

³The flow map $\mathbf{x}(t, \cdot)$ may not be differentiable everywhere. $\partial \mathbf{x} / \partial X$ may have discontinuity.

⁴In differential geometry, we express F as $d\varphi_t$.

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

$$\frac{\partial}{\partial X^\alpha} \frac{\partial}{\partial t} x^i(t, X) = \frac{\partial v^i}{\partial x^k} \frac{\partial x^k}{\partial X^\alpha}.$$

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

$$\boxed{\dot{F} = (\nabla \mathbf{v})F = LF.} \quad (8.2)$$

The term

$$L_k^i := \frac{\partial v^i}{\partial x^k}, \quad \text{or} \quad L = \nabla \mathbf{v}$$

is called the *rate-of-deformation*.⁵

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

$$\nabla \mathbf{v} + (\nabla \mathbf{v})^T = \dot{Q}Q^T + Q\dot{Q}^T = 0, \quad \because Q^T Q = I.$$

Let us characterize the rigid-body motion without proof.

Proposition 8.4. *Let $\varphi_t : \Omega \rightarrow \mathbb{R}^3$ be a flow map in \mathbb{R}^3 . Then $\varphi_t(X)$ is a rigid-body motion if and only if $F^T F \equiv I$, where $F := \nabla_X \varphi_t$.*

⁵Note that $(\nabla \mathbf{v})_k^i := \partial v^i / \partial x^k$, which is different from the notation of ordinary tensor product. There, $(\nabla \otimes \mathbf{v})_k^i := \partial_{x^i} v^j$. 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

$$v_1 = \dot{\gamma}_{21}x_2, \quad v_2 = 0, \quad v_3 = 0. \quad (8.3)$$

Here, $\dot{\gamma}_{21}$ is a constant, called the shear rate. The corresponding flow map is

$$x_1 = X_1 + \dot{\gamma}_{21}tX_2, \quad x_2 = X_2, \quad x_3 = X_3.$$

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 flow⁶ is given by

$$\begin{aligned} v_1 &= -\frac{1}{2}\dot{\epsilon}(1+b)x_1 \\ v_2 &= -\frac{1}{2}\dot{\epsilon}(1-b)x_2 \\ v_3 &= \dot{\epsilon}x_3. \end{aligned} \quad (8.4)$$

Here, $0 \leq b \leq 1$ and $\dot{\epsilon}$ are two constants, called the elongation rates. We have

$$\nabla \mathbf{v} = \begin{bmatrix} -\frac{1}{2}\dot{\epsilon}(1+b) & & \\ & -\frac{1}{2}\dot{\epsilon}(1-b) & \\ & & \dot{\epsilon} \end{bmatrix},$$

It satisfies

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

Thus, this flow map is volume preserving. The flow map is given by

$$\begin{bmatrix} x^1 \\ x^2 \\ x^3 \end{bmatrix} = \begin{bmatrix} \exp(-\frac{1}{2}\dot{\epsilon}(1+b)t) & & \\ & \exp(-\frac{1}{2}\dot{\epsilon}(1-b)t) & \\ & & \exp(\dot{\epsilon}t) \end{bmatrix} \begin{bmatrix} X^1 \\ X^2 \\ X^3 \end{bmatrix}.$$

Special cases are

- Elongational flow: $b = 0, \dot{\epsilon} > 0$. It elongates in x^3 direction and shrinks in x^1 and x^2 cross-section plane.
- Bi-axial stretching flow: $b = 0, \dot{\epsilon} < 0$. 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.

⁶This part of note mainly comes from Bird's book, Vol. I, Chapter 3.

4. Linear Deformation Consider an elastic motion satisfying $\nabla \mathbf{v} = \text{constant}$. 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 $\det(e^{tA}) = e^{t\text{Tr}(A)}$, we get $J(t) = \det F(t) = 1$ iff $\text{Tr}(A) = 0$.
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 ⁷

$$QQ^T = e^{tA}e^{tA^T} = e^{t(A+A^T)} = I.$$

That is, Q is a rotation. Thus, the flow is a rigid-body motion.

3. If $A = \lambda I$, then $e^{tA}X$ is an isotropic expansion/shrinking.
4. Suppose A is symmetric and $\text{Tr}(A) = 0$. We can diagonalize A , say $A = \text{diag}(\lambda_1, \lambda_2, \lambda_3)$ with $\sum_i \lambda_i = 0$. Then

$$e^{tA} = \text{diag}(e^{t\lambda_1}, e^{t\lambda_2}, e^{t\lambda_3}).$$

It expands in those directions where $\lambda_i > 0$ and shrinks in those where $\lambda_i < 0$.

⁷Note 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

$$A = \left(A - \frac{1}{3}\text{Tr}(A)I\right) + \frac{1}{3}\text{Tr}(A)I$$

The first term is trace free and the second term is isotropic.

$$e^{tA} = e^{t\left(A - \frac{1}{3}\text{Tr}(A)I\right)} e^{\frac{t}{3}\text{Tr}(A)}.$$

6. A general matrix can be decomposed into

$$A = \frac{1}{2}(A + A^T) + \frac{1}{2}(A - A^T) = S + \Omega.$$

Its exponential map in a short period of time 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:*

$$\boxed{F = O_{\mathbf{n}} \Lambda O_{\mathbf{N}}^T} \quad (8.5)$$

where

$$\Lambda = \text{diag}(\lambda_1, \lambda_2, \lambda_3), \quad \lambda_i \geq 0,$$

and

$$O_{\mathbf{n}} = [\mathbf{n}_1, \mathbf{n}_2, \mathbf{n}_3], \quad O_{\mathbf{N}} = [\mathbf{N}_1, \mathbf{N}_2, \mathbf{N}_3]$$

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 . λ_i are called 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

$$F_\alpha^i = \sum_k \lambda_k \mathbf{n}_k^i \mathbf{N}_k^\alpha.$$

The matrix $\mathbf{n}_k \mathbf{N}_k^T$ is a rank-1 matrix. It is a projection on 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 , $k = 1, 2, 3$. The 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 .⁸

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 $\{\mathbf{n}_k | \text{the corresponding } \lambda_k \neq 0\}$ 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 $\{\mathbf{n}_k\}$ 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

$$F \mathbf{N}_k = \lambda_k \mathbf{n}_k, \quad k = 1, 2, 3. \quad (8.6)$$

⁸The 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 $\Lambda = \text{diag}(\lambda_1, \lambda_2, \lambda_3)$. Then $O_{\mathbf{n}}$ and $O_{\mathbf{N}}$ are orthogonal matrices, and (8.6) can be expressed as

$$F[\mathbf{N}_1, \mathbf{N}_2, \mathbf{N}_3] = [\mathbf{n}_1, \mathbf{n}_2, \mathbf{n}_3] \text{diag}(\lambda_1, \lambda_2, \lambda_3),$$

or

$$F = O_{\mathbf{n}} \Lambda O_{\mathbf{N}}^T.$$

□

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.

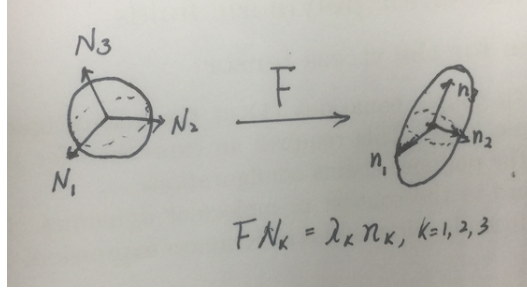
3. Let us restate the above argument by investigating the deformation of a small ball. Consider a small ball $\{|\Delta X|^2 = \varepsilon^2\}$ in the tangent space of material space TM_0 . Let us represent the tangent ΔX in terms of N_k as $\Delta X = \Delta X'^k \mathbf{N}_k$. The deformation gradient 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 . $FN_k = \lambda_k n_k$

Polar decomposition of F

1. Let $F = O_{\mathbf{n}} \Lambda O_{\mathbf{N}}^T$ be the singular value decomposition of F . Then

$$F = O_{\mathbf{n}} \Lambda O_{\mathbf{N}}^T = (O_{\mathbf{n}} O_{\mathbf{N}}^T) (O_{\mathbf{N}} \Lambda O_{\mathbf{N}}^T) = O S_r, \quad F_{\alpha}^i = O_{\beta}^i S_{r,\alpha}^{\beta}.$$

$$O := O_{\mathbf{n}}, \quad S_r := \Lambda O_{\mathbf{N}}^T.$$

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 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) on the material first, then map to the Eulerian space by an isometry (i.e. O).* We shall see in 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 equivalent $S_r^2 = C = F^T F$, the right Cauchy-Green strain. We shall see this in the material response to the deformation in later section.

2. Alternatively, we can have left polar decomposition:

$$F = O_{\mathbf{n}} \Lambda O_{\mathbf{N}}^T = (O_{\mathbf{n}} \Lambda O_{\mathbf{n}}^T) (O_{\mathbf{n}} O_{\mathbf{N}}^T) = S_l O^T, \quad F_{\alpha}^i = S_{l,k}^i O_{\alpha}^k,$$

$$O = O_{\mathbf{N}}, \quad S_l := O_{\mathbf{n}} \Lambda.$$

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 others are naturally defined in observer space M_t . These deformation tensors are also called the *strain tensors*.⁹

- Strain tensors defined in M_0 :

- Deformation gradient $F_\alpha^i(t, X) = \frac{\partial x^i}{\partial X^\alpha}$.

- Right Cauchy-Green deformation tensor: $C = F^T F$, or $C_\beta^\alpha = (F^T)_i^\alpha F_\beta^i = F_\beta^i F_\alpha^i$.

- Right stretch tensor $S_r := (F^T F)^{1/2}$.

- Strain tensors defined in M_t :

- Inverse deformation gradient: $(F^{-1})_i^\alpha(t, \mathbf{x}) = \frac{\partial X^\alpha}{\partial x^i}$.

- Left Cauchy-Green deformation tensor: $B := F F^T$, or $B_j^i = F_\alpha^i (F^T)_j^\alpha = F_\alpha^i F_\alpha^j$.

- Left stretch tensor $S_l := (F F^T)^{1/2}$.

2. The geometric meaning of deformation tensors can be analyzed through the change of arc length after deformation. We have

$$\langle d\mathbf{x}, d\mathbf{x} \rangle = \langle F dX, F dX \rangle = \langle F^T F dX, dX \rangle = \langle C dX, dX \rangle \quad (8.7)$$

and

$$\langle dX, dX \rangle = \langle F^{-1} d\mathbf{x}, F^{-1} d\mathbf{x} \rangle = \langle d\mathbf{x}, (F^{-T} F^{-1}) d\mathbf{x} \rangle = \langle d\mathbf{x}, B^{-1} d\mathbf{x} \rangle. \quad (8.8)$$

Thus, **the deformation tensors are the ratio of metric between Lagrangian and Eulerian coordinates**. C is the pullback of the metric $\langle d\mathbf{x}, d\mathbf{x} \rangle$ by the flow map φ_t . The principal eigenvalues of $C = F^T F$ are the stretching of the infinitesimal length $\|dX\|^2$.

⁹Some textbooks use the following names: Finger's tensor (FF^T), Cauchy ($F^T F$), Piola ($F^{-1} F^{-T}$), and Almansi ($F^{-T} F^{-1}$)

3. The right Cauchy-Green deformation tensor is also the first fundamental form of the domain $\Omega(t)$. The tangent vector $g_\alpha := \frac{\partial \mathbf{x}}{\partial X^\alpha}$ and the first fundamental form is defined to be $C_{\alpha\beta} := \langle g_\alpha, g_\beta \rangle$.
4. Deformation of an infinitesimal ellipsoid. Consider an infinitesimal sphere at $t = 0$. It is expressed as

$$dX \cdot dX = 1.$$

At time t , it is deformed to

$$d\mathbf{x} \cdot B^{-1} \cdot d\mathbf{x} = dX \cdot dX = 1.$$

This is an infinitesimal ellipsoid with three axes $\mathbf{n}_1, \mathbf{n}_2, \mathbf{n}_3$ and length λ_k^2 .

8.1.5 Displacement and Strain

- Displacement vector: $\mathbf{u} := \mathbf{x}(t, X) - X$.
- Lagrangian 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: $e := \frac{1}{2}(I - B^{-1})$.
- Eulerian strain tensor: $\varepsilon = \frac{1}{2} \left(\frac{\partial u^i}{\partial x^j} + \frac{\partial u^j}{\partial x^i} \right)$.

Let $ds^2 := d\mathbf{x} \cdot d\mathbf{x}$ and $dS^2 = dX \cdot dX$. 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

$$E = \frac{ds^2 - dS^2}{2dS^2}, \quad e = \frac{ds^2 - dS^2}{2ds^2}.$$

Infinitesimal strains We can also express strains in terms of displacement gradients. Note that

$$F = I + \nabla_X \mathbf{u}.$$

Define the following infinitesimal strain tensor

$$\mathbf{e} := \frac{1}{2} (\nabla_X \mathbf{u} + \nabla_X \mathbf{u}^T) = \frac{1}{2} (F + F^T) - I.$$

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

$$E = \frac{1}{2} \left((I + \nabla_X \mathbf{u})^T (I + \nabla_X \mathbf{u}) - I \right) = \mathbf{e} + o(\mathbf{e}). \quad (8.9)$$

Geometric meaning of infinitesimal strain. To understand the physical meaning of ε_{11} , let us consider an infinitesimal vector $dX_1 := (dl_1, 0, 0)^T$. The vector is deformed to

$$d\mathbf{x}_1 = \left(1 + \frac{\partial u^1}{\partial X^1}, \frac{\partial u^2}{\partial X^1}, \frac{\partial u^3}{\partial X^1} \right)^T dl_1.$$

Its length square

$$(d\tilde{l}_1)^2 = \langle d\mathbf{x}_1, d\mathbf{x}_1 \rangle \approx \left(1 + 2 \frac{\partial u^1}{\partial X^1} \right) (dl_1)^2.$$

Here, we have neglected the high order terms. Thus,

$$d\tilde{l}_1 \approx \sqrt{1 + 2 \frac{\partial u^1}{\partial X^1}} dl_1 \approx \left(1 + \frac{\partial u^1}{\partial X^1} \right) dl_1 \quad (8.10)$$

That is

$$e_{11} \approx \frac{d\tilde{l}_1 - dl_1}{dl_1}.$$

Thus, the physical meaning of e_{11} is the relative change of dl in the direction e_1 . Similarly, to understand the physical meaning of e_{12} , we consider two infinitesimal vectors

$$\begin{aligned} dX_1 &= (dl_1, 0, 0)^T \\ dX_2 &= (0, dl_2, 0)^T. \end{aligned}$$

The corresponding deformed vectors are

$$\begin{aligned} d\mathbf{x}_1 &= \left(1 + \frac{\partial u^1}{\partial X^1}, \frac{\partial u^2}{\partial X^1}, \frac{\partial u^3}{\partial X^1} \right)^T dl_1 \\ d\mathbf{x}_2 &= \left(\frac{\partial u^1}{\partial X^2}, 1 + \frac{\partial u^2}{\partial X^2}, \frac{\partial u^3}{\partial X^2} \right)^T dl_2. \end{aligned}$$

The inner product

$$\langle d\mathbf{x}_1, d\mathbf{x}_2 \rangle \approx \left(\frac{\partial u^1}{\partial X^2} + \frac{\partial u^2}{\partial X^1} \right) dl_1 dl_2.$$

Hence, we get

$$d\tilde{l}_1 d\tilde{l}_2 \cos \theta = 2e_{12} dl_1 dl_2$$

where θ is the angle between $d\mathbf{x}_1$ and $d\mathbf{x}_2$. Using (8.10) 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.

8.2 Stress

8.2.1 The stress tensor in Eulerian coordinate – Cauchy stress

The stress is a surface force. It is a restoration force in response to the 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 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 \mathbf{v} , there exists a surface force $\mathbf{t}(\mathbf{x}, \mathbf{v})$ on dS such that $\mathbf{t} = \mathbf{g}$ on the boundary $\partial\Omega_t$. We call $\mathbf{t}(\mathbf{x}, \mathbf{v})$ the Cauchy stress vector. The Cauchy stress vector is characterized by the following Cauchy theorem.

Theorem 8.6 (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 $\boldsymbol{\sigma}(\mathbf{x})$ such that

$$\mathbf{t}(\mathbf{x}, \mathbf{v}) = \boldsymbol{\sigma}(\mathbf{x}) \cdot \mathbf{v}. \quad (8.11)$$

- *In addition, assuming Principle of angular momentum:*

$$\int_G \rho \mathbf{x} \times \frac{d\mathbf{v}}{dt} d\mathbf{x} = \int_{\partial G} \mathbf{x} \times \boldsymbol{\sigma} \cdot \mathbf{v} dS + \int_G \mathbf{x} \times \mathbf{f} d\mathbf{x}$$

for any $G \subset \Omega_t$, then

$$\boldsymbol{\sigma}(\mathbf{x}) \text{ is symmetric.} \quad (8.12)$$

Proof. 1. To show (8.11), given \mathbf{v} , we consider a plane with normal \mathbf{v} . 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

$$\int_{\Delta G} \rho \frac{d\mathbf{v}}{dt} d\mathbf{x} = \int_{\Delta S} \mathbf{t}(\mathbf{x}, \mathbf{v}) dS + \sum_{i=1}^3 \int_{\Delta S_i} \mathbf{t}(\mathbf{x}, -\mathbf{e}_i) dS + \int_{\Delta G} \mathbf{f} d\mathbf{x}.$$

By dividing both sides by ΔS then take $\Delta S \rightarrow 0$, we can get

$$\int_{\Delta G} \rho \frac{d\mathbf{v}}{dt} d\mathbf{x} \rightarrow 0, \quad \int_{\Delta G} \mathbf{f} d\mathbf{x} \rightarrow 0$$

because $\Delta G/\Delta S \rightarrow 0$, and

$$\mathbf{t}(\mathbf{x}, \mathbf{v}) = - \sum_{i=1}^3 v_i \mathbf{t}(\mathbf{x}, -\mathbf{e}_i)$$

because

$$\mathbf{v} \Delta S = (\Delta S_1, \Delta S_2, \Delta S_3).$$

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 \mathbf{v} .

2. The principle of moments (conservation of angular momentum) reads

$$\int_G \rho \left(\mathbf{x} \times \frac{d\mathbf{v}}{dt} \right) d\mathbf{x} = \int_{\partial G} (\mathbf{x} \times \boldsymbol{\sigma} \cdot \mathbf{v}) dS + \int_G \mathbf{x} \times \mathbf{f} d\mathbf{x},$$

where the left-hand side is the change of total angular momentum. The first term on the right-hand side is the total torque from surface, the second term is the total torque from the body. In differential form:

$$\rho \mathbf{x} \times \frac{d\mathbf{v}}{dt} = \nabla_{\mathbf{x}} \cdot (\mathbf{x} \times \boldsymbol{\sigma}) + \mathbf{x} \times \mathbf{f}.$$

On the other hand, from linear momentum equation:

$$\rho \frac{d\mathbf{v}}{dt} = \nabla_{\mathbf{x}} \cdot \boldsymbol{\sigma} + \mathbf{f},$$

we take cross product with \mathbf{x} on both sides to get

$$\rho \mathbf{x} \times \frac{d\mathbf{v}}{dt} = \mathbf{x} \times (\nabla_{\mathbf{x}} \cdot \boldsymbol{\sigma}) + \mathbf{x} \times \mathbf{f}.$$

This leads to

$$\nabla_{\mathbf{x}} \cdot (\mathbf{x} \times \boldsymbol{\sigma}) = \mathbf{x} \times (\nabla_{\mathbf{x}} \cdot \boldsymbol{\sigma}). \quad (8.13)$$

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 $\mathbf{x} \times (\nabla_{\mathbf{x}} \cdot \boldsymbol{\sigma})$ in coordinate form is $\varepsilon_{ijk} x^j \partial_l \sigma^{kl}$. Comparing both sides of (8.13), 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. However, 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 states, 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.
- 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.

8.2.2 The stress tensor in Lagrangian coordinate – Piola-Kirchhoff stress

The Cauchy stress is measured in Eulerian coordinate system. We can transform it to the Lagrange coordinate system.

We want to express the linear momentum equation in Lagrangian coordinate. Suppose a material with domain G_0 is deformed to G_t , and its boundary S_0 is deformed to S_t . In Eulerian coordinate, the linear momentum equation is

$$\int_{G_t} \rho \frac{d\mathbf{v}}{dt} d\mathbf{x} = \int_{S_t} \boldsymbol{\sigma} \cdot \mathbf{v} dS_t. \quad (8.14)$$

Here, $\boldsymbol{\sigma}$ is the Cauchy stress. In Lagrangian coordinate, we have

$$\int_{G_0} \rho_0 \frac{d\mathbf{v}}{dt} dX = \int_{S_0} P \cdot \mathbf{n} dS_0 \quad (8.15)$$

The tensor P is called the Piola-Kirchhoff stress tensor or the first Piola-Kirchhoff stress tensor. Note that in the above two momentum equations, both are in the observer's coordinate. The difference is the domain of (8.14) is in Euler coordinate, while the domain of (8.15) is in Lagrange coordinate. Thus, P and $\boldsymbol{\sigma}$ represent the same surface force in the observer's coordinate system. We want to find the relation between $\boldsymbol{\sigma}$ and P .

First, the conservation of mass reads

$$\int_{G_t} \rho d\mathbf{x} = \int_{G_0} \rho_0 dX.$$

The left-hand side is $\int_{G_0} \rho J dX$. This is valid for any G_0 . This leads to

$$\rho J = \rho_0.$$

Using this,

$$\int_{G_t} \rho \frac{d\mathbf{v}}{dt} d\mathbf{x} = \int_{G_0} \rho \frac{d\mathbf{v}}{dt} J dX = \int_{G_0} \rho_0 \frac{d\mathbf{v}}{dt} dX.$$

In (8.15), the velocity \mathbf{v} at time t is the same vector, the stress $\boldsymbol{\sigma}$ is also the same vector in Lagrangian coordinate. We now change the surface force term to Lagrangian coordinate. We recall that

$$\boxed{v dS_t = J F^{-T} \mathbf{n} dS_0.} \quad (8.16)$$

With this, then

$$\int_{S_t} \boldsymbol{\sigma} \cdot \mathbf{v} dS_t = \int_{S_0} \boldsymbol{\sigma} \cdot J F^{-T} \mathbf{n} dS_0 = \int_{S_0} P \cdot \mathbf{n} dS_0.$$

This gives

$$\boxed{P = J \boldsymbol{\sigma} \cdot F^{-T}, \quad \boldsymbol{\sigma} = J^{-1} P F^T.}$$

In component form, it is

$$P_\alpha^i = J \sigma^{ij} (F^{-T})_\alpha^j = J \sigma^{ij} \frac{\partial X^\alpha}{\partial x^j}.$$

$$\sigma^{ij} = J^{-1} P_{\alpha}^i F_{\alpha}^j.$$

The first Piola-Kirchhoff stress P is the pullback of the Cauchy stress σ via φ_t .

Another stress is the second Piola-Kirchhoff stress, defined by

$$\Sigma := F^{-1} P = J F^{-1} \sigma F^{-T},$$

which has range in material space, not in observer's space. In component form, it is

$$\Sigma_{\alpha\beta} = (F^{-1})_i^{\alpha} P_{\beta}^i = \frac{\partial X^{\alpha}}{\partial x^i} P_{\beta}^i = J \sigma^{ij} \frac{\partial X^{\alpha}}{\partial x^i} \frac{\partial X^{\beta}}{\partial x^j},$$

which is also symmetric.

Chapter 9

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.

9.1 Lagrangian formulation for simple elasticity

9.1.1 Variational Approach for dynamics of 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:

$$\mathcal{X} := \{ \mathbf{x} : \Omega_0 \rightarrow \mathbb{R}^3 \mid \mathbf{x} \text{ is Lipschitz continuous, } \mathbf{x}(X) = \mathbf{x}_0(X), X \in \partial\Omega_0 \} \quad (9.1)$$

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

$$\mathbf{x} = \arg \min\{\mathcal{S}[\mathbf{x}] | \mathbf{x} \in \mathcal{X}\}. \quad (9.2)$$

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

$$\delta\mathbf{x}(t, X) := \left. \frac{\partial}{\partial \varepsilon} \right|_{\varepsilon=0} \mathbf{x}_\varepsilon(t, X),$$

the variation of the flow map $\mathbf{x}(\cdot, \cdot)$. We write the variation of \mathbf{x} by $\delta\mathbf{x}$ (or $\dot{\mathbf{x}}$). Since, for small ε , $\mathbf{x}_\varepsilon(t, \cdot)$ are flow maps, its variation

$$\delta\mathbf{x}(t, X) = \lim_{\varepsilon \rightarrow 0} \frac{\mathbf{x}_\varepsilon - \mathbf{x}_0}{\varepsilon}$$

is an infinitesimal variation of position, thus, is also called a pseudo-velocity. The derivative

$$\left. \frac{d}{d\varepsilon} \right|_{\varepsilon=0} \mathcal{S}[\mathbf{x}_\varepsilon]$$

is called the variation of the functional $\mathcal{S}[\mathbf{x}]$ in direction $\delta\mathbf{x}$. We denote it by

$$\delta\mathcal{S}[\mathbf{x}] \cdot \delta\mathbf{x} := \left. \frac{d}{d\varepsilon} \right|_{\varepsilon=0} \mathcal{S}[\mathbf{x}_\varepsilon].$$

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 δS :

$$\begin{aligned}
\delta S[\mathbf{x}] \cdot \delta \mathbf{x} &= \frac{d}{d\varepsilon} \Big|_{\varepsilon=0} \int_{t_0}^{t_1} \int_{\Omega_0} \left(\frac{1}{2} \rho_0(X) |\dot{\mathbf{x}}_\varepsilon(t, X)|^2 - W \left(\frac{\partial \mathbf{x}_\varepsilon(t, X)}{\partial X} \right) \right) dX dt \\
&= \int_{t_0}^{t_1} \int_{\Omega_0} (\rho_0(X) \dot{\mathbf{x}}(t, X) \cdot \delta \dot{\mathbf{x}} - W'(F) \delta F) dX dt \\
&= \int_{t_0}^{t_1} \int_{\Omega_0} \left(-\frac{d}{dt} (\rho_0(X) \dot{\mathbf{x}}(t, X)) \cdot \delta \mathbf{x} - W'(F) \frac{\partial \delta \mathbf{x}}{\partial X} \right) dX dt \\
&= \int_{t_0}^{t_1} \int_{\Omega_0} \left(-\rho_0(X) \ddot{\mathbf{x}}(t, X) \cdot \delta \mathbf{x} - W'(F) \frac{\partial \delta \mathbf{x}}{\partial X} \right) dX dt \\
&= \int_{t_0}^{t_1} \int_{\Omega_0} \left(-\rho_0(X) \ddot{\mathbf{x}}(t, X) \cdot \delta \mathbf{x} + \left(\frac{\partial}{\partial X} W'(F) \right) \cdot \delta \mathbf{x} \right) dX dt - B.C. \\
&= \int_{t_0}^{t_1} \int_{\Omega_0} \left[-\rho_0(X) \ddot{\mathbf{x}}(t, X) + \frac{\partial}{\partial X} W' \left(\frac{\partial \mathbf{x}}{\partial X} \right) \right] \cdot \delta \mathbf{x} dX dt - B.C.
\end{aligned}$$

Here,

$$\begin{aligned}
B.C. &= \int_{t_0}^{t_1} \int_{\Omega_0} \nabla_X \cdot (W'(F) \delta \mathbf{x}) dX dt \\
&= \int_{t_0}^{t_1} \int_{\partial \Omega_0} W'(F)_{\alpha}^i N^\alpha \delta x^i dX dt, \quad \mathbf{N} \text{ is the outer normal of } \partial \Omega_0
\end{aligned}$$

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

$$\delta S[\mathbf{x}] \cdot \delta \mathbf{x} = \int_{t_0}^{t_1} \int_{\Omega_0} \left[-\rho_0(X) \ddot{\mathbf{x}}(t, X) + \frac{\partial}{\partial X} W' \left(\frac{\partial \mathbf{x}}{\partial X} \right) \right] \cdot \delta \mathbf{x} dX dt = 0,$$

for all $\delta \mathbf{x}$ in the tangent space of \mathcal{X} . This leads to the following Euler-Lagrange equation

$$\boxed{\rho_0(X) \ddot{\mathbf{x}}(t, X) = \nabla_X \cdot P \left(\frac{\partial \mathbf{x}}{\partial X} \right) \quad \text{for } X \in \Omega_0,} \quad (9.3)$$

Here, $P := W'(F)$ is called the first Piola-Kirchhoff stress tensor, or just the Piola stress. Its component form is

$$P_\alpha^i = \frac{\partial W}{\partial F_\alpha^i}, \quad F_\alpha^i := \frac{\partial x^i}{\partial X_\alpha}.$$

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 (9.3) 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 (9.6), 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 condition**

$$\mathbf{x}(t, X) = \mathbf{x}_0(X) \quad \text{for } X \in \partial\Omega_0. \quad (9.4)$$

This condition is called the Dirichlet boundary condition which was inherited in our admissible class.

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 ;
- **traction:** we can apply traction \mathbf{g} on some part of the boundary, say Γ_0^n .

Here, the traction is only applied to certain portion of the boundary. This means that the boundary $\partial\Omega_0$ is decomposed into

$$\partial\Omega_0 = \Gamma_0^n \cup \Gamma_0^d.$$

The traction is applied on Γ_0^n . On Γ_0^d , we impose a Dirichlet boundary condition:

$$\mathbf{x}(t, X) = \mathbf{x}_0(X), \quad \text{for } X \in \Gamma_0^d.$$

In this situation, our admissible class is

$$\mathcal{X} = \{\mathbf{x} \mid \mathbf{x}(t, X) = \mathbf{x}_0(X) \text{ for } X \in \Gamma_0^d\}$$

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.

We also need to add the energies contributed from these two forces to our action functional:²

$$\begin{aligned} \mathcal{S}[\mathbf{x}] := & \int_{t_0}^{t_1} \int_{\Omega_0} \left(\frac{1}{2} \rho_0(X) |\dot{\mathbf{x}}(t, X)|^2 - W \left(\frac{\partial \mathbf{x}(t, X)}{\partial X} \right) \right) dX dt \\ & - \int_{t_0}^{t_1} \int_{\Omega_0} V(\mathbf{x}(t, X)) J dX dt + \int_{t_0}^{t_1} \int_{\Gamma_0^n} \mathbf{g}(X) \cdot \mathbf{x}(t, X) dS_0. \end{aligned} \quad (9.5)$$

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 respect to $\mathbf{x} \in \mathcal{X}$. This gives

$$\begin{aligned} \delta \mathcal{S}[\mathbf{x}] \cdot \delta \mathbf{x} = & \int_{t_0}^{t_1} \int_{\Omega_0} \left[-\rho_0(X) \ddot{\mathbf{x}}(t, X) + \frac{\partial}{\partial X} W' \left(\frac{\partial \mathbf{x}}{\partial X} \right) - \nabla_{\mathbf{x}} V(\mathbf{x}) J \right] \cdot \delta \mathbf{x} dX dt \\ & - \int_{t_0}^{t_1} \int_{\Gamma_0^n} (W' \cdot \mathbf{N} - \mathbf{g}) \cdot \delta \mathbf{x} dS_0 dt = 0, \end{aligned}$$

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

$$\boxed{\rho_0(X) \ddot{\mathbf{x}}(t, X) = \nabla_X \cdot P \left(\frac{\partial \mathbf{x}}{\partial X} \right) + \mathbf{f}(t, \mathbf{x}(t, X)) \det \left(\frac{\partial \mathbf{x}}{\partial X} \right) \text{ in } \Omega_0.} \quad (9.6)$$

where $\mathbf{f} = -\nabla_{\mathbf{x}} V(\mathbf{x})$ is the body force. The initial condition is the same. The boundary conditions are casted as

- Dirichlet: This is to impose

$$\mathbf{x}(t, X) = \mathbf{x}_0(X) \text{ for } X \in \Gamma_0^d. \quad (9.7)$$

- Neumann: This is to impose

$$P_\alpha^i(F(t, X)) N^\alpha(X) = \mathbf{g}^i(X) \text{ for } X \in \Gamma_0^n. \quad (9.8)$$

9.1.2 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:

$$\boxed{\begin{aligned} \dot{F} &= \frac{\partial \mathbf{v}}{\partial X} \\ \rho_0 \dot{\mathbf{v}} &= \nabla_X P(F) \end{aligned}} \quad (9.9)$$

The unknowns are (F, \mathbf{v}) . There are $9 + 3 = 12$ of them. The Piola stress $P(F)$ is given as a constitutive relation $P(F) = W'(F)$.

²The work is minus of force times displacement

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

$$\boxed{\nabla_X \times F^T = 0.} \quad (9.10)$$

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 (9.6), then $\dot{\mathbf{x}} = \mathbf{v}$ and $\frac{\partial \mathbf{x}}{\partial X}$ satisfy (9.9) and the compatibility condition. Conversely, if \mathbf{v} and F satisfy (9.9) 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

$$x^i(t, X) = \int^{(t, X)} \left(v^i dt + \sum_{\alpha=1}^3 F_{\alpha}^i dX^{\alpha} \right)$$

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

$$\boxed{\begin{aligned} \dot{\mathbf{x}} &= \mathbf{v} \\ \dot{F} &= \frac{\partial \mathbf{v}}{\partial X} \\ \rho_0 \dot{\mathbf{v}} &= \nabla_X \cdot P(F) + \mathbf{f}(t, \mathbf{x}) \det(F). \end{aligned}} \quad (9.11)$$

The unknowns are $\mathbf{x}, F, \mathbf{v}$. There are $3 + 9 + 3 = 15$ unknowns and equations.

Initial condition For the first order system (9.11), 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 (9.7) and (9.8) 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: ³

$$P_{\alpha}^i(F(t, X)) N^{\alpha}(X) = \mathbf{g}^i(X) \text{ for } X \in \Gamma_0^n.$$

³References:

Two examples:

1. One dimension: In one dimension, let us call $u = F_1^1 - 1$ the strain, and $P(F_1^1) = p(u)$. We also assume $\rho_0(X) \equiv 1$. Then the equation of motion is

$$\partial_t v = \partial_X p(u) \tag{9.12}$$

$$\partial_t u = \partial_X v. \tag{9.13}$$

Here, ∂_t means $\frac{\partial}{\partial t}|_X$. Such an equation is a 2×2 hyperbolic system. The stress $p(u)$ satisfies $p'(u) > 0$. This leads to the hyperbolicity of the 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. However, 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 spring. The stress tends to a constant as the strain increases.

2. Linear elasticity: In the Hookean case where $W(F) = \frac{k}{2}|F|^2$, the stress is $P(F) = kF$. The equation of motion becomes

$$\rho_0(X) \partial_t \mathbf{v} = k \nabla_X \cdot F \tag{9.14}$$

$$\partial_t F = \nabla_X \mathbf{v} \tag{9.15}$$

Eliminating F , we get

$$\rho_0(X) \partial_t^2 \mathbf{v} = k \nabla_X^2 \mathbf{v}.$$

This is the wave equation.

9.2 Variational approach for incompressible simple elasticity

A flow map $\mathbf{x}(t, X)$ is called incompressible if

$$J(t, X) := \det \left(\frac{\partial \mathbf{x}}{\partial X}(t, X) \right) = \det F = 1.$$

1. Antman, Nonlinear Problems in Elasticity, pp. 4243-426.
 2. Cialek 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

$$\delta(\det F) = \text{tr}(F^{-T}(\delta F)) \det F = \text{tr}(F^{-T}(\delta F)),$$

where

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

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

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

Thus, we obtain the constraint flow equation

$$\rho_0 \dot{\mathbf{x}} = \nabla_X \cdot (P - pF^{-T}).$$

Here, the divergence term in the integration by part is

$$(P - pF^{-T}) \cdot \delta \mathbf{x} \cdot \mathbf{N} = 0,$$

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

$$\begin{cases} \rho_0 \dot{\mathbf{v}} &= \nabla_X \cdot (P(F) - pF^{-T}) \\ \dot{F} &= \nabla_X \mathbf{v} \\ \det F &= 1 \end{cases}$$

The unknowns are (F, \mathbf{v}, p) .

Boundary conditions for incompressible elasticity The natural boundary condition is to have

$$(P - pF^{-1}) \cdot \mathbf{N} \cdot \delta \mathbf{x} = 0.$$

This leads to

$$\text{either } (P - pF^{-1}) \cdot \mathbf{N} = 0, \quad \text{or} \quad \delta \mathbf{x} = 0, \quad X \in \partial\Omega_0 = \Gamma_0.$$

Thus, we can decompose the boundary into two parts: $\Gamma_0 = \Gamma_0^n \cup \Gamma_0^d$. The boundary conditions are

$$(P - pF^{-1}) \cdot \mathbf{N} = 0 \quad \text{on } \Gamma_0^n,$$

and

$$\mathbf{v} \cdot \mathbf{N} = 0 \quad \text{on } \Gamma_0^d.$$

9.3 Eulerian formulation for simple elasticity

9.3.1 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):

$$\partial_t \mathcal{U} + \nabla_{\mathbf{x}} \cdot \mathcal{F} = \mathcal{R} \tag{9.16}$$

$$\frac{d}{dt} \mathcal{W} + \nabla_X \cdot \mathcal{G} = \mathcal{R}J. \tag{9.17}$$

where

$$\mathcal{U} = \begin{bmatrix} \rho \\ \rho \mathbf{v} \end{bmatrix}, \quad \mathcal{F} = \begin{bmatrix} \rho \mathbf{v} \\ \rho \mathbf{v} \mathbf{v} - \boldsymbol{\sigma} \end{bmatrix}, \quad \mathcal{R} = \begin{bmatrix} 0 \\ \mathbf{f} \end{bmatrix}$$

$$\mathcal{W} = \mathcal{U}J, \quad \mathcal{G} := (\mathcal{F} - \mathcal{U}\mathbf{v}) \cdot JF^{-T}. \tag{9.18}$$

Here, the Cauchy stress

$$\boldsymbol{\sigma}(F) = J^{-1} \frac{\partial W}{\partial F} \cdot F^T,$$

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:

$$\dot{F}_\alpha^i(t, X) = \frac{\partial v^i}{\partial X^\alpha}.$$

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

$$\boxed{\partial_t F + \mathbf{v} \cdot \nabla_{\mathbf{x}} F = (\nabla_{\mathbf{x}} \mathbf{v}) F \quad \text{for } \mathbf{x} \in \Omega_t} \quad (9.19)$$

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

$$\boxed{\begin{aligned} \partial_t \rho + \nabla \cdot (\rho \mathbf{v}) &= 0 \\ \rho (\partial_t \mathbf{v} + \mathbf{v} \cdot \nabla \mathbf{v}) &= \nabla \cdot \boldsymbol{\sigma} + \mathbf{f} \\ \partial_t F + \mathbf{v} \cdot \nabla F &= (\nabla \mathbf{v}) F \end{aligned}} \quad \text{in } \Omega_t. \quad (9.20)$$

The unknowns for this system are ρ, \mathbf{v}, F . The Cauchy stress is given by a constitutive relation

$$\boldsymbol{\sigma} = T(F).$$

The function \mathbf{f} is an external force. We also need the density constraint $\rho \det(F) = \rho_0$ as a compatibility condition.

Conservation form The advection equation for F is equivalent to

$$\partial_t (\rho F_{\alpha}^i) + \partial_k (\rho v^k F_{\alpha}^i - \rho v^i F_{\alpha}^k) = 0.$$

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

$$\rho(t, \mathbf{x}(t, X))J(t, X) = \rho_0(X) \quad (9.21)$$

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: $\boldsymbol{\sigma}(\mathbf{x}) \cdot \mathbf{v} = \mathbf{g}(F^{-1}(t, \mathbf{x}))$ 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 $(\partial_t + v\partial_x)F = -\frac{\sqrt{x^2-t}}{2x^3}$.

9.3.2 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

$$\begin{aligned} \frac{d}{dt} |_X (F^{-1}) &= -F^{-1} \dot{F} (F^{-1}) \\ &= -F^{-1} (\nabla_{\mathbf{x}} \mathbf{v}) F (F^{-1}) \\ &= -(F^{-1}) (\nabla_{\mathbf{x}} \mathbf{v}). \end{aligned}$$

$$\frac{d}{dt} (F^{-1})_i^\alpha = (F^{-1})_k^\alpha L_i^k, \quad L_i^k := \frac{\partial v^k}{\partial x^i}.$$

In the Eulerian coordinate, we have

$$\partial_t (F^{-1}) + \mathbf{v} \cdot \nabla_{\mathbf{x}} (F^{-1}) = -(F^{-1}) (\nabla_{\mathbf{x}} \mathbf{v})^T. \quad (9.22)$$

The compatibility condition for F^{-1} is just

$$\nabla_{\mathbf{x}} \times F^{-T} = 0, \quad \frac{\partial}{\partial x_j} (F^{-T})^i_{\alpha} = \frac{\partial}{\partial x^i} (F^{-T})^j_{\alpha}. \quad (9.23)$$

The advection equation for F^{-1} can be written in conservation form:

$$\partial_t (F^{-1})^{\alpha}_i + \partial_{x^i} ((F^{-1})^{\alpha}_j v^j) = 0. \quad (9.24)$$

This follows from (9.22) and (9.23):

$$\begin{aligned} \partial_t (F^{-1})^{\alpha}_i + \partial_{x^i} ((F^{-1})^{\alpha}_j v^j) &= \partial_t (F^{-1})^{\alpha}_i + v^j \partial_{x^j} (F^{-1})^{\alpha}_i - v^j \partial_{x^j} (F^{-1})^{\alpha}_i + \partial_{x^i} ((F^{-1})^{\alpha}_j v^j) \\ &= -(F^{-1})^{\alpha}_j \partial_{x^i} v^j - v^j \partial_{x^j} (F^{-1})^{\alpha}_i + \partial_{x^i} ((F^{-1})^{\alpha}_j v^j) = v^j (-\partial_{x^j} (F^{-1})^{\alpha}_i + \partial_{x^i} (F^{-1})^{\alpha}_j) = 0. \end{aligned}$$

Thus, the full set of equations are

$$\begin{cases} \partial_t \rho + \partial_{x^j} (v^j \rho) = 0 \\ \partial_t (\rho v^i) + \partial_{x^j} (\rho v^i v^j) = \partial_{x^j} \sigma^{ij} + f^i \\ \partial_t (F^{-1})^{\alpha}_k + \partial_{x^k} ((F^{-1})^{\alpha}_j v^j) = 0. \end{cases} \quad (9.25)$$

Plus the density constraint: $\rho J = \rho_0$ and the compatibility condition

$$\nabla_{\mathbf{x}} \times F^{-T} = 0. \quad (9.26)$$

There are $1 + 9 + 3 = 13$ unknowns and equations.

Boundary conditions in Euler coordinate

- Dirichlet: $\mathbf{v}(t, \mathbf{x}) = 0$ for $\mathbf{x} \in \Gamma_t^d$;
- Neumann: $\boldsymbol{\sigma}(\mathbf{x}) \cdot \boldsymbol{\nu} = \mathbf{g}(F^{-1}(t, \mathbf{x}))$ for $\mathbf{x} \in \Gamma_t^n$.

Remarks ⁴

- 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 (9.24) preserves the property $\nabla_{\mathbf{x}} \times (F^{-1}) = 0$.

⁴References:

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)

9.3.3 Formulation of compressible simple elasticity in terms of $B := FF^T$

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 addition, C should satisfy the compatibility condition.

Thus, the equations are

$$\begin{array}{l} \partial_t \rho + \nabla \cdot (\rho \mathbf{v}) = 0 \\ \rho (\partial_t \mathbf{v} + \mathbf{v} \cdot \nabla \mathbf{v}) = \nabla \cdot \sigma + \mathbf{f} \\ \partial_t B + \mathbf{v} \cdot \nabla B = (\nabla \mathbf{v})B + B(\nabla \mathbf{v})^T \end{array} \quad \text{in } \Omega_t. \quad (9.27)$$

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 10.9. 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].

9.3.4 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, $\dot{\mathbf{x}}(t, X) = \mathbf{v}(t, \mathbf{x}(t, X))$, then the incompressibility of $\mathbf{x}(t, X)$ is equivalent to $\nabla \cdot \mathbf{v}(t, \mathbf{x}) = 0$. This comes from the following formula

$$\delta \det(A) = \text{tr}((\delta A)A^{-T}) \det(A).$$

and the formula

$$\frac{\partial \dot{\mathbf{x}}}{\partial X} = (\nabla \mathbf{v}) \frac{\partial \mathbf{x}}{\partial X},$$

we get

$$\dot{J} = \text{tr}(\dot{F}F^{-T})J = \text{tr}(\nabla \mathbf{v})J = (\nabla \cdot \mathbf{v})J.$$

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 $\delta \mathbf{x}(t, X) := \left. \frac{\partial}{\partial \varepsilon} \right|_{\varepsilon=0} \mathbf{x}_\varepsilon(t, X)$. Let $\mathbf{w}(t, \mathbf{x}(t, X)) = \delta \mathbf{x}(t, X)$. Let $F_\varepsilon = \partial \mathbf{x}_\varepsilon / \partial X$. $\delta F := \left. \frac{\partial}{\partial \varepsilon} \right|_{\varepsilon=0} F_\varepsilon$. Then

$$\delta F = (\nabla \mathbf{w})F.$$

Similarly,

$$\delta J = (\nabla \cdot \mathbf{w})J.$$

Thus, the volume preserving of \mathbf{x}_ε 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

$$\begin{aligned} 0 &= \int_{t_0}^{t_1} \int (-\rho \frac{D\mathbf{v}}{Dt} + \nabla \cdot \boldsymbol{\sigma}) \cdot \mathbf{w} + p(\nabla \cdot \mathbf{w}) dx dt \\ &= \int_{t_0}^{t_1} \int (-\rho \frac{D\mathbf{v}}{Dt} + \nabla \cdot \boldsymbol{\sigma} - \nabla p) \cdot \mathbf{w} dx dt \end{aligned}$$

This gives

$$\rho \frac{D\mathbf{v}}{Dt} + \nabla p = \nabla \cdot \boldsymbol{\sigma}.$$

Here, $\boldsymbol{\sigma}(F) = W'(F)F^T$. 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

$$\left\{ \begin{array}{l} \frac{D\rho}{Dt} = 0 \\ \nabla \cdot \mathbf{v} = 0 \\ \rho \frac{D\mathbf{v}}{Dt} = -\nabla p + \nabla \cdot \boldsymbol{\sigma}(F) \\ \frac{DF}{Dt} = (\nabla \mathbf{v})F. \end{array} \right.$$

9.4. ADVECTION EQUATIONS AND THE COMPATIBILITY CONDITIONS FOR OTHER TYPES OF STRAINS

with the constitutive equation $\sigma(F) = J^{-1}W'(F)F^T$ and the density constraint $\rho J = \rho_0$. The unknowns are (ρ, p, \mathbf{v}, F) . We notice that these equations can be written in conservation form

$$\begin{cases} \partial_t \rho + \nabla \cdot (\rho \mathbf{v}) = 0 \\ \nabla \cdot \mathbf{v} = 0 \\ \partial_t (\rho \mathbf{v}) + \nabla \cdot (\rho \mathbf{v} \mathbf{v}) = -\nabla p + \nabla \cdot \sigma(F) \\ \partial_t F + \mathbf{v} \cdot \nabla F = (\nabla \mathbf{v})F. \end{cases}$$

9.4 Advection equations and the compatibility conditions for other types of strains

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.

9.4.1 Advection equations for the deformation tensors

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

$$\frac{d}{dt} F^{-1} = -F^{-1} \dot{F} F^{-1} = -F^{-1} L F F^{-1} = -F^{-1} L.$$

3. For the right Cauchy-Green tensor,

$$\dot{C} = \frac{d}{dt} (F^T F) = \dot{F}^T F + F^T \dot{F} = F^T L^T F + F^T L F = F^T L^T F^{-T} F^T F + F^T F F^{-1} L F = R^T C + C R,$$

where $R = F^{-1} L F$.

4. For the left Cauchy-Green tensor,

$$\dot{B} = \frac{d}{dt} (F F^T) = \dot{F} F^T + F \dot{F}^T = L F F^T + F F^T L^T = L B + B L^T.$$

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. Since B is symmetric, we can also decompose L into symmetric part and antisymmetric part:

$$L = D + \Omega, \quad D = \frac{1}{2}(\nabla \mathbf{v} + (\nabla \mathbf{v})^T), \quad \Omega = \frac{1}{2}((\nabla \mathbf{v})^T - \nabla \mathbf{v}).$$

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

$$\frac{d}{dt}C^{-1} = -C^{-1}\dot{C}C^{-1} = -C^{-1}(CR + R^TC)C^{-1} = -RC^{-1} - C^{-1}R^T.$$

7. For B^{-1} , we have

$$\frac{d}{dt}B^{-1} = -B^{-1}\dot{B}B^{-1} = -B^{-1}(LB + BL^T)B^{-1} = -B^{-1}L - L^TB^{-1}.$$

9.4.2 Compatibility condition for the deformation gradients

- For $F_\alpha^i := \frac{\partial x^i}{\partial X^\alpha}$, we have

$$\frac{\partial F_\alpha^i}{\partial X^\beta} = \frac{\partial^2 x^i}{\partial X^\beta \partial X^\alpha} = \frac{\partial^2 x^i}{\partial X^\alpha \partial X^\beta} = \frac{\partial F_\beta^i}{\partial X^\alpha}.$$

This is called the compatibility condition for F . Sometimes, we write it as

$$\nabla_X \times F^T = 0.$$

- For $(F^{-1})_i^\alpha = \frac{\partial X^\alpha}{\partial x^i}$, the corresponding compatibility condition reads

$$\frac{\partial (F^{-1})_i^\alpha}{\partial x^j} = \frac{\partial (F^{-1})_i^\alpha}{\partial x^i}.$$

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

$$\Gamma_{\alpha\gamma\beta} = \frac{1}{2} (\partial_\beta C_{\alpha\gamma} - \partial_\alpha C_{\beta\gamma} - \partial_\gamma C_{\alpha\beta}), \quad \Gamma_{\alpha\beta}^\gamma = (C^{-1})_{\gamma\delta} \Gamma_{\alpha\delta\beta}.$$

And the corresponding compatibility condition for C reads

$$\partial_\delta \Gamma_{\alpha\gamma}^\beta - \partial_\gamma \Gamma_{\alpha\delta}^\beta + \Gamma_{\alpha\gamma}^\tau \Gamma_{\tau\delta}^\beta - \Gamma_{\alpha\delta}^\tau \Gamma_{\tau\gamma}^\beta = 0.$$

The above expression states that the Riemann-Christoffel curvature tensor is zero. See [Cialet, pp. 55], [Antman pp. 423-426].

- We should also derive the compatibility condition for $B = FF^T$.

9.5 Hyperbolicity

9.5.1 Hyperbolicity for simple elasticity in Lagrangian coordinate

The equation of motion for simple elasticity reads

$$\rho_0 \ddot{\mathbf{x}} = \nabla_X \cdot P, \quad P = \frac{\partial W}{\partial F}. \quad (9.28)$$

Let

$$a_{ijkl}(F) := \frac{\partial^2 W(F)}{\partial F_j^i \partial F_l^k}.$$

For stability purpose, we usually consider a linearized equation where the coefficient $a_{ijkl}(F_0)$ is frozen at a particular F_0 . In this case, the linearized equation reads

$$\rho_0 \ddot{x}^i = \sum_{j,k,l=1}^3 a_{ijkl}(F_0) \frac{\partial^2 x^k}{\partial X^j \partial X^l}. \quad (9.29)$$

We look for plane wave solution of the form $\mathbf{x}(t, X) = \xi e^{i(X \cdot \eta - \lambda t)}$. It means that, given a direction η , we look for a plane wave with speed $\lambda(\eta)$ and amplitude $\xi(\eta)$. Plug this expression into the linearized equation, we get

$$\rho_0 \lambda^2 \xi_i = \sum_{j,k,l=1}^3 a_{ijkl} \xi_k \eta_j \eta_l = \sum_{k=1}^3 \left(\sum_{j,l=1}^3 a_{ijkl} \eta_j \eta_l \right) \xi_k,$$

or in matrix form

$$A(\eta) \xi = \rho_0 \lambda^2 \xi, \quad A(\eta)_{ik} := \left(\sum_{j,l=1}^3 a_{ijkl} \eta_j \eta_l \right)_{3 \times 3}$$

Thus, equation (9.29) supports plane wave solution in direction η if $A(\eta)$ has positive eigenvalue $\rho_0 \lambda^2$ with eigenvector ξ .

Proposition 9.6. *Given a stored energy $W(F)$, define $a_{ijkl} = \frac{\partial^2 W}{\partial F_j^i \partial F_l^k}$. Then for any $\eta \in \mathbb{R}^3$, the matrix $A(\eta) := (\sum_{j,l} a_{ijkl} \eta_j \eta_l)_{ik}$ is symmetric.*

Proof. This is due to

$$A(\eta)_{ik} = \sum_{j,l=1}^3 a_{ijkl} \eta_j \eta_l = \sum_{j,l=1}^3 a_{ijkl} \eta_l \eta_j = \sum_{j,l=1}^3 a_{ilkj} \eta_j \eta_l = \sum_{j,l=1}^3 a_{kjil} \eta_j \eta_l = A(\eta)_{ki}. \quad (9.30)$$

Here, the 2nd equality is due to $\eta_j \eta_l = \eta_l \eta_j$. The 3rd equality is a change of indices. The 4th equality uses $a_{ilkj} = a_{kjil}$, which is resulted in hyper-elasticity assumption:

$$\frac{\partial^2 W}{\partial F_l^i \partial F_j^k} = \frac{\partial^2 W}{\partial F_l^k \partial F_j^i}.$$

□

To support plane wave solutions, we need $A(\eta)$ to be positive definite for $\eta \neq 0$. This means

$$\sum_{i,j,k,l=1}^3 a_{ijkl} \xi_i \xi_k \eta_j \eta_l > 0, \text{ for all } \eta, \xi \neq 0. \quad (9.31)$$

This condition is called the *strong ellipticity condition* for the 4-tensor a_{ijkl} .

Definition 9.4. *System (9.28) is called hyperbolic if*

$$\frac{\partial^2 W(F)}{\partial F_\alpha^i \partial F_\beta^j} \xi_i \xi_j \eta^\alpha \eta^\beta > 0, \text{ for every } F \in \mathbb{M}_3^+, \xi \neq 0, \eta \neq 0. \quad (9.32)$$

9.5.2 Hyperbolicity for the first-order system in Lagrangian coordinate

Equation of motion in Lagrangian coordinate We study the system of simple elasticity

$$\dot{F}_{kl} - \frac{\partial v^k}{\partial X^l} = 0, \quad k, l = 1, 2, 3, \quad (9.33)$$

$$\rho_0 \dot{v}^i - \sum_{j=1}^3 \frac{\partial P_{ij}}{\partial X^j} = 0, \quad i = 1, 2, 3. \quad (9.34)$$

where the first Piola stress P is given by

$$P_{ij} = \frac{\partial W}{\partial F_{ij}}, \quad i, j = 1, 2, 3. \quad (9.35)$$

for some potential function $W(F)$, and the deformation gradient F satisfies the compatibility condition

$$\frac{\partial F_{ij}}{\partial X^l} = \frac{\partial F_{il}}{\partial X^j}.$$

There are 12 equations with 12 unknowns are (F, \mathbf{v}) . The compatibility condition is satisfied automatically for $t > 0$ if it is satisfied at $t = 0$. Writing these equations in vector form, they are

$$\boxed{\begin{aligned} \dot{F} &= \frac{\partial \mathbf{v}}{\partial X} \\ \rho_0 \dot{\mathbf{v}} &= \nabla_X \cdot P(F). \end{aligned}} \quad (9.36)$$

The compatibility condition reads

$$\nabla \times F^T = 0. \quad (9.37)$$

Let us take $\rho_0 \equiv 1$ for simplicity. It is not hard to put them back in the theory below.

Hyperbolicity and characteristic modes The system can be rewritten in the following conservation form

$$\partial_t \mathcal{W} + \sum_{j=1}^3 \partial_{X^j} \mathcal{G}_j = 0,$$

where

$$\mathcal{W} = \begin{bmatrix} F_{11} \\ F_{21} \\ F_{31} \\ F_{12} \\ F_{22} \\ F_{32} \\ F_{13} \\ F_{23} \\ F_{33} \\ v^1 \\ v^2 \\ v^3 \end{bmatrix}, \quad \mathcal{G}_1 = - \begin{bmatrix} v^1 \\ v^2 \\ v^3 \\ 0 \\ 0 \\ 0 \\ 0 \\ 0 \\ 0 \\ P_{11} \\ P_{21} \\ P_{31} \end{bmatrix}, \quad \mathcal{G}_2 = - \begin{bmatrix} 0 \\ 0 \\ 0 \\ v^1 \\ v^2 \\ v^3 \\ 0 \\ 0 \\ 0 \\ P_{12} \\ P_{22} \\ P_{32} \end{bmatrix}, \quad \mathcal{G}_3 = - \begin{bmatrix} 0 \\ 0 \\ 0 \\ 0 \\ 0 \\ 0 \\ v^1 \\ v^2 \\ v^3 \\ P_{13} \\ P_{23} \\ P_{33} \end{bmatrix}$$

This system can be written as a quasi-linear form

$$\partial_t \mathcal{W} + \sum_{j=1}^3 \mathcal{B}_j \partial_{X^j} \mathcal{W} = 0, \quad \mathcal{B}_j = \frac{\partial \mathcal{G}_j}{\partial \mathcal{W}}.$$

The matrix \mathcal{B}_j has the form

$$\mathcal{B}_j = - \begin{bmatrix} \mathbf{0}_{9 \times 9} & E_{j9 \times 3} \\ A_{j3 \times 9} & \mathbf{0}_{3 \times 3} \end{bmatrix}$$

where

$$E_1 = \begin{bmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 1 \\ 0 & 0 & 0 \\ 0 & 0 & 0 \\ 0 & 0 & 0 \\ 0 & 0 & 0 \\ 0 & 0 & 0 \\ 0 & 0 & 0 \end{bmatrix}, \quad E_2 = \begin{bmatrix} 0 & 0 & 0 \\ 0 & 0 & 0 \\ 0 & 0 & 0 \\ 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 1 \\ 0 & 0 & 0 \\ 0 & 0 & 0 \\ 0 & 0 & 0 \end{bmatrix}, \quad E_3 = \begin{bmatrix} 0 & 0 & 0 \\ 0 & 0 & 0 \\ 0 & 0 & 0 \\ 0 & 0 & 0 \\ 0 & 0 & 0 \\ 0 & 0 & 0 \\ 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 1 \end{bmatrix},$$

$$A_j = \begin{bmatrix} a_{1j11} & a_{1j12} & \cdots & a_{1j33} \\ a_{2j11} & a_{2j12} & \cdots & a_{2j33} \\ a_{3j11} & a_{3j12} & \cdots & a_{3j33} \end{bmatrix}_{3 \times 9}, \quad a_{ijkl} := \frac{\partial P_{ij}}{\partial F_{kl}} = \frac{\partial^2 W(F)}{\partial F_{kl} \partial F_{ij}}.$$

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

$$\Lambda(\mathcal{W}, \eta) := \sum_{j=1}^3 \mathcal{B}_j \eta_j$$

and

$$\Lambda(\mathcal{W}, \eta) = - \begin{bmatrix} 0 & 0 & 0 & \eta & 0 & 0 \\ 0 & 0 & 0 & 0 & \eta & 0 \\ 0 & 0 & 0 & 0 & 0 & \eta \\ \mathbf{b}_{11} & \mathbf{b}_{12} & \mathbf{b}_{13} & 0 & 0 & 0 \\ \mathbf{b}_{21} & \mathbf{b}_{22} & \mathbf{b}_{23} & 0 & 0 & 0 \\ \mathbf{b}_{31} & \mathbf{b}_{32} & \mathbf{b}_{33} & 0 & 0 & 0 \end{bmatrix}_{12 \times 12} := - \begin{bmatrix} \mathbf{0}_{9 \times 9} & C_{9 \times 3} \\ \mathbf{B}_{3 \times 9} & \mathbf{0}_{3 \times 3} \end{bmatrix},$$

$$\eta = \begin{bmatrix} \eta_1 \\ \eta_2 \\ \eta_3 \end{bmatrix}_{3 \times 1}, \quad \mathbf{b}_{ik}(\eta) = [\sum_j a_{ijk1} \eta_j \quad \sum_j a_{ijk2} \eta_j \quad \sum_j a_{ijk3} \eta_j]_{1 \times 3}$$

The characteristic equation of the matrix $\Lambda(\mathcal{W}, \eta)$ is:

$$\det(\lambda - \Lambda(\mathcal{W}, \eta)) = \det \begin{bmatrix} \lambda I_{9 \times 9} & C_{9 \times 3} \\ B_{3 \times 9} & \lambda I_{3 \times 3} \end{bmatrix} = \det \begin{bmatrix} \lambda I_{9 \times 9} & C_{9 \times 3} \\ 0_{3 \times 9} & -\frac{1}{\lambda} B_{3 \times 9} C_{9 \times 3} + \lambda I_{3 \times 3} \end{bmatrix}$$

$$\lambda^9 \det \left(\lambda \delta_{ik} - \frac{1}{\lambda} \sum_{j,l=1}^3 a_{ijkl} \eta_j \eta_l \right) = \lambda^6 \det(\lambda^2 I - A(\eta)) = 0.$$

Strong ellipticity and hyperbolicity

- There are 6 eigenvalues of $\Lambda(\mathcal{W}, \eta)$ which are 0
- The rest 6 eigenvalues are real provided $(A(\eta))$ is positive definite.

Note that the 3×3 matrix

$$A(\eta)_{ik} := \sum_{j,l=1}^3 a_{ijkl} \eta_j \eta_l$$

is symmetric due to

$$a_{ijkl}(F) := \frac{\partial^2 W(F)}{\partial F_{ij} \partial F_{kl}} = \frac{\partial^2 W(F)}{\partial F_{kl} \partial F_{ij}} = a_{klij}.$$

The strong ellipticity assumption for (a_{ijkl}) 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:

$$\begin{bmatrix} 0 & 0 & 0 & \eta & 0 & 0 \\ 0 & 0 & 0 & 0 & \eta & 0 \\ 0 & 0 & 0 & 0 & 0 & \eta \\ \mathbf{b}_{11} & \mathbf{b}_{12} & \mathbf{b}_{13} & 0 & 0 & 0 \\ \mathbf{b}_{21} & \mathbf{b}_{22} & \mathbf{b}_{23} & 0 & 0 & 0 \\ \mathbf{b}_{31} & \mathbf{b}_{32} & \mathbf{b}_{33} & 0 & 0 & 0 \end{bmatrix} \begin{bmatrix} \zeta_1 \\ \zeta_2 \\ \zeta_3 \\ \xi_1 \\ \xi_2 \\ \xi_3 \end{bmatrix} = 0, \quad \text{where } \zeta_i = \begin{bmatrix} \zeta_{i1} \\ \zeta_{i2} \\ \zeta_{i3} \end{bmatrix}, i = 1, 2, 3.$$

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_{ijkl}) . 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 $\eta = (1, 0, 0)^T$,

$$\mathbf{b}_{ik} = [a_{i1k1} \ a_{i1k2} \ a_{i1k3}], \quad i, k = 1, 2, 3. \quad (9.38)$$

The last three equations for ζ_i , $i = 1, 2, 3$ read

$$\sum_{k=1}^3 b_{ik} \zeta_k = 0, \quad i = 1, 2, 3. \quad (9.39)$$

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 (9.39) to find the corresponding ζ_1 . This gives 6 eigenvectors corresponding to the zero eigenvalue.

Eigenvectors corresponding to nonzero eigenvalues We solve the eigen system

$$\begin{bmatrix} \lambda I & 0 & 0 & \eta & 0 & 0 \\ 0 & \lambda I & 0 & 0 & \eta & 0 \\ 0 & 0 & \lambda I & 0 & 0 & \eta \\ \mathbf{b}_{11} & \mathbf{b}_{12} & \mathbf{b}_{13} & \lambda & 0 & 0 \\ \mathbf{b}_{21} & \mathbf{b}_{22} & \mathbf{b}_{23} & 0 & \lambda & 0 \\ \mathbf{b}_{31} & \mathbf{b}_{32} & \mathbf{b}_{33} & 0 & 0 & \lambda \end{bmatrix} \begin{bmatrix} \zeta_1 \\ \zeta_2 \\ \zeta_3 \\ \xi_1 \\ \xi_2 \\ \xi_3 \end{bmatrix} = 0, \quad (9.40)$$

with $\lambda \neq 0$. The first 9 equations give

$$\zeta_k = -\frac{\xi_k}{\lambda} \eta \quad (9.41)$$

Plug into the last three equations. Then from (9.38), the last three equations read

$$\sum_{k=1}^3 \sum_{l=1}^3 \left(\sum_{j=1}^3 a_{ijkl} \eta_j \right) \left(-\frac{\xi_k}{\lambda} \eta_l \right) + \lambda \xi_i = 0, \quad i = 1, 2, 3.$$

This shows (λ^2, ξ) are eigen pair of the matrix

$$A(\eta) = \sum_{j,l=1}^3 a_{ijkl} \eta_j \eta_l.$$

Note that A is positive definite from strong ellipticity of (a_{ijkl}) . Thus, the eigenvalues of A are positive. We thus get $\pm\lambda$ are the eigenvalues of (9.40). The corresponding eigenvectors of (9.40) are also obtained from the eigenvectors of A and (9.41).

Definition 9.5. *System (9.28) is called hyperbolic if*

$$\frac{\partial^2 W(F)}{\partial F_\alpha^i \partial F_\beta^j} \xi_i \xi_j \eta^\alpha \eta^\beta > 0, \quad \text{for every } F \in \mathbb{M}_3^+, \xi \neq 0, \eta \neq 0. \quad (9.42)$$

This hyperbolicity condition is a basic requirement for the restored energy W for the well-posedness of system (9.28).

9.5.3 Hyperbolicity for first-order system in Eulerian formulation

Let us denote

$$G_{\alpha i} = (F^{-1})_i^\alpha.$$

The system can be rewritten in the following conservation form

$$\partial_t \mathcal{U} + \sum_{j=1}^3 \partial_{x_j} \mathcal{F}_j = 0,$$

where

$$\mathcal{U} = \begin{bmatrix} G_{11} \\ G_{21} \\ G_{31} \\ G_{12} \\ G_{22} \\ G_{32} \\ G_{13} \\ G_{23} \\ G_{33} \\ \rho v^1 \\ \rho v^2 \\ \rho v^3 \\ \rho \end{bmatrix}, \quad \mathcal{F}_1 = \begin{bmatrix} G_{11}v^1 \\ G_{12}v^2 \\ G_{13}v^3 \\ 0 \\ 0 \\ 0 \\ 0 \\ 0 \\ 0 \\ \rho v^1 v^1 - \sigma_{11} \\ \rho v^1 v^2 - \sigma_{21} \\ \rho v^1 v^3 - \sigma_{31} \\ \rho v^1 \end{bmatrix}, \quad \mathcal{F}_2 = \begin{bmatrix} 0 \\ 0 \\ 0 \\ G_{21}v^1 \\ G_{22}v^2 \\ G_{23}v^3 \\ 0 \\ 0 \\ 0 \\ \rho v^2 v^1 - \sigma_{12} \\ \rho v^2 v^2 - \sigma_{22} \\ \rho v^2 v^3 - \sigma_{32} \\ \rho v^2 \end{bmatrix}, \quad \mathcal{F}_3 = \begin{bmatrix} 0 \\ 0 \\ 0 \\ 0 \\ 0 \\ 0 \\ G_{31}v^1 \\ G_{32}v^2 \\ G_{33}v^3 \\ \rho v^3 v^1 - \sigma_{13} \\ \rho v^3 v^2 - \sigma_{23} \\ \rho v^3 v^3 - \sigma_{33} \\ \rho v^3 \end{bmatrix}$$

TOBE CONTINUED

Chapter 10

Stress-Strain relation for Elasticity

10.1 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. $\{F(s)|s \leq t\}$). 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** *are materials whose mechanical stresses are conservative.* This means that the work done by the stress through a closed-loop deformation is zero. Thus, the definition of conservative mechanical stress is equivalent to: *there exists a mechanical potential function $W(F)$ such that the Piola stress is $P = W'(F)$.*

We shall mainly focus on hyper-elastic materials.

Below, we shall characterize the response functions of Cauchy-elastic materials and hyper-elastic materials. The basic property the response should satisfy is the frame-indifference property.

10.1.1 Frame indifference

1. **Frame-indifference property for Cauchy stress** *The response function $T(F)$ should satisfy*

$$\boxed{T(OF) = OT(F)O^T \text{ for any rotation } O \in O(3).} \quad (10.1)$$

This is also called the *axiom of material frame-indifference*. The reason is the following. 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 $\mathbf{v}^* = Ov$, $\mathbf{t}^* = Ot$. In terms of the response function, it reads

$$\begin{aligned} \mathbf{t}^* &= T(OF)\mathbf{v}^* = T(OF)Ov \\ Ot &= OT(F)v. \end{aligned}$$

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,

$$P(OF) = OP(F) \text{ for any rotation } O \in O(3). \quad (10.2)$$

2. **Frame indifference for hyper-elastic materials** means that the potential energy W remains the same when we change to a new frame through rotation. That is

$$\boxed{W(OF) = W(F) \text{ for any rotation } O \in O(3).} \quad (10.3)$$

This definition is equivalent to the above definition. Indeed, we differentiate $P(F) = \frac{\partial W}{\partial F}(F)$ in F to get

$$P(F) = \frac{\partial}{\partial F} W(F) \stackrel{?}{=} \frac{\partial}{\partial F} W(OF) = O^T \frac{\partial W(OF)}{\partial(OF)} = O^T P(OF).$$

Thus, $P(OF) = OP(F)$ if and only if $\frac{\partial}{\partial F} (W(OF) - W(F)) = 0$.

10.1.2 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

$$\boxed{T(FO) = T(F)}. \quad (10.4)$$

This isotropic property can be expressed in terms of the Piola stress as the follows.

$$P(FO) = P(F)O \quad \text{for all rotation } O. \quad (10.5)$$

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

$$\boxed{W(FO) = W(F) \text{ for all } O \in O(3)}. \quad (10.6)$$

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

$$\partial_{F_\alpha^i} W(F_\beta^j O_\gamma^\beta) = W_{F_\gamma^j} \frac{\partial F_\beta^j O_\gamma^\beta}{\partial F_\alpha^i} = P_\gamma^j \delta^{ij} \delta_{\alpha\beta} O_\gamma^\beta = P_\gamma^i O_\gamma^\alpha.$$

Thus, $P(F)O = P(FO)$ is equivalent to $\frac{\partial}{\partial F} (W(FO) - W(F)) = 0$.

10.1.3 Representation of 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 $\lambda_1, \lambda_2, \lambda_3$ of A as below:

$$\iota_1 = \operatorname{tr} A = \lambda_1 + \lambda_2 + \lambda_3 \quad (10.7)$$

$$\iota_2 = \frac{1}{2} ((\operatorname{tr} A)^2 - \operatorname{tr}(A^2)) = \operatorname{tr}(\operatorname{Cof} A) = \lambda_1 \lambda_2 + \lambda_2 \lambda_3 + \lambda_3 \lambda_1 \quad (10.8)$$

$$\iota_3 = \det A = \lambda_1 \lambda_2 \lambda_3. \quad (10.9)$$

The set of these principal invariants of A is denoted by ι_A .

Characterization of response functions

Proposition 10.7. *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 (10.4), we have

$$T(F) = T(S_l O) \stackrel{(10.4)}{=} T(S_l) = \hat{T}(S_l^2) = \hat{T}(B) = \hat{T}(FF^T).$$

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

$$\hat{T}(OBO^T) = \hat{T}(OS_l^2 O^T) = \hat{T}(OS_l(OS_l)^T) = T(OS_l) \stackrel{(10.1)}{=} OT(S_l)O^T = O\hat{T}(B)O^T.$$

□

Representation of isotropic Cauchy stress

Theorem 10.7 (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 10.8 (Rivlin-Ericksen Representation Theorem). *Suppose a function $\hat{T} : \mathbb{S}^3 \rightarrow \mathbb{S}^3$ satisfying*

$$\hat{T}(OQO^T) = O\hat{T}(Q)O^T \quad \text{for all } O \in O(3),$$

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

$$\begin{aligned} I &= p_1p_1^T + p_2p_2^T + p_3p_3^T \\ Q &= \lambda_1p_1p_1^T + \lambda_2p_2p_2^T + \lambda_3p_3p_3^T \\ Q^2 &= \lambda_1^2p_1p_1^T + \lambda_2^2p_2p_2^T + \lambda_3^2p_3p_3^T. \end{aligned}$$

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 $\hat{T}(OQO^T) = O\hat{T}(Q)O^T$, we see that $\hat{T}(Q)$ can be diagonalized by $O = [p_1, p_2, p_3]$. That is

$$\hat{T}(Q) = \mu_1p_1p_1^T + \mu_2p_2p_2^T + \mu_3p_3p_3^T.$$

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

$$\begin{aligned} I &= p_1p_1^T + (p_2p_2^T + p_3p_3^T) \\ Q &= \lambda_1p_1p_1^T + \lambda_2(p_2p_2^T + p_3p_3^T) \end{aligned}$$

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 $\hat{T}(OQO^T) = O\hat{T}(Q)O^T$ and taking $O = [p_1, p_2, p_3]$, we see that O can diagonalize Q as well as $T(Q)$. Since in the subspace spanned by p_2 and p_3 , the matrix B is $\lambda_2 I$, we get $T(Q)$ 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.

10.1.4 Representation of isotropic hyper-elastic stress

The goal of this subsection is to have representation of Cauchy stress in terms of invariants of F . First, we have an important property of the hyper-elastic materials.

Proposition 10.8. *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

$$\begin{aligned}
\sigma_{ij} &= J^{-1} P_{\alpha}^i F_{\alpha}^j = J^{-1} \frac{\partial W}{\partial F_{\alpha}^i} F_{\alpha}^j \\
&= J^{-1} \frac{\partial \check{W}}{\partial C_{\beta\gamma}} \frac{\partial C_{\beta\gamma}}{\partial F_{\alpha}^i} F_{\alpha}^j = J^{-1} \frac{\partial \check{W}}{\partial C_{\beta\gamma}} \frac{\partial (F_{\beta}^k F_{\gamma}^k)}{\partial F_{\alpha}^i} F_{\alpha}^j \\
&= J^{-1} \frac{\partial \check{W}}{\partial C_{\beta\gamma}} \left(\delta^{ik} \delta_{\beta\alpha} F_{\gamma}^k + \delta^{ik} \delta_{\gamma\alpha} F_{\beta}^k \right) F_{\alpha}^j \\
&= J^{-1} \frac{\partial \check{W}}{\partial C_{\beta\gamma}} \left(F_{\gamma}^i F_{\beta}^j + F_{\beta}^i F_{\gamma}^j \right) \\
&= 2J^{-1} \frac{\partial \check{W}}{\partial C_{\beta\gamma}} F_{\gamma}^i F_{\beta}^j \\
&= 2J^{-1} \frac{\partial \check{W}}{\partial C_{\gamma\beta}} F_{\beta}^j F_{\gamma}^i = \sigma_{ji}
\end{aligned}$$

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 10.9. *For isotropic hyper-elastic material, σ can also be represented in terms of B :*

$$\boxed{\sigma = 2J^{-1} \hat{W}_B B.} \quad (10.10)$$

Proof. Recall $B^{k\ell} = F_{\beta}^k F_{\beta}^{\ell}$. We have

$$\begin{aligned}
P_{\alpha}^i &= W_{F_{\alpha}^i} = \frac{\partial \hat{W}(FF^T)}{\partial F_{\alpha}^i} = \hat{W}_{B^{k\ell}} \frac{\partial B^{k\ell}}{\partial F_{\alpha}^i} = \hat{W}_{B^{k\ell}} \frac{\partial F_{\beta}^k F_{\beta}^{\ell}}{\partial F_{\alpha}^i} \\
&= \hat{W}_{B^{k\ell}} \left(\delta^{ik} \delta_{\alpha\beta} F_{\beta}^{\ell} + F_{\beta}^k \delta^{i\ell} \delta_{\alpha\beta} \right) = \hat{W}_{B^{i\ell}} F_{\alpha}^{\ell} + \hat{W}_{B^{ki}} F_{\alpha}^k \\
&= 2\hat{W}_{B^{ik}} F_{\alpha}^k
\end{aligned}$$

Here, we have used symmetries of $B = FF^T$ and \hat{W}_B . Thus,

$$\sigma^{ij} = J^{-1} P_{\alpha}^i F_{\alpha}^j = 2J^{-1} \hat{W}_{B^{ik}} F_{\alpha}^k F_{\alpha}^j = 2J^{-1} \hat{W}_{B^{ik}} B^{kj}.$$

□

Proposition 10.10. *The stored energy $W(F)$ of an isotropic hyper-elastic material satisfies*

$$W(F) = \bar{W}(\mathfrak{I}(FF^T)).$$

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 $\{\mathfrak{I}(F)\}$ and $\{\mathfrak{I}(FF^T)\}$, thus we can express

$$W(F) = \bar{W}(\iota_1(B), \iota_2(B), \iota_3(B)),$$

where $B = FF^T$.

□

Homework Check (11.7).

Theorem 10.9 (Representation of stress). *Let us denote the invariants $\iota_k(B)$ by I_k . The Cauchy stress for an isotropic hyper-elastic material with restoration energy function $\bar{W}(I_1, I_2, I_3)$ is given by*

$$\sigma = \frac{2}{\sqrt{I_3}} (I_3 \bar{W}_{I_3} I + (\bar{W}_{I_1} + I_1 \bar{W}_{I_2}) B - \bar{W}_{I_2} B^2) \quad (10.11)$$

Another Finger's formula is

$$\sigma = \frac{2}{\sqrt{I_3}} ((I_2 \bar{W}_{I_2} + I_3 \bar{W}_{I_3}) I + \bar{W}_{I_1} B - I_3 \bar{W}_{I_2} B^{-1}). \quad (10.12)$$

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 .

$$\begin{aligned} \sigma &= 2J^{-1} \hat{W}_B B \\ &= 2J^{-1} [(\bar{W}_{I_1} + I_1 \bar{W}_{I_2}) I - \bar{W}_{I_2} B + I_3 \bar{W}_{I_3} B^{-1}] B \\ &= 2J^{-1} [I_3 \bar{W}_{I_3} I + (\bar{W}_{I_1} + I_1 \bar{W}_{I_2}) B - \bar{W}_{I_2} B^2] \end{aligned}$$

3. $J = \sqrt{I_3}$ because $I_3 = \det(FF^T) = J^2$.

4. The first Finger's formula can be obtained by the second Finger's formula and the Caley-Hamilton formula

$$\iota_3 B^{-1} = B^2 - \iota_1 B + \iota_2 I.$$

□

Proposition 10.11 (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*

$$\begin{aligned} W_Q &= [W_{\iota_1} + \iota_1(Q)W_{\iota_2} + \iota_2(Q)W_{\iota_3}]I \\ &\quad - [W_{\iota_2} + \iota_1(Q)W_{\iota_3}]Q^T + W_{\iota_3}(Q^T)^2. \end{aligned} \quad (10.13)$$

It can also be expressed as

$$W_Q = [W_{\iota_1} + \iota_1(Q)W_{\iota_2}]I - W_{\iota_2}Q^T + \iota_3(Q)W_{\iota_3}Q^{-T}. \quad (10.14)$$

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 $n = 2$.

$$\delta \iota_1(Q^2) = \delta(I:Q^2) = 2I:(Q \cdot \delta Q) = 2Q:\delta Q = 2Q^T:\delta Q^T.$$

4. By direct computation, we get

$$\begin{aligned} \iota_2(Q) &= \frac{1}{2}(\iota_1^2(Q) - \iota_1(Q^2)) \\ \iota_3(Q) &= \frac{1}{3}(\iota_1(Q^3) - \iota_1^3(Q) + 3\iota_1(Q)\iota_2(Q)) \end{aligned}$$

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

$$\begin{aligned} [\iota_3(Q)]_Q &= \iota_2(Q)I - \iota_1(Q)Q^T + (Q^T)^2 \\ &= (\iota_2(Q)Q^T - \iota_1(Q)(Q^T)^2 + (Q^T)^3)(Q^T)^{-1} \\ &= \iota_3(Q)(Q^T)^{-1} \end{aligned}$$

In the last step, the Caley-Hamilton formula:

$$-Q^3 + \iota_1 Q^2 - \iota_2 Q + \iota_3 I = 0,$$

is used. □

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

$$\Sigma = 2(\psi_0(C)C^{-1} + \psi_1(C)I + \psi_2(C)C). \quad (10.15)$$

where

$$\psi_0 = I_3 \bar{W}_{I_3}, \quad \psi_1 = \bar{W}_{I_1} + I_1 \bar{W}_{I_2}, \quad \psi_2 = -\bar{W}_{I_2}. \quad (10.16)$$

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

$$\begin{aligned} \Sigma &= 2 \left(\frac{\psi_0}{I_3} (C^2 - I_1 C + I_2 I) + \psi_1 I + \psi_2 C \right) \\ &= 2 \left(\psi_1 + \frac{\psi_0 I_2}{I_3} \right) I + 2 \left(\psi_2 - \frac{\psi_0 I_1}{I_3} \right) C + 2 \frac{\psi_0}{I_3} C^2 \\ &= 2 (\gamma_0 I + \gamma_1 C + \gamma_2 C^2). \end{aligned} \quad (10.17)$$

The first Piola stress is represented as

$$P = F\Sigma \quad (10.18)$$

with Σ represented by (10.15) or (10.17).

10.1.5 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

¹Cialet V. I, pp. 155

Theorem 10.10. For an isotropic elastic material, by normalizing $\check{\Sigma}(I) = 0$, the second Piola stress tensor has the following representation:

$$\check{\Sigma}(C) = \lambda(\text{tr}E)I + 2\mu E + o(E). \quad (10.19)$$

Here, λ and μ are called the Lamé moduli, $E = \frac{1}{2}(C - I)$. The potential W has the following representation:

$$W(E) = \frac{\lambda}{2}(\text{tr}E)^2 + \mu \text{tr}(E^2) + o(E^2), \quad (10.20)$$

or

$$W(E) = \bar{W}(I_1, I_2, I_3) = \mu(I_1 - 3) + \frac{\lambda + 2\mu}{8}(I_1 - 3)^2 - \frac{\mu}{3}(I_2 - 3) + o(E^2). \quad (10.21)$$

where I_k are invariants of C .

Proof. 1. We want to expand Σ in terms of E . Recall that

$$\Sigma = 2(\psi_0 C^{-1} + \psi_1 I + \psi_2 C).$$

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

$$\begin{aligned} \psi_0 &= I_3 \bar{W}_{I_3} = (1 + 2\text{tr}(E)) \bar{W}_{I_3} + o(E) \\ \psi_1 &= \bar{W}_{I_1} + I_1 \bar{W}_{I_2} = \bar{W}_{I_1} + \bar{W}_{I_2}(3 + 2\text{tr}(E)) + o(E) \\ \psi_2 &= -\bar{W}_{I_2} \end{aligned}$$

where we have used the expansion of invariants I_1, I_2, I_3 in terms of E , which is shown in the next item.

3. Expand the invariants:

$$\begin{aligned} I_1(C) &= \text{tr}C = 3 + 2\text{tr}(E) \\ I_2(C) &= \frac{1}{2}((\text{tr}C)^2 - \text{tr}C^2) = 3 + 4\text{tr}(E) + o(E) \\ I_3(C) &= \frac{1}{6}(\text{tr}C)^3 - \frac{1}{2}\text{tr}C \text{tr}C^2 + \frac{1}{3}\text{tr}C^3 \\ &= 1 + 2\text{tr}(E) + o(E). \end{aligned}$$

Here, we have used

$$\begin{aligned} \text{tr}C &= 3 + 2\text{tr}(E) \\ \text{tr}C^2 &= 3 + 4\text{tr}(E) + o(E) \\ \text{tr}C^3 &= 3 + 6\text{tr}(E) + o(E). \end{aligned}$$

4. Thus,

$$\begin{aligned}\Sigma &= 2 \left((1 + 2\text{tr}(E))\bar{W}_{I_3}(I - 2E) + (\bar{W}_{I_1} + \bar{W}_{I_2}(3 + 2\text{tr}(E)))I - \bar{W}_{I_2}(I + 2E) \right) \\ &= 2 \left[(\bar{W}_{I_1} + 2\bar{W}_{I_2} + \bar{W}_{I_3}) + (\bar{W}_{I_2} + 2\bar{W}_{I_3})\text{tr}(E) \right] I - 4(\bar{W}_{I_2} + \bar{W}_{I_3})E + o(E)\end{aligned}$$

Since $\Sigma(0) = 0$ when there is no strain (i.e. $E = 0$), we get

$$\bar{W}_{I_1} + 2\bar{W}_{I_2} + \bar{W}_{I_3} = 0, \quad (10.22)$$

and

$$\Sigma = \left[2(\bar{W}_{I_2} + 2\bar{W}_{I_3})\text{tr}(E) \right] I - 4(\bar{W}_{I_2} + \bar{W}_{I_3})E + o(E).$$

5. Let us call

$$2(\bar{W}_{I_2} + 2\bar{W}_{I_3}) = \lambda, \quad -2(\bar{W}_{I_2} + \bar{W}_{I_3}) = \mu$$

or

$$\bar{W}_{I_2} = -\frac{\lambda}{2} - \mu, \quad \bar{W}_{I_3} = \frac{\lambda}{2} + \frac{\mu}{2},$$

we then get

$$\Sigma = \lambda(\text{tr}E)I + 2\mu E + o(E).$$

Remark In the linear elasticity theory, we use the infinitesimal strain

$$\mathbf{e} := \frac{1}{2}(\mathbf{u}_X + \mathbf{u}_X^T),$$

which satisfies

$$\mathbf{e} = E + o(E).$$

In the above stress-strain relation for infinitesimal strain, we can replace E by \mathbf{e} . □

10.2 Elastic Models

To establish mathematical models for hyperelastic materials, there are two requirements that the stored energy W should satisfy:

- $W \rightarrow \infty$ as $J \rightarrow 0$,
- 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.

10.2.1 Hyperbolicity for isotropic materials

Below, we want to find the condition on $\bar{W}(I_1, I_2, I_3)$ 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

$$\frac{\partial^2 \bar{W}}{\partial F \partial F}(I_1, I_2, I_3) = \sum_{p=1}^3 \left(\bar{W}_{I_p} \frac{\partial^2 I_p}{\partial F \partial F} + \sum_{q=1}^3 \bar{W}_{I_p I_q} \left(\frac{\partial I_p}{\partial F} \right) \left(\frac{\partial I_q}{\partial F} \right) \right). \quad (10.23)$$

Recall I_p has the following expression: let $C = F^T F$,

- $I_1(C) = \text{Tr}(C)$,
- $I_2(C) = \frac{1}{2} (\text{Tr}(C)^2 - \text{Tr}(C^2))$,
- $I_3(C) = \det(C) = J^2 = \frac{1}{6} (\text{Tr} C)^3 - \frac{1}{2} (\text{Tr} C) (\text{Tr} C^2) + \frac{1}{3} (\text{Tr} C^3)$.
- $J = \det(F)$,

Lemma 10.7. *We have the following formulae for I_p :*

$$\frac{\partial I_1}{\partial F} = 2F, \quad (10.24)$$

$$\frac{\partial I_2}{\partial F_\alpha^i} = 2I_1 F_\alpha^i - 2F_\beta^i F_\beta^k F_\alpha^k, \quad (10.25)$$

$$\frac{\partial I_3}{\partial F_\alpha^i} = 2J^2 (F^{-1})_i^\alpha \quad (10.26)$$

$$\frac{\partial^2 I_1}{\partial F_\alpha^i \partial F_\beta^j} = 2\delta^{ij} \delta_{\alpha\beta}, \quad (10.27)$$

$$\frac{\partial^2 I_2}{\partial F_\beta^j \partial F_\alpha^i} = 2I_1 \delta^{ij} \delta_{\alpha\beta} + 4F_\alpha^i F_\beta^j - 2 \left(\delta^{ij} F_\alpha^k F_\beta^k + \delta_{\alpha\beta} F_\gamma^i F_\gamma^j + F_\beta^i F_\alpha^j \right) \quad (10.28)$$

$$\frac{\partial^2 I_3}{\partial F_\alpha^i \partial F_\beta^j} = 4J^2 (F^{-1})_i^\alpha (F^{-1})_j^\beta - 2J^2 (F^{-1})_j^\alpha (F^{-1})_i^\beta \quad (10.29)$$

Proof. 1. From $I_1(C) = F_\alpha^i F_\alpha^i$, we get $I_{1,F} = 2F$.

2. From $\frac{\partial I_1}{\partial F} = 2F$, we get $\frac{\partial^2 I_1}{\partial F_\alpha^i \partial F_\beta^j} = 2\delta^{ij} \delta_{\alpha\beta}$.

3. $I_{2,F} = I_1 I_{1,F} - \frac{1}{2} \frac{\partial \text{Tr}(C^2)}{\partial C} \frac{\partial C}{\partial F} = 2I_1 F - C(F + F^T) = 2I_1 F - 2CF$.

4. From $I_3 = J^2$, we get $\frac{\partial I_3}{\partial F_\alpha^i} = 2J \frac{\partial J}{\partial F_\alpha^i} = 2J (F^{-1})_i^\alpha$. Here, we have used

$$\frac{\partial J}{\partial F_\alpha^i} = J (F^{-T})_\alpha^i = J (F^{-1})_i^\alpha.$$

We also have

$$\begin{aligned} \frac{\partial^2 I_3}{\partial F_\beta^j \partial F_\alpha^i} &= 4J \cdot J (F^{-1})_j^\beta (F^{-1})_i^\alpha + 2J^2 \frac{\partial (F^{-1})_i^\alpha}{\partial F_\beta^j} \\ &= 4J^2 (F^{-1})_j^\beta (F^{-1})_i^\alpha - 2J^2 (F^{-1})_k^\alpha \frac{\partial F_\gamma^k}{\partial F_\beta^j} (F^{-1})_i^\gamma \\ &= 4J \cdot J (F^{-1})_j^\beta (F^{-1})_i^\alpha - 2J^2 (F^{-1})_j^\alpha (F^{-1})_i^\beta. \end{aligned}$$

□

Separable case Let us assume \bar{W} is separable. This means that

$$\frac{\partial^2 \bar{W}}{\partial I_p \partial I_q} = 0, \text{ if } p \neq q.$$

Effect of I_1 Suppose \bar{W}_1 is only a function of I_1 . We have

$$\frac{\partial^2 \bar{W}_1(I_1)}{\partial F_\beta^j \partial F_\alpha^i} = 2\bar{W}_{1,I_1} \delta^{ij} \delta_{\alpha\beta} + 4\bar{W}_{1,I_1 I_1} F_\alpha^i F_\beta^j. \quad (10.30)$$

The hyperbolicity condition for \bar{W}_1 reads

$$\sum_{i,j,\alpha,\beta} \frac{\partial^2 \bar{W}_1(I_1)}{\partial F_\beta^j \partial F_\alpha^i} \xi^i \xi^j \eta^\alpha \eta^\beta > 0.$$

Using (10.30), this condition is

$$2\bar{W}'_1 |\xi|^2 |\eta|^2 + 4\bar{W}''_1 (\xi^1 + \xi^2 + \xi^3)^2 (\eta^1 + \eta^2 + \eta^3)^2 > 0. \quad (10.31)$$

By choosing $\xi \neq 0$ but $\xi^1 + \xi^2 + \xi^3 = 0$, we see that a necessary condition for (10.31) is

$$\bar{W}'_1 > 0. \quad (10.32)$$

We note that

$$(\xi^1 + \xi^2 + \xi^3)^2 \leq 3|\xi|^2, \quad (\eta^1 + \eta^2 + \eta^3)^2 \leq 3|\eta|^2.$$

Then a necessary and sufficient condition for hyperbolicity (10.31) is

$$\bar{W}'_1 > 0 \quad \text{and} \quad \bar{W}'_1 - 18|\bar{W}''_1| > 0. \quad (10.33)$$

Examples of \bar{W}_1 :

- $\bar{W}_1 = \frac{H}{2}I_1$. $\bar{W}'_1 = \frac{H}{2} > 0$. Thus, this model is hyperbolic.
- $\bar{W}_1 = \frac{\lambda}{2}I_1^2 + \mu I_1$. In this model, $\bar{W}'_1 = \lambda I_1 + \mu$; $\bar{W}''_1 = \lambda$. The hyperbolicity $\bar{W}'_1 - 18|\bar{W}''_1|$ 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 do not allow the density $\rho \rightarrow \infty$, which is equivalent to the specific volume $V \rightarrow 0$, or equivalently, $J \rightarrow 0$, or $I_3 \rightarrow 0$. This means that the stored energy should satisfy

$$\bar{W} \rightarrow \infty \text{ as } I_3 \rightarrow 0.$$

One example is the γ -law

$$\bar{W}_3(I_3) = \frac{\mu}{\gamma-1} I_3^{(1-\gamma)/2}, \quad \gamma > 1,$$

Another is the Log law

$$\bar{W}_3(I_3) = cI_3 - \frac{d}{2} \log(I_3).$$

TO BE Continued for hyperbolicity in terms of I_k .

10.2.2 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

$$F = \mathbf{u}_X + I,$$

$$E := \frac{1}{2}(C - I) = \frac{1}{2}((\mathbf{u}_X + I)^T(\mathbf{u}_X + I) - I) = \frac{1}{2}(\mathbf{u}_X + \mathbf{u}_X^T + \mathbf{u}_X^T \mathbf{u}_X).$$

The infinitesimal strain theory is to study elastic motions when $|u_X|$ is small. The infinitesimal strain is defined to be

$$\mathbf{e} := \frac{1}{2}(\mathbf{u}_X + \mathbf{u}_X^T). \quad (10.34)$$

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 10.12. *The coefficients $a_{ijkl} := \frac{\partial^2 W}{\partial F_j^i \partial F_l^k}(I)$ has the following symmetries:*

- $a_{ijkl} = a_{klij}$
- $a_{ijkl} = a_{ijlk}$
- $a_{ijkl} = a_{jikl}$
- $P_{ij} = P_{ji}$

Proof. 1. $a_{ijkl} = a_{klij}$ is due to $\frac{\partial^2 W}{\partial F_j^i \partial F_l^k} = \frac{\partial^2 W}{\partial F_l^k \partial F_j^i}$.

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, $C = F^T F$, $\mathbf{e} = \frac{1}{2}(F + F^T) - I$. 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

Linear isotropic material When a linear elastic material is also isotropic, that is $F^T F \sim I$, then W has the expansion: (Theorem 10.10)

$$W(E) = \frac{\lambda}{2} (Tr E)^2 + \mu Tr(E^2) + o(E).$$

Note that

$$E = \frac{1}{2}(C - I) = \frac{1}{2}(\mathbf{u}_X + (\mathbf{u}_X)^T) + (\mathbf{u}_X)^T(\mathbf{u}_X) = \mathbf{e} + o(\mathbf{e})$$

and

$$P = F\Sigma = \Sigma + o(\mathbf{e}).$$

Thus, from Theorem 10.10, we have

$$W = \frac{\lambda}{2} (Tr(\mathbf{e}))^2 + \mu Tr(\mathbf{e}^2), \quad (10.35)$$

$$P = \lambda Tr(\mathbf{e})I + 2\mu\mathbf{e}, \quad P_{ij} = \lambda(e_{11} + e_{22} + e_{33})\delta_{ij} + 2\mu e_{ij}. \quad (10.36)$$

That is,

$$a_{ijkl} = \lambda \delta_{ij} \delta_{kl} + \mu (\delta_{ik} \delta_{jl} + \delta_{il} \delta_{jk}). \quad (10.37)$$

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

$$E := \frac{P_{11}}{e_{11}} \quad (10.38)$$

²From $a_{ijkl} = a_{jikl}$, 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

$$(11, 11), (11, 21), (11, 22), (11, 31), (11, 32), (11, 33), (21, 21), (21, 22), \dots, (33, 33).$$

The total number of these list is $6 + 5 + \dots + 1 = 21$.

is called the *Young modulus*. (Modulus means a ratio between stress and strain.) The shrinking of the material can be measured by

$$\nu := -\frac{e_{22}}{e_{11}} = -\frac{e_{33}}{e_{11}}. \quad (10.39)$$

This parameter is called the *Poisson ratio*. From (10.36), we get

$$\begin{aligned} P_{11} &= \lambda (e_{11} - 2\nu e_{11}) + 2\mu e_{11} \\ 0 &= \lambda (e_{11} - 2\nu e_{11}) - 2\mu \nu e_{11}. \end{aligned}$$

We can express λ and μ in terms of E and ν , and vice versa:

$$\lambda = \frac{E\nu}{(1+\nu)(1-2\nu)}, \quad \mu = \frac{E}{2(1+\nu)}, \quad (10.40)$$

$$E = \frac{\mu(3\lambda + 2\mu)}{\lambda + \mu}, \quad \nu = \frac{\lambda}{2(\lambda + \mu)}. \quad (10.41)$$

The inversion of (10.36) reads

$$e_{ij} = \frac{1}{2\mu} P_{ij} - \frac{\lambda}{2\mu(3\lambda + 2\mu)} \text{Tr}(P) \delta_{ij}. \quad (10.42)$$

In terms of E and ν , it reads

$$\begin{aligned} e_{11} &= \frac{1}{E} (P_{11} - \nu(P_{22} + P_{33})) \\ e_{22} &= \frac{1}{E} (P_{22} - \nu(P_{33} + P_{11})) \\ e_{33} &= \frac{1}{E} (P_{33} - \nu(P_{11} + P_{22})) \\ e_{ij} &= \frac{1}{2\mu} P_{ij}, \quad i \neq j. \end{aligned}$$

Another parameters are the shear modulus and bulk modulus. Let us decompose \mathbf{e} into

$$\mathbf{e} = \left(\mathbf{e} - \frac{1}{3} \text{Tr}(\mathbf{e}) \mathbf{I}\right) + \frac{1}{3} \text{Tr}(\mathbf{e}) \mathbf{I} := \mathbf{e}^D + \mathbf{e}^S,$$

Then P can be expressed as

$$P = 2\mu \mathbf{e}^D + (3\lambda + 2\mu) \mathbf{e}^S.$$

$$P^D = 2\mu \mathbf{e}^D$$

$$P^S = (3\lambda + 2\mu) \mathbf{e}^S$$

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 found in [Cialet pp. 129].

Hookean model The Hookean law is

$$W(F) = \frac{H}{2} \sum_{i,\alpha} |F_\alpha^i|^2 = \frac{H}{2} \text{tr}(F^T F), \quad H > 0.$$

This gives $P_\alpha^i = HF_\alpha^i$. The equation of motion is

$$\rho_0(X)\ddot{\mathbf{x}} = \nabla_X \cdot P, \quad \text{or} \quad \rho_0 \ddot{x}^i = \partial_{X^\alpha} P_\alpha^i = \partial_{X^\alpha} H \partial_{X^\alpha} x^i = H \sum_\alpha \partial_{X^\alpha}^2 x^i.$$

This is the standard wave equation. This is equivalent to the above linear isotropic model with $\mu = H$ and $\lambda = -H$.

10.2.3 St. Venant-Kirchhoff Model

The model is express as

$$\Sigma = \lambda(\text{Tr}E) + 2\mu E, \quad E = \frac{1}{2}(C - I).$$

or

$$W = \frac{\lambda}{2}(\text{Tr}E)^2 + \mu \text{Tr}(E^2).$$

It is the simplest nonlinear elastic model. Its linearization, which replaces

$$E = \frac{1}{2}(F^T F - I) = \frac{1}{2}(\nabla_X \mathbf{u} + (\nabla_X \mathbf{u})^T + \nabla_X \mathbf{u}^T \nabla_X \mathbf{u}) \quad \text{by} \quad \mathbf{e} = \frac{1}{2}(\nabla_X \mathbf{u} + (\nabla_X \mathbf{u})^T),$$

is the linear isotropic model we have seen earlier. Note that the St. Venant-Kirchhoff model is not polyconvex, which is a 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

$$\bar{W}(I_1, I_2) = \frac{\lambda}{8} I_1^2 + \frac{\mu}{4} (I_1^2 - 2I_1 + 2I_2) - 9 \left(\frac{\lambda}{8} + \frac{\mu}{4} \right).$$

10.2.4 Fluid-solid model

When $W = \bar{W}_3(I_3)$, 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)

$$\boldsymbol{\sigma} = \frac{2}{\sqrt{I_3}} I_3 \bar{W}_{I_3} \mathbf{I} = -p(\rho) \mathbf{I}.$$

A particular example is the γ -law simple gas, where

$$\bar{W}_3(I_3) = \frac{\mu}{\gamma-1} I_3^{(1-\gamma)/2}, \quad \gamma > 1,$$

$$p = -2\sqrt{I_3} \bar{W}_{I_3} = \mu I_3^{-\gamma/2} = \mu \left(\frac{\rho}{\rho_0} \right)^\gamma.$$

10.2.5 Ogden 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:

$$W := \bar{W}_1 + \bar{W}_2 + \bar{W}_3,$$

$$\bar{W}_1 := \sum_{i=1}^M a_i (\mu_1^{\alpha_i} + \mu_2^{\alpha_i} + \mu_3^{\alpha_i} - 3)$$

$$\bar{W}_2 := \sum_{i=1}^N b_i \left((\mu_2 \mu_3)^{\beta_i} + (\mu_3 \mu_1)^{\beta_i} + (\mu_1 \mu_2)^{\beta_i} - 3 \right)$$

$$\bar{W}_3 := \bar{W}_3(\mu_1 \mu_2 \mu_3), \quad \bar{W}_3(I_3) \rightarrow \infty \text{ as } I_3 \rightarrow 0+.$$

Examples of \bar{W}_3 are

$$\bar{W}_3(I_3) = \frac{\mu}{\gamma-1} I_3^{(1-\gamma)/2}, \quad \gamma > 1,$$

$$\bar{W}_3(I_3) = c I_3 - \frac{d}{2} \ln I_3$$

Special cases are

- **neo-Hookean model:**

$$\bar{W} = \frac{\mu}{2} (I_1 - 3) + \bar{W}_3(I_3) = \frac{\mu}{2} \left[(I_1 - 3) + \frac{1}{k} (I_3^{-k} - 1) \right], \quad k = \frac{\gamma-1}{2}.$$

Here, we normalize \bar{W} so that $\bar{W}(3, 3, 1) = 0$. The term I_1 gives the Hookean elastic model, whereas $\bar{W}_3(I_3)$ gives the compressible fluid model.

- **Mooney-Rivlin compressible solid**

$$\bar{W} = c_1(I_1 - 3) + c_2(I_2 - 3) + \bar{W}_3(I_3).$$

- **Knowles solid**

$$\bar{W} = \frac{\mu}{2}[(I_1 - 3)\bar{W}_1(I_3) + (I_2 - 3)\bar{W}_2(I_3) + \bar{W}_3(I_3)]$$

For more models, see Drozdov (pp. 103-118).

10.3 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:** $\text{Cof}(\mathbf{A}) := ((-1)^{i+j}A_{ij})$ is called the cofactor of \mathbf{A} ,
- **Adjugate of A** is defined to be $\text{adj}(\mathbf{A}) := (\text{Cof}A)^T$,
- An important property of adjugate of \mathbf{A} is

$$\mathbf{A} \text{adj}(\mathbf{A}) = \text{adj}(\mathbf{A})\mathbf{A} = \det(A)\mathbf{I}.$$

Thus,

$$\text{adj}(A) = \det(A)A^{-1}, \quad \text{Cof}(\mathbf{A}) = \det(A)A^{-T}$$

Theorem 10.11 (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 $\text{adj}(M)$ 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 i th row and j th column of the matrix M . The adjugate matrix has the following property:

$$\text{adj}(\mathbf{M}) \cdot \mathbf{M} = \mathbf{M} \cdot \text{adj}(\mathbf{M}) = \det(\mathbf{M})\mathbf{I}_n.$$

Applying this property to $\mathbf{M} = \lambda\mathbf{I}_n - \mathbf{A}$, we get

$$(\lambda\mathbf{I}_n - \mathbf{A}) \cdot \text{adj}(\lambda\mathbf{I}_n - \mathbf{A}) = \det(\lambda\mathbf{I}_n - \mathbf{A})\mathbf{I}_n.$$

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 $\text{adj}(\lambda \mathbf{I} - \mathbf{A})$ can be expressed as polynomial in λ of degree $(n - 1)$:

$$\text{adj}(\lambda \mathbf{I} - \mathbf{A}) = \sum_{i=0}^{n-1} \mathbf{B}_i \lambda^i.$$

Thus, the left-hand side is

$$\begin{aligned} (\lambda \mathbf{I}_n - \mathbf{A}) \cdot \text{adj}(\lambda \mathbf{I} - \mathbf{A}) &= \sum_{i=0}^{n-1} (\lambda \mathbf{I} - \mathbf{A}) \cdot \mathbf{B}_i \lambda^i \\ &= \lambda^n \mathbf{B}_{n-1} + \sum_{i=1}^{n-1} \lambda^i (\mathbf{B}_{i-1} - \mathbf{A} \mathbf{B}_i) - \mathbf{A} \mathbf{B}_0. \end{aligned}$$

4. By comparing both polynomials, we obtain

$$\mathbf{I}_n = \mathbf{B}_{n-1}, \quad c_i \mathbf{I}_n = \mathbf{B}_{i-1} - \mathbf{A} \mathbf{B}_i, \quad 1 \leq i \leq n-1, \quad c_0 \mathbf{I}_n = -\mathbf{A} \mathbf{B}_0.$$

5. Multiply the above i th 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 $\lambda_1, \lambda_2, \lambda_3$ of A as below:

$$\iota_1 = \text{tr}A = \lambda_1 + \lambda_2 + \lambda_3 \quad (10.43)$$

$$\iota_2 = \frac{1}{2} ((\text{tr}A)^2 - \text{tr}(A^2)) = \text{tr}(\text{Cof}A) = \lambda_1 \lambda_2 + \lambda_2 \lambda_3 + \lambda_3 \lambda_1 \quad (10.44)$$

$$\iota_3 = \det A = \lambda_1 \lambda_2 \lambda_3. \quad (10.45)$$

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 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 $\left. \frac{d}{ds} \right|_{s=0} \mathbf{x}^s(X)$ is called a variation of $\mathbf{x}(X)$. We denote it by $\dot{\mathbf{x}}$. An infinitesimal variation of the deformation is denoted by \dot{F} . If $\mathbf{x}^s(X)$ is the time-evolution flow maps $\mathbf{x}(s, X)$ with s being the time, we denote its variation by $\dot{\mathbf{x}}$.
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

$$\dot{W} = P : \dot{F}.$$

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 w.r.t. F and W can be obtained from F through integration:

$$P = \frac{\partial W}{\partial F}, \quad W(F) = \int_I^F P : \dot{F} ds.$$

4. The specific internal energy $U(F)$ is defined to be

$$\rho_0(X)U(F(X)) = W(F(X)).$$

Then the variation of internal energy is due to the variation of work, which is

$$\rho_0 \dot{U} = P : \dot{F}. \quad (11.1)$$

5. In Eulerian coordinate, we have

$$\rho \dot{U} = \sigma : \dot{\varepsilon}. \quad (11.2)$$

Here,

$$\sigma_{ij} = \rho \frac{\partial U}{\partial F_\alpha^i} F_\alpha^j, \quad \varepsilon_{ij} = \frac{1}{2} \left(\frac{\partial \dot{x}^i}{\partial x^j} + \frac{\partial \dot{x}^j}{\partial x^i} \right)$$

are the Cauchy stress and the pseudo-strain, respectively. Formula (11.2) is obtained from (11.1) and the symmetry of σ .¹

¹We have used

$$\dot{F}_\alpha^i = \frac{\partial \dot{x}^i}{\partial X^\alpha} = \frac{\partial \dot{x}^i}{\partial x^k} \frac{\partial x^k}{\partial X^\alpha} = \frac{\partial \dot{x}^i}{\partial x^k} F_\alpha^k.$$

and

$$\rho \dot{U} = \rho \frac{\partial U}{\partial F_\alpha^i} \dot{F}_\alpha^i = \rho \frac{\partial U}{\partial F_\alpha^i} F_\alpha^k \frac{\partial \dot{x}^i}{\partial x^k} = \sigma_{ik} \frac{\partial \dot{x}^i}{\partial x^k} = \sigma_{ij} \frac{1}{2} \left(\frac{\partial \dot{x}^i}{\partial x^j} + \frac{\partial \dot{x}^j}{\partial x^i} \right).$$

Heat and 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

$$\rho_0 \dot{U} = \rho_0 \dot{Q} + P : \dot{F}. \quad (11.3)$$

This is called the Gibbs relation.

2. An adiabatic process is a process with $\dot{Q} = 0$. 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 absolute temperature, such that

$$\dot{Q} = T \dot{S}.$$

The Gibbs relation is expressed as

$$\boxed{\rho_0 \dot{U} = \rho_0 T \dot{S} + P : \dot{F}.} \quad (11.4)$$

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

$$\boxed{\rho \dot{U} = \rho T \dot{S} + \sigma : \dot{\varepsilon}.} \quad (11.5)$$

Representation of stresses in terms of internal energy

1. We have seen from the existence of entropy function $S(U, F)$. We can invert the relation $S \leftrightarrow U$ 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:

²This is due to Carathéodory's theory of geometric thermodynamics.

- 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,

$$U(S, F) = \bar{U}(S, I_1, I_2, I_3).$$

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:

$$\sigma = \rho U_F F^T, \quad \sigma_i^j = \rho \frac{\partial U}{\partial F_\alpha^i} F_\alpha^j. \quad (11.6)$$

$$\sigma = -\rho (F^{-T}) U_{(F^{-1})}, \quad \sigma_i^j = -\rho (F^{-1})_i^\alpha \frac{\partial U}{\partial (F^{-1})_j^\alpha}. \quad (11.7)$$

$$\sigma = -\rho U_{(F^{-T})} (F^{-1}), \quad \sigma_i^j = -\rho \frac{\partial U}{\partial (F^{-T})_i^\alpha} (F^{-1})_j^\alpha. \quad (11.8)$$

$$\sigma = 2\rho B U_B, \quad \sigma_j^i = 2\rho B^{ik} \frac{\partial U}{\partial B^{kj}}, \quad \text{where } B = F F^T. \quad (11.9)$$

$$\sigma^{ij} = 2\rho \frac{\partial U}{\partial C_{\alpha\beta}} F_\alpha^i F_\beta^j \quad (11.10)$$

7. Using the representation formulae (10.11) and (10.12), 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

$$\sigma = 2\rho [(I_3 \bar{U}_{I_3}) I + (\bar{U}_{I_1} + I_1 \bar{U}_{I_2}) B - \bar{U}_{I_2} B^2] \quad (11.11)$$

or

$$\sigma = 2\rho [(I_2 \bar{U}_{I_2} + I_3 \bar{U}_{I_3}) I + \bar{U}_{I_1} B - I_3 \bar{U}_{I_2} B^{-1}]. \quad (11.12)$$

8. Using (10.15) and (10.17), the Piola stress can be represented as

$$P = 2\rho_0 F (\psi_0 C^{-1} + \psi_1 I + \psi_2 C)$$

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

$$P = 2\rho_0 F (\gamma_0 I + \gamma_1 C + \gamma_2 C^2)$$

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 is: there exists an internal energy $U(S, F)$ such that

$$\boxed{\rho_0 \dot{U} = \rho_0 T \dot{S} + P : \dot{F}}$$

where

$$T := \frac{\partial U}{\partial S}, \quad P := \frac{\partial U}{\partial F}.$$

In Eulerian coordinate, it reads

$$\boxed{\rho \dot{U} = \rho T \dot{S} + \sigma : \dot{\varepsilon}}.$$

The stability conditions are

- U_{FF} is strongly elliptic, that is

$$\frac{\partial^2 U}{\partial F_\alpha^i \partial F_\beta^j} \xi^i \xi^j \eta_\alpha \eta_\beta > 0,$$

- $U_{SS} > 0$

First law of thermo-elasticity in terms of 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

$$\boxed{\rho_0 \dot{\Psi} = -\rho_0 S \dot{T} + P : \dot{F}}. \quad (11.13)$$

From this formula, we get

$$S = - \left(\frac{\partial \Psi}{\partial T} \right)_F, \quad P = \rho_0 \left(\frac{\partial \Psi}{\partial F} \right)_T. \quad (11.14)$$

We can also express this first law of thermodynamics in Eulerian coordinate:

$$\boxed{\rho \dot{\Psi} = -\rho S \dot{T} + \sigma : \dot{\varepsilon}.} \quad (11.15)$$

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 σ 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

$$\Psi = \bar{\Psi}(T, I_1, I_2, I_3), \quad \text{where } I_k = \iota_k(C).$$

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
- $\Psi_{TT} < 0$

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

$$\boxed{\rho_0 \dot{S} + \nabla_X \cdot \left(\frac{\mathbf{Q}}{T} \right) - \frac{\rho_0 r}{T} \geq 0.} \quad (11.16)$$

This is called the *Clausius-Duhem inequality*. The integral form of the Clausius-Duhem inequality is

$$\frac{d}{dt} \int_{\Omega_0} \rho_0(X) S(t, X) dX \geq - \int_{\partial \Omega_0} \frac{\mathbf{Q} \cdot \mathbf{N}}{T} dS_0 + \int_{\Omega_0} \frac{\rho_0 r}{T} dX.$$

2. The above Clausius-Duhem inequality can be expressed in Eulerian coordinate:

$$\boxed{\rho \dot{S} + \nabla_{\mathbf{x}} \cdot \left(\frac{\mathbf{q}}{T} \right) - \frac{\rho r}{T} \geq 0.} \quad (11.17)$$

Here, the heat fluxes in Lagrangian and Eulerian coordinates are related by

$$\mathbf{q} = J^{-1} \mathbf{Q} F^T.$$

The integral form is

$$\frac{d}{dt} \int_{\Omega(t)} \rho S d\mathbf{x} + \int_{\partial\Omega(t)} \frac{\mathbf{q} \cdot \mathbf{v}}{T} dS_t - \int_{\Omega(t)} \frac{\rho r}{T} d\mathbf{x} \geq 0. \quad (11.18)$$

Here $\Omega(t) = \varphi_t(\Omega_0)$. The terms $-\int_{\partial\Omega(t)} \frac{\mathbf{q} \cdot \mathbf{v}}{T} dS_t$ 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 postulate by: there exists function $U(S, F)$ such that the specific internal energy $U = U(S, F)$. From variational approach and the Euler-Lagrange transformation formula, we can get the same equation of motion

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

with stress

$$\sigma_{ij} = \rho \frac{\partial U}{\partial F_{\alpha}^i} F_{\alpha}^j.$$

Note that the Cauchy stress $\boldsymbol{\sigma}$ is symmetric. By multiplying the equation of motion by \mathbf{v} and using

$$(\nabla \cdot \boldsymbol{\sigma}) \cdot \mathbf{v} = \nabla \cdot (\boldsymbol{\sigma} \mathbf{v}) - \boldsymbol{\sigma} \cdot \nabla \mathbf{v} = \nabla \cdot (\boldsymbol{\sigma} \mathbf{v}) - \boldsymbol{\sigma} : \dot{\boldsymbol{\varepsilon}},$$

we get the equation for the kinetic energy density $E_k = \frac{1}{2} |\mathbf{v}|^2$:

$$\partial_t(\rho E_k) + \nabla \cdot [(\rho E_k \mathbf{I} - \boldsymbol{\sigma}) \cdot \mathbf{v}] = -\boldsymbol{\sigma} : \dot{\boldsymbol{\varepsilon}}.$$

Here, $\dot{\boldsymbol{\varepsilon}} = \frac{1}{2} (\nabla \mathbf{v} + (\nabla \mathbf{v})^T)$ is the rate of strain. The term $\boldsymbol{\sigma} : \dot{\boldsymbol{\varepsilon}}$ is the rate of work done by the elastic material. Next, the energy equation reads

$$\boxed{\frac{\partial(\rho E)}{\partial t} + \nabla \cdot [(\rho E \mathbf{I} - \boldsymbol{\sigma}) \cdot \mathbf{v}] = -\nabla \cdot \mathbf{q}.} \quad (11.19)$$

where the energy density $E := \frac{1}{2}|\mathbf{v}|^2 + U$, and \mathbf{q} is the heat flux. Subtract the kinetic energy equation from this energy equation, we get an equation for the internal energy

$$\boxed{\rho\dot{U} = \boldsymbol{\sigma} : \dot{\boldsymbol{\varepsilon}} - \nabla \cdot \mathbf{q}.} \quad (11.20)$$

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

$$\rho\dot{U} = \rho T \dot{S} + \boldsymbol{\sigma} : \dot{\boldsymbol{\varepsilon}}. \quad (11.21)$$

Putting (11.20) and (11.21) together, we get an equation for entropy

$$\boxed{\rho\dot{S} = -\frac{\nabla \cdot \mathbf{q}}{T}, \quad \text{or} \quad \rho\dot{S} + \nabla \cdot \left(\frac{\mathbf{q}}{T}\right) = -\frac{\mathbf{q} \cdot \nabla T}{T^2}.} \quad (11.22)$$

Adding $S(\rho_t + \nabla \cdot (\rho\mathbf{v})) = 0$, we get entropy production equation

$$\partial_t(\rho S) + \nabla \cdot (\rho S \mathbf{v}) + \nabla \cdot \left(\frac{\mathbf{q}}{T}\right) = -\frac{1}{T^2} \mathbf{q} \cdot \nabla T. \quad (11.23)$$

Its integral form reads

$$\boxed{\frac{d}{dt} \int_{\Omega(t)} \rho S d\mathbf{x} + \int_{\partial\Omega(t)} \frac{\mathbf{q} \cdot \mathbf{n}}{T} dS = - \int_{\Omega(t)} \frac{1}{T^2} \mathbf{q} \cdot \nabla T d\mathbf{x}.} \quad (11.24)$$

Thus, the Clausius-Duhem inequality (11.18) with $r = 0$ is equivalent to

$$\mathbf{q} \cdot \nabla T \leq 0. \quad (11.25)$$

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: $\rho \dot{U} = \rho T \dot{S} + \sigma : \dot{\varepsilon}$. 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

$$\text{Clausius-Duhem inequality} \Leftrightarrow \mathbf{q} \cdot \nabla T \leq 0 \Leftrightarrow \mathbf{Q} \cdot \nabla_X T \leq 0.$$

- 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

11.2.1 Constitutive laws

Kinematic constitutive law Let us consider a linear elastic material which is in natural steady state at temperature T_0 . This means the stress

$$P(T_0, I) = 0.$$

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

$$\rho_0 \Psi_{FF}(T_0, I) = a_{ijkl}, \quad \rho_0 \Psi_{FT}(T_0, I) = G = (g_{ij}), \quad \rho_0 \Psi_{TT}(T_0, I) = -a.$$

The term $(F - I)_j^i = \frac{\partial u^i}{\partial X^j}$. 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

$$\Sigma_{ij} \approx P_{ij} = \rho_0 \frac{\partial \Psi}{\partial F_j^i} = \sum_{k,l} a_{ijkl} e_{kl} + g_{ij} \theta.$$

From the symmetry of Σ , we obtain g_{ij} is also symmetric, thus $g_{ij} \frac{\partial u^i}{\partial X^j} = g_{ij} \frac{\partial u^j}{\partial X^i}$ and

$$\sum_{i,j} g_{ij} \frac{\partial u^i}{\partial X^j} = \sum_{i,j} g_{ij} e_{ij} := \mathbf{G} : \mathbf{e}.$$

Dropping high-order terms, Ψ can be approximated as

$$\rho_0 \Psi = \frac{1}{2} \langle \mathbf{A} \mathbf{e}, \mathbf{e} \rangle + (\mathbf{G} : \mathbf{e}) \theta - \frac{a}{2} \theta^2.$$

for $F \sim I$. The kinematic constitutive laws are

- The Piola stress:

$$P(\theta, \mathbf{e}) = \mathbf{A} \mathbf{e} + \mathbf{G} \theta, \quad P_{ij} = \sum_{k,l=1}^3 a_{ijkl} e_{kl} + g_{ij} \theta. \quad (11.26)$$

- The entropy S :

$$\rho_0 S = -\rho_0 \frac{\partial \Psi}{\partial T} = -\rho_0 \frac{\partial \Psi}{\partial \theta} = -\mathbf{G} : \mathbf{e} + a \theta. \quad (11.27)$$

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

$$\mathbf{Q} = -K \nabla_X T. \quad (11.28)$$

From $\mathbf{Q} \cdot \nabla_X T \leq 0$, we get a condition for K :

$$K_{ij} \Theta_i \Theta_j \geq 0 \text{ for any vector } \Theta = (\Theta_i)_{i=1}^3.$$

³This 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 $f(0) = 0$.

11.2.2 The full set of equations

Momentum equation The equation of motion is

$$\rho_0 \ddot{u}^i = \sum_{j,k,l=1}^3 a_{ijkl} \frac{\partial u^k}{\partial X^j} \frac{\partial X^l}{\partial X^i} + \sum_{j=1}^3 g_{ij} \frac{\partial \theta}{\partial X^j}. \quad (11.29)$$

Energy equation Recall the energy equation in terms of entropy and the heat flux as:

$$\rho_0 \dot{S} = -\frac{\nabla_X \mathbf{Q}}{T}. \quad (11.30)$$

It can be approximated by

$$\rho_0 \dot{S} = -\frac{\nabla_X \mathbf{Q}}{T_0},$$

Plug (11.27) and (11.28) into this linear energy 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

$$a \dot{\theta} = \frac{1}{T_0} \sum_{i,j=1}^3 K_{ij} \frac{\partial^2 \theta}{\partial X^i \partial X^j} + \sum_{i,j=1}^3 g_{ij} \frac{\partial^2 u^i}{\partial t \partial X^j} \quad (11.31)$$

The conditions for the coefficients are

- $a_{ijkl} = a_{klij} = a_{ijlk} = a_{kjil}$,
- $g_{ij} = g_{ji}$,
- $K + K^T \geq 0$,
- $a > 0$.

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

$$\frac{d}{dt} \int_{\Omega_0} \frac{a}{2} \theta^2 dX = \frac{1}{T_0} \int_{\Omega_0} \theta \nabla_X \cdot K \nabla_X \theta + \int_{\Omega_0} \sum_{i,j} g_{ij} \theta \frac{\partial^2 u^i}{\partial t \partial X^j} dX.$$

Adding these two equations together, we get

$$\boxed{\frac{d}{dt} \int_{\Omega_0} \frac{1}{2} \left(\rho_0 \left| \frac{\partial \mathbf{u}}{\partial t} \right|^2 + \sum_{i,j,k,l} a_{ijkl} \frac{\partial u^i}{\partial X^j} \frac{\partial u^k}{\partial X^l} + a \theta^2 \right) dX = - \int_{\Omega_0} \frac{1}{T_0} \sum_{j,l} k_{jl} \frac{\partial \theta}{\partial X^j} \frac{\partial \theta}{\partial X^l} dX.} \quad (11.32)$$

This shows energy dissipation law.

11.2.3 Stability Analysis

We look for solution of the form:

$$\begin{aligned} u^i &= \xi^i \exp(i(X \cdot \eta - \lambda t)), i = 1, 2, 3, \\ \theta &= \Theta \exp(i(X \cdot \eta - \lambda t)). \end{aligned}$$

The system is called stable if

$$\text{Im}(\lambda) \leq 0.$$

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):

$$\begin{aligned} -\rho_0 \lambda^2 \xi^i &= - \sum_{j,k,l} a_{ijkl} \eta^j \eta^l \xi^k + \sum_j g_{ij} i \eta^j \Theta \\ -i a \lambda \Theta &= - \frac{1}{T_0} \sum_{j,l} K_{jl} \eta^j \eta^l \Theta + \lambda \sum_{i,j} g_{ij} \eta^j \xi^i. \end{aligned}$$

In matrix form, it is

$$\begin{bmatrix} A(\boldsymbol{\eta}) - \rho_0 \lambda^2 & -\mathbf{i} G \boldsymbol{\eta} \\ -\lambda (G \boldsymbol{\eta})^T & \frac{1}{T_0} K(\boldsymbol{\eta}) - \mathbf{i} a \lambda \end{bmatrix} \begin{bmatrix} \boldsymbol{\xi} \\ \Theta \end{bmatrix} = 0.$$

The characteristic equation is

$$0 = \det \begin{bmatrix} A(\boldsymbol{\eta}) - \rho_0 \lambda^2 I & -\mathbf{i} G \boldsymbol{\eta} \\ -\lambda (G \boldsymbol{\eta})^T & \frac{1}{T_0} K(\boldsymbol{\eta}) - \mathbf{i} a \lambda \end{bmatrix} = \det \begin{bmatrix} A(\boldsymbol{\eta}) - \rho_0 \lambda^2 I & -\mathbf{i} G \boldsymbol{\eta} \\ 0 & \lambda (G \boldsymbol{\eta})^T (A - \rho_0 \lambda^2)^{-1} (-\mathbf{i} G \boldsymbol{\eta}) + \frac{1}{T_0} K(\boldsymbol{\eta}) - \mathbf{i} a \lambda \end{bmatrix}$$

This leads to

$$\det (A(\boldsymbol{\eta}) - \rho_0 \lambda^2 I) = 0, \quad (11.33)$$

and

$$\lambda (G \boldsymbol{\eta})^T (A(\boldsymbol{\eta}) - \rho_0 \lambda^2 I)^{-1} (-\mathbf{i} G \boldsymbol{\eta}) + \frac{1}{T_0} K(\boldsymbol{\eta}) - \mathbf{i} a \lambda = 0. \quad (11.34)$$

From hyperbolicity condition of a_{ijkl} , the matrix $A(\boldsymbol{\eta})$ is symmetric positive definite. Thus, it has the following eigenvalues and eigenvectors:

$$A(\boldsymbol{\eta}) \boldsymbol{\xi}_p = \rho_0 \lambda_p^2 \boldsymbol{\xi}_p, \quad \lambda_p > 0, \quad p = 1, 2, 3.$$

The corresponding solutions for thermo elasticity are pure elastic waves, which include

- forward waves: $\mathbf{u} = \boldsymbol{\xi}_p \exp(\mathbf{i}(X \cdot \boldsymbol{\eta} - \lambda_p t))$, $\boldsymbol{\theta}_p \equiv 0$, $p = 1, 2, 3$
- backward waves: $\mathbf{u} = \boldsymbol{\xi}_p \exp(\mathbf{i}(X \cdot \boldsymbol{\eta} + \lambda_p t))$, $\boldsymbol{\theta}_p \equiv 0$, $p = 1, 2, 3$.

The other family of solutions are obtained by solving equation (11.34). Let $(\lambda_p^2, \boldsymbol{\xi}_p)$, $p = 1, 2, 3$ be the eigen-expansion of $A(\boldsymbol{\eta})$. We expand $G \boldsymbol{\eta}$ in $\{\boldsymbol{\xi}_p\}$ as

$$G \boldsymbol{\eta} = \sum_{p=1}^3 g_p \boldsymbol{\xi}_p, \quad \text{where } g_p = G \boldsymbol{\eta} \cdot \boldsymbol{\xi}_p.$$

The term

$$(G \boldsymbol{\eta})^T (A(\boldsymbol{\eta}) - \rho_0 \lambda^2 I)^{-1} G \boldsymbol{\eta} = \sum_{p=1}^3 (\rho_0 (\lambda_p^2 - \lambda^2))^{-1} g_p^2.$$

Equation (11.34) becomes

$$a \lambda + \sum_{p=1}^3 \frac{\rho_0 g_p^2}{(\lambda_p^2 - \lambda^2)} = -\mathbf{i} \frac{K(\boldsymbol{\eta})}{T_0}. \quad (11.35)$$

Here, $K(\boldsymbol{\eta}) = \sum_{j,l} K_{jl} \eta_j \eta_l > 0$. After rescaling, this equation is equivalent to

$$a \lambda + \mathbf{i} + \sum_{p=1}^3 b_p \left(\frac{1}{\lambda_p - \lambda} + \frac{1}{\lambda_p + \lambda} \right) = 0,$$

where the coefficients b_p, λ_p are positive.

Proposition 11.13. *The root of the equation (11.35) satisfies $\text{Im}(\lambda) < 0$ if and only if $a > 0$.*

Proof. **TO BE COMPLETED.** □

With this λ , we find the corresponding vector (ξ, Θ) by solving

$$A(\eta) - \rho_0 \lambda^2 I \xi - i G \eta \Theta = 0.$$

We set Θ as a free parameter and find the solution ξ . This thermo-elastic has negative $\text{Im}(\lambda)$. It decays to zero as $t \rightarrow \infty$.

Remarks

1. The condition

$$\Psi_{TT} < 0 \tag{11.36}$$

is called the thermo 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 heat capacity of the material at constant deformation. The parameter a is

$$a := -\rho_0 \frac{\partial^2 \Psi}{\partial T^2}.$$

2. The thermo 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.

4. For polytropic gases,

$$T = \frac{A(S)}{R} V^{-\gamma+1}, \quad U = c_v T, \quad A(S) = e^{\frac{S-S_0}{c_v}}.$$

Thus,

$$\begin{aligned} S &= S_0 + c_v \ln(RTV^{-\gamma+1}), \\ \Psi &= U - TS = c_v T - T(S_0 + c_v \ln(RTV^{-\gamma+1})). \\ -\frac{\partial^2 \Psi}{\partial T^2} &= \frac{\partial S}{\partial T} = \frac{c_v}{T} > 0. \end{aligned}$$

See also (1.24).

11.3 Equations for Nonlinear Thermo-elasticity

11.3.1 Lagrangian formulation

The full set of equations are the equation of motion (9.36) + energy equation (11.30):

$$\begin{aligned}\dot{F} &= \frac{\partial \mathbf{v}}{\partial X} \\ \rho_0 \dot{\mathbf{v}} &= \nabla_X \cdot \mathbf{P} \\ \rho_0 \dot{S} &= -\frac{\nabla_X \mathbf{Q}}{T}.\end{aligned}\tag{11.38}$$

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: $F_\alpha^i = \frac{\partial x^i}{\partial X^\alpha}$, 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

$$\rho_0 \left(\frac{\partial^2 \Psi}{\partial F_\alpha^i \partial F_\beta^j} \right)_T \xi^i \xi^j \eta^\alpha \eta^\beta > 0, \text{ for all } \xi = (\xi^1, \xi^2, \xi^3)^T \neq 0 \text{ and } \eta = (\eta^1, \eta^2, \eta^3)^T \neq 0.$$

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:

$$\mathbf{Q} \cdot \nabla_{\mathbf{x}} T \leq 0.$$

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 .

$$\begin{cases} \partial_t \rho + \partial_{x^j} (v^j \rho) = 0 \\ \partial_t (\rho v^i) + \partial_{x^j} (\rho v^i v^j) = \partial_{x^j} \sigma^{ij} + f^i \\ \partial_t (F^{-1})_k^\alpha + \partial_{x^k} \left((F^{-1})_j^\alpha v^j \right) = 0 \\ \partial_t (\rho E) + \partial_{x^j} (v^j \rho E - v^i \sigma^{ij}) + \partial_{x^j} q^j = v^i f^i \end{cases} \quad (11.41)$$

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

$$\nabla_{\mathbf{x}} \times F^{-T} = 0. \quad (11.42)$$

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**

$$\frac{\partial^2 \Psi}{\partial F_\alpha^i \partial F_\beta^j} \eta^\alpha \eta^\beta \xi^i \xi^j > 0, \text{ for all } \eta, \xi \in \mathbb{R}^3 \setminus \{0\},$$

or

$$\frac{\partial^2 U}{\partial F_\alpha^i \partial F_\beta^j} \eta^\alpha \eta^\beta \xi^i \xi^j > 0, \text{ for all } \eta, \xi \in \mathbb{R}^3 \setminus \{0\},$$

- **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

$$\rho = \rho_0 I_3^{-1/2}, \quad P(\rho) = 72 \left(\frac{\rho}{\rho_0} - 1 \right) + 172 \left(\frac{\rho}{\rho_0} - 1 \right)^2 + 40 \left(\frac{\rho}{\rho_0} - 1 \right)^3.$$

$$\rho_0 = 2.7 \times 10^3 \text{ kg/m}^3, \quad \mu_0 = 24.8 \text{ GPa}.$$

3. Copper [Miller 2004] The internal energy is decomposed into hydrostatic (H), thermo (T), and shear (S) energies:

$$U = U_H(I_3) + U_T(S, I_3) + U_S(I_1, I_2, I_3),$$

$$U_H = -\frac{4K}{\rho_0(K' - 1)^2} (1 + r(I_3, K')) \exp(-r(I_3, K')),$$

$$U_T = c_v T_0 \left[\exp\left(\frac{S - S_0}{c_v}\right) - 1 \right] \exp\left(\frac{\gamma_0 - \gamma(I_3)}{q}\right),$$

$$U_S = \frac{G(I_3)}{2\rho_0} \sqrt{I_3} \left[\beta I_1 I_3^{-1/3} + (1 - \beta) I_2 I_3^{-2/3} - 3 \right]$$

where

$$r(x, y) = \frac{3}{2}(y - 1) \left(x^{1/6} - 1 \right), \quad \gamma(x) = \gamma_0 x^q,$$

$$G(x) = \exp \left[-r \left(x, \frac{KG'}{G_0} \right) \right] g(x),$$

$$g(x) = G_0 \left\{ \left[1 - r \left(x, \frac{KG'}{G_0} \right) \right] x^{-1/6} - \frac{4}{3} r \left(x, \frac{KG'}{G_0} \right) \left(\frac{x^{-1/3}}{\frac{KG'}{G_0} - 1} \right) \right\}.$$

Chapter 12

Elastoplasticity

References

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4. Miller and Colella, A high-order Eulerian Godunov Method for Elastic-Plastic Flow in Solid J. Comput. Phys. (2001).
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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)

$$F = F^e F^p, \quad F_{\alpha}^i = (F^e)^i_{\beta} (F^p)_{\alpha}^{\beta}.$$

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

$$\begin{cases} \dot{F}^p = h(\rho, F, F^p, U, \xi), \\ \dot{\xi} = K(\rho, F, F^p, U, \xi). \end{cases}$$

The functions h and K 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 a modified Mooney-Rivlin equation-of-state:

$$\begin{aligned} \rho U(S, F^e, \xi) = & \frac{\lambda(S)}{2} \left(\ln \sqrt{\det C^e} \right)^2 + \frac{\mu(S)}{2} \text{tr} C^e \\ & - \frac{\mu(S)}{2} \ln(\det C^e) + \frac{\rho_0}{\vartheta_0} \rho \left(\xi + \frac{1}{\vartheta_1} e^{-\vartheta_1 \xi} \right), \end{aligned}$$

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).

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,

$$\partial_t(\rho E) + \nabla \cdot ((\rho E \mathbf{I} - \boldsymbol{\sigma}) \mathbf{v}) = \nabla \cdot (\kappa \nabla T),$$

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 $E_k := \frac{1}{2} |\mathbf{v}|^2$

$$\partial_t(\rho E_k) + \nabla \cdot [(\rho E_k \mathbf{I} - \boldsymbol{\sigma}) \cdot \mathbf{v}] = -\boldsymbol{\sigma} : D,$$

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:

$$\rho \dot{U} = \boldsymbol{\sigma} : D + \nabla \cdot (\kappa \nabla T). \quad (12.1)$$

On the other hand, by differentiating $U = U(S, F^e, \xi)$ in time with fixed material variable, and treating $F^e = F(F^p)^{-1}$, we get

$$\dot{U} = \frac{\partial U}{\partial S} \dot{S} + \frac{\partial U}{\partial F} : \dot{F} + \frac{\partial U}{\partial F^p} : \dot{F}^p + \frac{\partial U}{\partial \xi} \cdot \dot{\xi}.$$

Here, the partial derivatives $\frac{\partial U}{\partial F}$ and $\frac{\partial U}{\partial F^p}$ fix (S, ξ) . Multiplying this equation by ρ , we get

$$\rho \dot{U} = \rho T \dot{S} + \rho \frac{\partial U}{\partial F} : \dot{F} + \rho \frac{\partial U}{\partial F^p} : \dot{F}^p + \chi \cdot \dot{\xi}. \quad (12.2)$$

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

$$\begin{aligned} \rho \frac{\partial U}{\partial F_{\alpha\beta}^p} &= \rho \frac{\partial F_{\gamma}^i}{\partial F_{\alpha\beta}^p} \frac{\partial U}{\partial F_{\gamma}^i} = \left(\rho \frac{\partial U}{\partial F_{\gamma}^i} \right) \frac{\partial}{\partial F_{\alpha\beta}^p} ((F^e)^i_{\tau} (F^p)_{\tau\gamma}) \\ &= \sigma_{ij} (F^{-1})_j^{\gamma} (F^e)_{\tau}^i \delta_{\alpha\tau} \delta_{\beta\gamma} = \sigma_{ij} (F^{-1})_j^{\beta} (F^e)_{\alpha}^i \\ &= \sigma_{ij} (F^{-1})_j^{\beta} F_{\gamma}^i ((F^p)^{-1})_{\gamma\alpha} \end{aligned}$$

Thus,

$$\rho \frac{\partial U}{\partial F_{\alpha\beta}^p} \dot{F}_{\alpha\beta}^p = \sigma_{ij} (F^{-1})_j^{\beta} F_{\gamma}^i ((F^p)^{-1})_{\gamma\alpha} \dot{F}_{\alpha\beta}^p = [(F^{-1})_j^{\beta} \sigma_{ji} F_{\gamma}^i] [((F^p)^{-1})_{\gamma\alpha} \dot{F}_{\alpha\beta}^p] := \Sigma^T : L^p,$$

where

$$\Sigma = F^{-1} \sigma F, \quad L^p := (F^p)^{-1} \dot{F}^p.$$

Equating (12.1) and (12.2), we get an evolution equation for the thermo variables:

$$\rho T \dot{S} + \Sigma^T : L^p + \chi \cdot \dot{\xi} = \nabla \cdot (\kappa \nabla T).$$

The entropy production is

$$\dot{S} = -\frac{1}{\rho T} \left(\Sigma^T : L^p + \chi \cdot \dot{\xi} \right) + \frac{1}{\rho T} \nabla \cdot (\kappa \nabla T) = \frac{1}{\rho T} (\Psi_{plast} + \Psi_{therm})$$

The term

$$\Psi_{plas} := -\Sigma^T : L^p - \chi \cdot \dot{\xi}$$

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

$$f(\boldsymbol{\sigma}, \boldsymbol{\chi}) = \|\text{dev}(\boldsymbol{\sigma})\| - \sqrt{\frac{2}{3}}(\sigma_Y + \boldsymbol{\chi}). \quad (12.3)$$

Here, $\text{dev}(\boldsymbol{\sigma}) := \boldsymbol{\sigma} - \frac{1}{3}(\text{tr}\boldsymbol{\sigma})I$ is the deviatorial part of $\boldsymbol{\sigma}$, σ_Y is a constant yield stress parameter. During material deformation, when the deviatorial stress is greater than $\sqrt{\frac{2}{3}}(\sigma_Y + \boldsymbol{\chi})$, the material lattice is broken and the material undergoes a plastic deformation. The broken process is described by the internal variable $\boldsymbol{\xi}$ 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 $\boldsymbol{\xi}$ are determined by

$$\max_{\Sigma, \boldsymbol{\chi}} \Psi_{plast}(\Sigma, \boldsymbol{\chi}, L^P, \dot{\boldsymbol{\xi}})$$

subject to the constraint

$$f(\boldsymbol{\sigma}, \boldsymbol{\chi}) \leq 0.$$

Recall

$$\Psi_{plast} = -\Sigma^T : L^P - \boldsymbol{\chi} \cdot \dot{\boldsymbol{\xi}},$$

and use method of Lagrange multiplier, we get the corresponding Euler-Lagrange equation is

$$\frac{\partial}{\partial \Sigma^T} (\Psi_{plast} + \zeta f) = 0, \quad \frac{\partial}{\partial \boldsymbol{\chi}} (\Psi_{plast} + \zeta f) = 0.$$

Here, ζ is the Lagrange multiplier. Recall $L^P := (F^P)^{-1} \dot{F}^P$, the Euler-Lagrange equations are

$$\dot{F}^P = \zeta F^P \frac{\partial f}{\partial \Sigma^T}, \quad (12.4)$$

$$\dot{\boldsymbol{\xi}} = \zeta \frac{\partial f}{\partial \boldsymbol{\chi}}. \quad (12.5)$$

The Lagrange multiplier ζ should satisfy the KKT condition

$$f = 0 \quad (12.6)$$

$$\zeta \geq 0 \quad (12.7)$$

$$\zeta f = 0. \quad (12.8)$$

In addition, in the plastic regime (i.e. $f = 0, \zeta > 0$), it should satisfy the consistency condition

$$\zeta \dot{f} = 0 \quad \text{when } f = 0. \quad (12.9)$$

It means that the material stays in plastic mode during $f = 0$ and this gives $\dot{f} = 0$ in this regime.

Chapter 13

*Geometric Elasticity

13.1 Geometric view of strain and stress

Let $\varphi_t : M_0 \rightarrow M_t \subset \mathcal{S}$ 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 target space.

- 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 . We also assume M_0 has a Riemannian metric: $(g_0)_{\alpha,\beta} = \langle \partial_{X^\alpha}, \partial_{X^\beta} \rangle$,
- The target space is a Cartesian space with metric $(g_t)_{ij}$, basis $\{\partial_{x^i}\}$ in TM_t and dual basis $\{dx^i\}$ in the cotangent space T^*M_t .
- The deformation gradient F is $d\varphi_t$, which maps a tangent vector ∂_{X^α} in TM_0 to a vector $F_\alpha^i \partial_{x^i}$ in TM_t . Thus, 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 $F \in \Gamma(\text{Hom}(TM_0, TM_t))$, the space of all section maps from M_0 to $\text{Hom}(TM_0, TM_t)$. Here, $\text{Hom}(V, W)$ is the space of all linear maps from vector space V to vector space W . Note that $\text{Hom}(V, W) = V^* \otimes W$. 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 $\mathbf{x} = \mathbf{x}(t, X)$.¹ F has the following representation

$$F(X) = F_\alpha^i(X) dX^\alpha \otimes \partial_{x^i}, \quad F_\alpha^i := \frac{\partial x^i}{\partial X^\alpha}. \quad (13.1)$$

- Inverse deformation gradient (F^{-1}) which maps a vector ∂_{x^i} in TM_t to a vector $(F^{-1})_i^\alpha \partial_{X^\alpha}$ in TM_0 . Thus, $(F^{-1})(\mathbf{x}) \in T_{\mathbf{x}}(M_0) \otimes T_{\mathbf{x}}^*M_t$ with $\mathbf{x} = \mathbf{x}(t, X)$. The rep-

¹In Marsden & Hughes's book, F is called a two-point tensor of type $\begin{bmatrix} 0 & 1 \\ 1 & 0 \end{bmatrix}$.

resentation of (F^{-1}) is

$$(F^{-1})(\mathbf{x}) = (F^{-1})_i^\alpha \frac{\partial}{\partial X^\alpha} \otimes dx^i.$$

- Right Cauchy-Green tensor: $C = F^T F$.

$$F : TM_0 \rightarrow TM_t, \quad F^* : T^*M_t \rightarrow T^*M_0$$

Using metric g_0 and g_t , we can identify T^*M_0 to TM_0 and T^*M_t to TM_t . Thus F^* induces

$$F^T : TM_t \rightarrow TM_0,$$

with

$$(F^T)_i^\alpha = (g_0)^{\alpha\beta} F_\beta^j(g_t)_{ij}.$$

Define $C = F^T F$, $C : TM_0 \rightarrow TM_0$ with

$$C = C_\beta^\alpha dX^\beta \otimes \partial_{X^\alpha}$$

$$C_\beta^\alpha = (g_0)^{\alpha\gamma} F_\gamma^j(g_t)_{ij} F_\beta^i.$$

Note that

$$g_{\alpha\beta} = (g_0)_{\alpha\delta} C_\beta^\delta = F_\alpha^j(g_t)_{ij} F_\beta^i = \varphi^*(g_t)$$

is the pullback metric of g_t in M_0 .

- Left Cauchy-Green tensor $B := FF^T : TM_t \rightarrow TM_t$ is defined as

$$B = B_j^i dx^j \otimes \partial_{x^i},$$

$$B_j^i = F_\alpha^i (F^T)_j^\alpha = F_\alpha^i (g_0)^{\alpha\beta} F_\beta^k(g_t)_{jk}.$$

- vdS_t is an Eulerian vector-valued 2-form on M_t . Its pull-back by φ_t is $\mathbf{nd}S_0$, which is a Lagrangian vector-valued 2-form on M_0 . Indeed,

$$vdS_t = (dx^2 \wedge dx^3, dx^3 \wedge dx^1, dx^1 \wedge dx^2) = (\star dx^1, \star dx^2, \star dx^3) \text{ in Eulerian coordinate}$$

$$\mathbf{nd}S_0 = (dX^2 \wedge dX^3, dX^3 \wedge dX^1, dX^1 \wedge dX^2) = (\star dX^1, \star dX^2, \star dX^3) \text{ in Lagrangian coordinate.}$$

The pull-back of vdS_t is

$$\varphi_t^*(vdS_t) = JF^{-T} \mathbf{nd}S_0.$$

- 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 $F = F_\alpha^i dX^\alpha \otimes \partial_{x^i}$, P must have the form

$$P(F) = P_i^\alpha(F)(\star dX^\alpha) \otimes dx^i. \quad (13.2)$$

This means that $P \in \Omega^{n-1}(M_0) \otimes T^*M_t$, or covector-valued $(n-1)$ -form $\Omega^{n-1}(M_0, T^*M_t)$. Recall that F is a vector-valued 1-form. The pairing of P and F is

$$W(F)\hat{\mu} := F \wedge P = F_\alpha^i P_i^\alpha dX^\alpha \wedge (\star dX^\alpha) \langle \partial_{x^i} | dx^i \rangle = F_\alpha^i P_i^\alpha \hat{\mu}. \quad (13.3)$$

Given an equation of state:

$$\mathcal{E}(F) = \int_{\hat{M}} W(F)\hat{\mu},$$

define

$$P(F) := \frac{\delta \mathcal{E}(F)}{\delta F} = \frac{\partial W}{\partial F_\alpha^i} (\star dX^\alpha) \otimes dx^i, \quad P_i^\alpha := \frac{\partial W}{\partial F_\alpha^i}.$$

- Cauchy stress. The Cauchy stress has the form

$$\sigma = \sigma_i^j (\star dx^j) \otimes dx^i.$$

It is a covector-valued $(n-1)$ -form $\Omega^{n-1}(M_t, T^*M_t)$. The pullback of σ for the $(n-1)$ -form part is the first Piola stress:

$$\begin{aligned} \varphi_t^*(\sigma) &= \sigma_i^j \varphi_t^*(\star dx^j) \otimes dx^i \\ &= \sigma_i^j J(F^{-T})_j^\alpha (\star dX^\alpha) \otimes dx^i \\ &= P_i^\alpha (\star dX^\alpha) \otimes dx^i \\ &= P. \end{aligned}$$

- The second Piola stress is the pull-back of P to M_0 . That is

$$\Sigma := F^{-1}P.$$

It is the Lagrangian covector-valued 2-form in Lagrangian coordinate. It is symmetric.

13.2 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. $\eta = v_i dx^i$ 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

$$d_t \varphi_t^* = \varphi_t^* (\partial_t + \mathcal{L}_{\mathbf{v}}).$$

Continuity equation

$$\boxed{(\partial_t + \mathcal{L}_{\mathbf{v}})(\rho_t \mu_t) = 0.} \quad (13.4)$$

Advection equation for deformation gradient F Recall that

$$F(X) = F_\alpha^i(X) dX^\alpha \otimes \partial_{x^i}, \quad F_\alpha^i := \frac{\partial x^i}{\partial X^\alpha}. \quad (13.5)$$

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

$$\boxed{\partial_t F + \mathcal{L}_{\mathbf{v}} F = 0.} \quad (13.6)$$

This follows from

$$\begin{aligned} \partial_t F + \mathcal{L}_{\mathbf{v}} F &= \frac{d}{dt} (F_\alpha^i(X) dX^\alpha \otimes \partial_{x^i}) \\ &= \frac{d}{dt} \left(F_\alpha^i(X) dX^\alpha \otimes \frac{\partial X^\beta}{\partial x^i} \partial_{X^\beta} \right) \\ &= \left(\partial_t F_\alpha^i + v^k \partial_{x^k} F_\alpha^i - F_\alpha^k \frac{\partial v^j}{\partial x^k} \right) dX^\alpha \otimes \partial_{x^i} \end{aligned}$$

Note that the pull-back is only for ∂_{x^k} .

Advection of the left Cauchy-Green deformation tensor Define the left Cauchy-Green tensor

$$B(\mathbf{x}) = F_\alpha^i F_\alpha^j \partial_{x^i} \otimes \partial_{x^j},$$

which is a tensor of type $(2,0)$. The Lie derivative of a type $(2,0)$ tensor A is given by

$$\begin{aligned} \mathcal{L}_v A &= (\mathcal{L}_v A^{ij}) \frac{\partial}{\partial x^i} \otimes \frac{\partial}{\partial x^j} + A^{kj} \mathcal{L}_v \left(\frac{\partial}{\partial x^k} \right) \otimes \frac{\partial}{\partial x^j} + A^{il} \frac{\partial}{\partial x^i} \otimes \mathcal{L}_v \left(\frac{\partial}{\partial x^l} \right) \\ &= \left(\partial_t A^{ij} + v^k \partial_{x^k} A^{ij} - A^{kj} \frac{\partial v^i}{\partial x^k} - A^{il} \frac{\partial v^j}{\partial x^l} \right) \frac{\partial}{\partial x^i} \otimes \frac{\partial}{\partial x^j} \end{aligned}$$

This is also known as the upper-convected derivative of the tensor A . Thus,

$$(\partial_t + \mathcal{L}_v)B = (\partial_t + \mathbf{v} \cdot \nabla)B - LB - BL^T = 0.$$

Equation of motion Let $\eta = v_i dx^i$ be the momentum 1-form. The Piola stress has the form

$$P(F) = P_i^\alpha(F) (\star dX^\alpha) \otimes dx^i. \quad (13.7)$$

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

$$W(F)\hat{\mu} := F \wedge P = F_\alpha^i P_i^\alpha dX^\alpha \wedge (\star dX^\alpha) \langle \partial_{x^i} | dx^i \rangle = F_\alpha^i P_i^\alpha \hat{\mu}. \quad (13.8)$$

The equation of motion is

$$\boxed{(\partial_t + \mathcal{L}_v)\eta - d \left(\frac{1}{2} |\mathbf{v}|^2 \right) = \frac{1}{\rho} \star d\sigma.} \quad (13.9)$$

The connection between P and σ is

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

Chapter 14

*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

$$L(\mathbf{v}, \rho, S, F) := \frac{1}{2} \rho |\mathbf{v}|^2 - \rho U(S, F).$$

$$\mathcal{L}[\mathbf{q}] := \int_{\Omega_0} L(\dot{\mathbf{q}}, \frac{\partial \mathbf{q}}{\partial X}) dX$$

The momentum

$$\mathbf{p}(X) := \frac{\delta \mathcal{L}}{\delta \mathbf{v}} = \rho_0(X) \mathbf{v}(X).$$

The internal energy U depends on the conformation tensor

$$\mathbf{c}^{ij} = F_{\alpha}^i F_{\beta}^j \mathbf{c}_0^{\alpha\beta}.$$

Let us define

$$\mathfrak{s}(\mathbf{x}) = \rho(\mathbf{x}) S(\mathbf{x}), \quad \mathbf{c}(\mathbf{x}) = \rho(\mathbf{x}) \mathbf{c}\left(\frac{\partial \mathbf{x}}{\partial X}\right), \quad \mathbf{m}(\mathbf{x}) = \rho(\mathbf{x}) \mathbf{v}(\mathbf{x}).$$

Then \mathfrak{s} and \mathbf{c} satisfy

$$\partial_t \mathfrak{s} + \nabla \cdot (\mathbf{v} \mathfrak{s}) = 0, \quad \partial_t \mathbf{c} + \nabla_{\mathbf{x}} \cdot (\mathbf{v} \mathbf{c}) - (\nabla \mathbf{v}) \mathbf{c} - \mathbf{c} (\nabla \mathbf{v})^T = 0.$$

¹Reference: 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

$$\begin{aligned}\rho(\mathbf{x}) &= \int_{\Omega_0} \rho_0(X) \delta(\mathbf{x} - \mathbf{q}(X)) dX \\ \mathfrak{s}(\mathbf{x}) &= \int_{\Omega_0} \mathfrak{s}_0(X) \delta(\mathbf{x} - \mathbf{q}(X)) dX \\ \mathbf{m}(\mathbf{x}) &= \int_{\Omega_0} \mathbf{p}(X) \delta(\mathbf{x} - \mathbf{q}(X)) dX\end{aligned}\tag{14.1}$$

And

$$\begin{aligned}\mathfrak{c}(\mathbf{x}) &= \int_{\Omega} \delta(\mathbf{x} - \mathbf{y}) \mathfrak{c}(\mathbf{y}) d\mathbf{y} \\ &= \int_{\Omega_0} \delta(\mathbf{x} - \mathbf{q}(X)) \rho(\mathbf{q}(X)) \mathfrak{c}\left(\frac{\partial \mathbf{q}}{\partial X}\right) J^{-1} dX \\ &= \int_{\Omega_0} \delta(\mathbf{x} - \mathbf{q}(X)) \rho_0(X) \mathfrak{c}\left(\frac{\partial \mathbf{q}}{\partial X}\right) dX.\end{aligned}$$

A functional $\mathcal{F}[\mathbf{q}, \mathbf{p}]$ can also be represented as a functional of $[\rho, \mathfrak{s}, \mathfrak{c}, \mathbf{m}]$ by

$$\bar{\mathcal{F}}[\rho, \mathfrak{s}, \mathfrak{c}, \mathbf{m}] = \mathcal{F}[\mathbf{q}, \mathbf{p}],$$

with variation

$$\begin{aligned}\delta \mathcal{F} &= \int_{\Omega_0} \left(\frac{\delta \mathcal{F}}{\delta \mathbf{q}} \delta \mathbf{q} + \frac{\delta \mathcal{F}}{\delta \mathbf{p}} \delta \mathbf{p} \right) dX \\ &= \int_{\Omega} \left(\frac{\delta \bar{\mathcal{F}}}{\delta \rho} \delta \rho + \frac{\delta \bar{\mathcal{F}}}{\delta \mathfrak{s}} \delta \mathfrak{s} + \frac{\delta \bar{\mathcal{F}}}{\delta \mathfrak{c}} \delta \mathfrak{c} + \frac{\delta \bar{\mathcal{F}}}{\delta \mathbf{m}} \delta \mathbf{m} \right) d\mathbf{x}\end{aligned}$$

In this expression, $\frac{\delta \bar{\mathcal{F}}}{\delta \rho}$ 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 (14.1). We get

$$\begin{aligned}\frac{\delta \rho}{\delta \mathbf{q}} &= -\rho_0(X) \nabla_{\mathbf{x}} \delta(\mathbf{x} - \mathbf{q}(X)) \\ \frac{\delta \mathfrak{s}}{\delta \mathbf{q}} &= -\mathfrak{s}_0(X) \nabla_{\mathbf{x}} \delta(\mathbf{x} - \mathbf{q}(X)) \\ \frac{\delta \mathbf{m}}{\delta \mathbf{q}} &= -\mathbf{p}(X) \nabla_{\mathbf{x}} \delta(\mathbf{x} - \mathbf{q}(X)) \\ \frac{\delta \mathbf{m}}{\delta \mathbf{p}} &= \delta(\mathbf{x} - \mathbf{q}(X))\end{aligned}$$

$$\delta c^{ij} = \int_{\Omega_0} -\partial_{x^k} \delta(\mathbf{x} - \mathbf{q}(X)) \delta q^k \rho_0(X) \mathbf{c} \left(\frac{\partial \mathbf{q}}{\partial X} \right) + \delta(\mathbf{x} - \mathbf{q}(X)) \rho_0(X) \delta c^{ij} dX.$$

Recall that $c^{ij} = F_\alpha^i F_\beta^j c_0^{\alpha\beta} = \frac{\partial x^i}{\partial X^\alpha} \frac{\partial x^j}{\partial X^\beta} c_0^{\alpha\beta}(X)$. With $\mathbf{x} = \mathbf{q}(t, X)$, we have

$$\delta c^{ij} = \frac{\partial \delta q^i}{\partial X^\alpha} F_\beta^j c_0^{\alpha\beta} + \frac{\partial \delta q^j}{\partial X^\beta} F_\alpha^i c_0^{\alpha\beta} = \left(\delta_k^i F_\beta^j c_0^{\alpha\beta} + \delta_k^j F_\beta^i c_0^{\beta\alpha} \right) \frac{\partial}{\partial X^\alpha} \delta q^k.$$

Thus,

$$\begin{aligned} \frac{\delta c^{ij}}{\delta q^k} &= -\frac{\partial}{\partial x^k} \delta(\mathbf{x} - \mathbf{q}(X)) \rho_0 c^{ij} - \frac{\partial}{\partial X^\alpha} \left[\delta(\mathbf{x} - \mathbf{q}(X)) \rho_0 \left(\delta_k^i F_\beta^j c_0^{\alpha\beta} + \delta_k^j F_\beta^i c_0^{\beta\alpha} \right) \right] \\ &= -\frac{\partial}{\partial x^k} \delta(\mathbf{x} - \mathbf{q}(X)) \rho_0 c^{ij} - J \frac{\partial}{\partial x^m} \left[\delta(\mathbf{x} - \mathbf{q}(X)) J^{-1} \rho_0(X) \left(\delta_k^i F_\beta^j c_0^{\alpha\beta} + \delta_k^j F_\beta^i c_0^{\beta\alpha} \right) F_\alpha^m \right] \\ &= -\frac{\partial}{\partial x^k} \delta(\mathbf{x} - \mathbf{q}(X)) \rho_0 c^{ij} - J \frac{\partial}{\partial x^m} \left[\delta(\mathbf{x} - \mathbf{q}(X)) \rho \left(\delta_k^i c^{mj} + \delta_k^j c^{im} \right) \right]. \end{aligned}$$

Here, we have used

$$\frac{\partial}{\partial X^\alpha} P_\alpha^i = J \frac{\partial}{\partial x^m} \sigma_m^i, \quad \sigma_m^i = J^{-1} P_\alpha^i F_\alpha^m.$$

The function $\bar{\mathcal{F}}$ maps $(\rho, \mathbf{s}, \mathbf{c}, \mathbf{m})$ to \mathbb{R} and $\mathcal{F} = \bar{\mathcal{F}} \circ \mathbf{q}$ maps \mathbf{q} to \mathbb{R} . Therefore, $\frac{\delta \bar{\mathcal{F}}}{\delta \mathbf{p}}$ and $\frac{\delta \mathcal{F}}{\delta \mathbf{q}}$, which are functions of X , can be expressed as

$$\begin{aligned} \frac{\delta \bar{\mathcal{F}}}{\delta \mathbf{q}}(X) &= \int_{\Omega_0} \left(\frac{\delta \bar{\mathcal{F}}}{\delta \rho} \frac{\delta \rho}{\delta \mathbf{q}} + \frac{\delta \bar{\mathcal{F}}}{\delta \mathbf{s}} \frac{\delta \mathbf{s}}{\delta \mathbf{q}} + \frac{\delta \bar{\mathcal{F}}}{\delta \mathbf{c}} \frac{\delta \mathbf{c}}{\delta \mathbf{q}} + \frac{\delta \bar{\mathcal{F}}}{\delta \mathbf{m}} \frac{\delta \mathbf{m}}{\delta \mathbf{q}} \right) d\mathbf{x} \\ &= I + II. \\ I &= - \int_{\Omega} \left(\rho_0 \frac{\delta \bar{\mathcal{F}}}{\delta \rho} + s_0 \frac{\delta \bar{\mathcal{F}}}{\delta \mathbf{s}} + \rho_0 \mathbf{c} \frac{\delta \bar{\mathcal{F}}}{\delta \mathbf{c}} + \mathbf{p} \cdot \frac{\delta \bar{\mathcal{F}}}{\delta \mathbf{m}} \right) \cdot \nabla_{\mathbf{x}} \delta(\mathbf{x} - \mathbf{q}(X)) d\mathbf{x} \\ &= \int_{\Omega} \left(\rho_0 \nabla_{\mathbf{x}} \cdot \frac{\delta \bar{\mathcal{F}}}{\delta \rho} + s_0 \nabla_{\mathbf{x}} \cdot \frac{\delta \bar{\mathcal{F}}}{\delta \mathbf{s}} + \rho_0 \mathbf{c} \cdot \frac{\delta \bar{\mathcal{F}}}{\delta \mathbf{c}} + \mathbf{p} \cdot \nabla_{\mathbf{x}} \frac{\delta \bar{\mathcal{F}}}{\delta \mathbf{m}} \right) \delta(\mathbf{x} - \mathbf{q}(X)) d\mathbf{x} \\ II &= - \int_{\Omega} \frac{\delta \bar{\mathcal{F}}}{\delta \mathbf{c}^{ij}} \frac{\delta c^{ij}}{\delta \mathbf{q}} d\mathbf{x} \\ &= - \int_{\Omega} \frac{\delta \bar{\mathcal{F}}}{\delta c^{ij}} J \frac{\partial}{\partial x^m} \left[\delta(\mathbf{x} - \mathbf{q}(X)) \rho \left(\delta_k^i c^{mj} + \delta_k^j c^{im} \right) \right] d\mathbf{x} \\ \frac{\delta \mathcal{F}}{\delta \mathbf{p}}(X) &= \int_{\Omega} \frac{\delta \bar{\mathcal{F}}}{\delta \mathbf{m}} \delta(\mathbf{x} - \mathbf{q}(X)) d\mathbf{x} = \frac{\delta \bar{\mathcal{F}}}{\delta \mathbf{m}}(\mathbf{q}(X)) \end{aligned}$$

The Poisson bracket $\{\mathcal{F}, \mathcal{G}\}$ defined by

$$\{\mathcal{F}, \mathcal{G}\} := \int_{\Omega_0} \left(\frac{\delta \mathcal{F}}{\delta \mathbf{q}} \cdot \frac{\delta \mathcal{G}}{\delta \mathbf{p}} - \frac{\delta \mathcal{G}}{\delta \mathbf{q}} \cdot \frac{\delta \mathcal{F}}{\delta \mathbf{p}} \right) dX$$

can be expressed in terms of $(\rho, \mathfrak{s}, \mathfrak{c}, \mathbf{m})$ as

$$\begin{aligned}
\{\bar{\mathcal{F}}, \bar{\mathcal{G}}\} &= \{\mathcal{F}, \mathcal{G}\} \\
&= \int_{\Omega_0} \int_{\Omega} \delta(\mathbf{x} - \mathbf{q}(X)) \left(\rho_0 \nabla_{\mathbf{x}} \frac{\delta \bar{\mathcal{F}}}{\delta \rho} + \mathfrak{s}_0 \nabla_{\mathbf{x}} \frac{\delta \bar{\mathcal{F}}}{\delta \mathfrak{s}} + \rho_0 \mathfrak{c} \nabla_{\mathbf{x}} \frac{\delta \bar{\mathcal{F}}}{\delta \mathfrak{c}} + \mathbf{p} \cdot \nabla_{\mathbf{x}} \frac{\delta \bar{\mathcal{F}}}{\delta \mathbf{m}} \right) \cdot \frac{\delta \bar{\mathcal{G}}}{\delta \mathbf{m}} \\
&\quad - \delta(\mathbf{x} - \mathbf{q}(X)) \left(\rho_0 \nabla_{\mathbf{x}} \frac{\delta \bar{\mathcal{G}}}{\delta \rho} + \mathfrak{s}_0 \nabla_{\mathbf{x}} \frac{\delta \bar{\mathcal{G}}}{\delta \mathfrak{s}} + \rho_0 \mathfrak{c} \nabla_{\mathbf{x}} \frac{\delta \bar{\mathcal{G}}}{\delta \mathfrak{c}} + \mathbf{p} \cdot \nabla_{\mathbf{x}} \frac{\delta \bar{\mathcal{G}}}{\delta \mathbf{m}} \right) \cdot \frac{\delta \bar{\mathcal{F}}}{\delta \mathbf{m}} d\mathbf{x} dX \\
&+ \int_{\Omega_0} \int_{\Omega} \frac{\delta \bar{\mathcal{F}}}{\delta \mathfrak{c}^{ij}} J \frac{\partial}{\partial x^m} \left[\delta(\mathbf{x} - \mathbf{q}(X)) \rho \left(\delta_k^i \mathfrak{c}^{mj} + \delta_k^j \mathfrak{c}^{im} \right) \right] d\mathbf{x} \frac{\delta \bar{\mathcal{G}}}{\delta \mathbf{m}^k} dX \\
&- \int_{\Omega_0} \int_{\Omega} \frac{\delta \bar{\mathcal{G}}}{\delta \mathfrak{c}^{ij}} J \frac{\partial}{\partial x^m} \left[\delta(\mathbf{x} - \mathbf{q}(X)) \rho \left(\delta_k^i \mathfrak{c}^{mj} + \delta_k^j \mathfrak{c}^{im} \right) \right] d\mathbf{x} \frac{\delta \bar{\mathcal{F}}}{\delta \mathbf{m}^k} dX
\end{aligned}$$

We use (5.6) and a lemma below to get

$$\begin{aligned}
\{\mathcal{F}, \mathcal{G}\} &= \int_{\Omega} \left(\rho \nabla_{\mathbf{x}} \frac{\delta \bar{\mathcal{F}}}{\delta \rho} + \mathfrak{s} \nabla_{\mathbf{x}} \frac{\delta \bar{\mathcal{F}}}{\delta \mathfrak{s}} + \mathbf{m} \cdot \nabla_{\mathbf{x}} \frac{\delta \bar{\mathcal{F}}}{\delta \mathbf{m}} \right) \cdot \frac{\delta \bar{\mathcal{G}}}{\delta \mathbf{m}} \\
&\quad - \left(\rho \nabla_{\mathbf{x}} \frac{\delta \bar{\mathcal{G}}}{\delta \rho} + \mathfrak{s} \nabla_{\mathbf{x}} \frac{\delta \bar{\mathcal{G}}}{\delta \mathfrak{s}} + \mathbf{m} \cdot \nabla_{\mathbf{x}} \frac{\delta \bar{\mathcal{G}}}{\delta \mathbf{m}} \right) \cdot \frac{\delta \bar{\mathcal{F}}}{\delta \mathbf{m}} d\mathbf{x} \\
&+ \int_{\Omega} \mathfrak{c} \nabla_{\mathbf{x}} \frac{\delta \bar{\mathcal{F}}}{\delta \mathfrak{c}} \cdot \frac{\delta \bar{\mathcal{G}}}{\delta \mathbf{m}} - \mathfrak{c} \nabla_{\mathbf{x}} \frac{\delta \bar{\mathcal{G}}}{\delta \mathfrak{c}} \cdot \frac{\delta \bar{\mathcal{F}}}{\delta \mathbf{m}} d\mathbf{x} \\
&+ \int_{\Omega} \left(\frac{\partial}{\partial x^m} \frac{\delta \bar{\mathcal{F}}}{\delta \mathfrak{c}^{ij}} \right) \left(\delta_k^i \mathfrak{c}^{mj} + \delta_k^j \mathfrak{c}^{im} \right) \frac{\delta \bar{\mathcal{G}}}{\delta \mathbf{m}^k} \\
&\quad - \left(\frac{\partial}{\partial x^m} \frac{\delta \bar{\mathcal{G}}}{\delta \mathfrak{c}^{ij}} \right) \left(\delta_k^i \mathfrak{c}^{mj} + \delta_k^j \mathfrak{c}^{im} \right) \frac{\delta \bar{\mathcal{F}}}{\delta \mathbf{m}^k} d\mathbf{x}
\end{aligned}$$

Here,

$$\left(\mathbf{m} \cdot \nabla_{\mathbf{x}} \frac{\delta \bar{\mathcal{G}}}{\delta \mathbf{m}} \right) \cdot \frac{\delta \bar{\mathcal{F}}}{\delta \mathbf{m}} := \mathbf{m}^i \left(\frac{\partial}{\partial x^j} \frac{\delta \bar{\mathcal{G}}}{\delta \mathbf{m}^i} \right) \frac{\delta \bar{\mathcal{F}}}{\delta \mathbf{m}^j}$$

We need a lemma.

Lemma 14.8. *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

$$\begin{aligned} & \int_{\Omega} \int_{\Omega} \delta(\mathbf{x} - \mathbf{y}) \rho_0(\mathbf{q}^{-1}(\mathbf{y})) \phi(\mathbf{x}) \psi(\mathbf{y}) d\mathbf{x} J^{-1}(\mathbf{q}^{-1}(\mathbf{y})) d\mathbf{y} \\ &= \int_{\Omega} \int_{\Omega} \delta(\mathbf{x} - \mathbf{y}) \rho(\mathbf{y}) \phi(\mathbf{x}) \psi(\mathbf{y}) d\mathbf{x} d\mathbf{y} \\ &= \int_{\Omega} \rho(\mathbf{x}) \phi(\mathbf{x}) \psi(\mathbf{x}) d\mathbf{x}. \end{aligned}$$

$$\begin{aligned} & \int_{\Omega_0} \int_{\Omega} \phi(\mathbf{x}) J(X) \nabla_{\mathbf{x}} [\delta(\mathbf{x} - \mathbf{q}(X)) \theta(\mathbf{x})] \psi(\mathbf{q}(X)) d\mathbf{x} dX = \int_{\Omega} \int_{\Omega} \phi(\mathbf{x}) \nabla_{\mathbf{x}} [\delta(\mathbf{x} - \mathbf{y}) \theta(\mathbf{x})] \psi(\mathbf{y}) d\mathbf{x} d\mathbf{y} \\ &= - \int_{\Omega} \int_{\Omega} \nabla_{\mathbf{x}} \phi(\mathbf{x}) [\delta(\mathbf{x} - \mathbf{y}) \theta(\mathbf{x})] \psi(\mathbf{y}) d\mathbf{x} d\mathbf{y} = - \int_{\Omega} \nabla_{\mathbf{x}} \phi(\mathbf{x}) \theta(\mathbf{x}) \psi(\mathbf{x}) d\mathbf{x} \end{aligned}$$

□

14.1 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

$$\mathcal{Q} := \{\mathbf{q} : \hat{M} \rightarrow M \text{ is 1-1, onto and Lipschitz continuous.}\}$$

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 $L : \mathcal{T}\mathcal{Q} \rightarrow \mathbb{R}$ 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

$$A(\mathbf{c}) = E(\mathbf{c}) - TS(\mathbf{c}), \quad \mathbf{c} := \frac{\partial \mathbf{q}}{\partial X} \mathbf{c}_0(X) \left(\frac{\partial \mathbf{q}}{\partial X} \right)^T = F \mathbf{c}_0 F^T.$$

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,

$$E(\mathbf{c}) = \frac{1}{2}nK(\text{Tr}(\mathbf{c}))$$

$$S(\mathbf{c}) = \frac{1}{2}nk_B \ln \det(\mathbf{c}).$$

Here n is number density of polymer spring and K is the spring constant.

The action is defined as

$$\begin{aligned} \mathcal{S}[\mathbf{q}, \frac{\partial \mathbf{q}}{\partial X}, \dot{\mathbf{q}}] &= \int_{\Omega} \frac{1}{2} \rho(\mathbf{q}) |\dot{\mathbf{q}}|^2 d\mathbf{x} - \int_{\Omega} A(\mathbf{c}) d\mathbf{x} \\ &= \int_{\Omega_0} \frac{1}{2} \rho_0(X) |\dot{\mathbf{q}}|^2 dX - \int_{\Omega_0} A(F\mathbf{c}_0F^T) J dX \\ &= \mathcal{K}[\dot{\mathbf{q}}] - \mathcal{A}[\mathbf{q}, F] \end{aligned}$$

Note that both \mathbf{c} and \mathbf{c}_0 are symmetric. The variation of \mathcal{A} w.r.t. \mathbf{q} gives the stress term:

$$\begin{aligned} \delta \mathcal{A} &= \delta \int_{\Omega_0} A(F\mathbf{c}_0F^T) J dX \\ &= \int_{\Omega_0} [A'(\mathbf{c}) : ((\delta F)\mathbf{c}_0F^T + F\mathbf{c}_0(\delta F^T)) J + A\delta J] dX \end{aligned}$$

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

$$A'(\mathbf{c}) : ((\delta F)\mathbf{c}_0F^T + F\mathbf{c}_0(\delta F^T)) = 2A'(\mathbf{c}) : (\delta F)\mathbf{c}_0F^T.$$

$$\begin{aligned} \delta \mathcal{A} &= 2 \int_{\Omega_0} A'_{ij} (\delta F)_k^i \mathbf{c}_0^{kl} (F^T)_j^\ell J dX \\ &= 2 \int_{\Omega_0} A'_{ij} \frac{\partial \delta x^i}{\partial X^k} \mathbf{c}_0^{kl} F_\ell^j J dX \\ &= -2 \int_{\Omega_0} \frac{\partial}{\partial X^k} (A'_{ij} \mathbf{c}_0^{kl} F_\ell^j J) \delta q^i dX \\ &:= - \int_{\Omega_0} \frac{\partial}{\partial X^k} P \cdot \delta \mathbf{q} dX \end{aligned}$$

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

$$\boldsymbol{\sigma} = J^{-1} P F^T.$$

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 $\boldsymbol{\sigma}$ are symmetric. We have

$$\boldsymbol{\sigma} = 2A' \mathbf{c} = 2\mathbf{c}A'.$$

In the case of viscosity, we add the rate-of-strain to the extra stress. Thus

$$\boldsymbol{\sigma} = 2\mathbf{c}A' + \eta_p (\nabla \mathbf{v} + (\nabla \mathbf{v})^T).$$

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 \mathcal{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

$$\mathcal{H}[\mathbf{q}, \frac{\partial \mathbf{q}}{\partial X}, \mathbf{p}] := \int_{\Omega_0} H(\mathbf{q}, \frac{\partial \mathbf{q}}{\partial X}, \mathbf{p}) dX.$$

2. The Lagrangian dynamics is equivalent to the following Hamiltonian dynamics:

$$\begin{aligned}\dot{\mathbf{q}} &= \frac{\delta \mathcal{H}}{\delta \mathbf{p}} = \rho_0 \mathbf{v} \\ \dot{\mathbf{p}} &= -\frac{\delta \mathcal{H}}{\delta \mathbf{q}} = \nabla_X P.\end{aligned}$$

This equation can also be formulated in terms of Poisson bracket. Namely

$$\dot{\mathbf{q}} = \{\mathbf{q}, \mathcal{H}\}, \quad \dot{\mathbf{p}} = \{\mathbf{p}, \mathcal{H}\},$$

where the Poisson bracket is defined by

$$\{\mathcal{F}, \mathcal{G}\} := \int_{\Omega_0} \left(\frac{\partial \mathcal{F}}{\partial \mathbf{q}} \frac{\partial \mathcal{G}}{\partial \mathbf{p}} - \frac{\partial \mathcal{G}}{\partial \mathbf{q}} \frac{\partial \mathcal{F}}{\partial \mathbf{p}} \right) dX$$

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

$$\begin{aligned}\rho(\mathbf{x}) &= \int_{\Omega_0} \rho_0(X) \delta(\mathbf{x} - \mathbf{q}(X)) dX \\ \mathbf{m}(\mathbf{x}) &= \int_{\Omega_0} \mathbf{p}(X) \delta(\mathbf{x} - \mathbf{q}(X)) dX \\ \mathbf{c}(\mathbf{x}) &= \left(\frac{\partial \mathbf{q}}{\partial X} \mathbf{c}_0(X) \left(\frac{\partial \mathbf{q}}{\partial X} \right)^T \right)_{X=\mathbf{q}^{-1}(\mathbf{x})}\end{aligned}$$

Here, we have assumed that ρ_0 and \mathbf{c}_0 are pre-given function on Ω_0 .

2. Variations

$$\begin{aligned}\delta \rho &= - \int_{\Omega_0} \rho_0(X) \nabla_{\mathbf{x}} \delta(\mathbf{x} - \mathbf{q}(X)) \cdot \delta \mathbf{q}(X) dX \\ \delta \mathbf{m} &= \int_{\Omega_0} (-\mathbf{p} \nabla_{\mathbf{x}} \delta(\mathbf{x} - \mathbf{q}(X))) \cdot \delta \mathbf{q} + \delta(\mathbf{x} - \mathbf{q}(X)) \delta \mathbf{p} dX\end{aligned}$$

For

$$c^{ij}(\mathbf{q}(X)) := \frac{\partial q^i}{\partial X^k} \frac{\partial q^j}{\partial X^\ell} C^{kl}(X)$$

its variation is

$$\begin{aligned}\delta c^{ij}(\mathbf{q}(X)) &= \frac{\partial \delta q^i}{\partial X^k} \frac{\partial q^j}{\partial X^\ell} C^{kl} + \frac{\partial \delta q^j}{\partial X^\ell} \frac{\partial q^i}{\partial X^k} C^{kl} \\ &= \frac{\partial (\delta q^m)}{\partial X^k} \left((\delta^{im} \frac{\partial q^j}{\partial X^\ell} + \delta^{jm} \frac{\partial q^i}{\partial X^\ell}) C^{kl} \right)\end{aligned}$$

Here, we have used $C^{kl} = C^{\ell k}$. Hence, for a functional $\mathcal{F}[\mathbf{q}, \mathbf{p}] = \bar{\mathcal{F}}[\rho, \mathbf{m}, \mathbf{c}] = \int F(\rho, \mathbf{m}, \mathbf{c}) dX$, we have

$$\begin{aligned}
\delta \mathcal{F} &= \int_{\Omega_0} \left(\frac{\delta \mathcal{F}}{\delta \mathbf{q}} \delta \mathbf{q} + \frac{\delta \mathcal{F}}{\delta \mathbf{p}} \right) dX \\
&= \int_{\Omega} \left(\frac{\delta \bar{\mathcal{F}}}{\delta \rho} \delta \rho + \frac{\delta \bar{\mathcal{F}}}{\delta \mathbf{m}} \delta \mathbf{m} + \frac{\delta \bar{\mathcal{F}}}{\delta \mathbf{c}} \delta \mathbf{c} \right) d\mathbf{x} \\
&= \int_{\Omega} \frac{\partial F}{\partial \rho} \int_{\Omega_0} -\rho_0(X) \nabla_{\mathbf{x}} \delta(\mathbf{x} - \mathbf{q}(X)) \cdot \delta \mathbf{q}(X) dX d\mathbf{x} \\
&\quad + \int_{\Omega} \frac{\partial F}{\partial \mathbf{m}} \int_{\Omega_0} (-\mathbf{p} \nabla_{\mathbf{x}} \delta(\mathbf{x} - \mathbf{q}(X))) \cdot \delta \mathbf{q} + \delta(\mathbf{x} - \mathbf{q}(X)) \delta \mathbf{p} dX d\mathbf{x} \\
&\quad + \int_{\Omega} \frac{\partial F}{\partial c^{ij}} \frac{\partial(\delta q^m)}{\partial X^k} \left(\frac{\partial \delta q^i}{\partial X^k} \frac{\partial q^j}{\partial X^\ell} C^{k\ell} + \frac{\partial \delta q^j}{\partial X^\ell} \frac{\partial q^i}{\partial X^k} C^{\ell k} \right) d\mathbf{x} \\
&= \int_{\Omega_0} \int_{\Omega} \left(\delta(\mathbf{x} - \mathbf{q}(X)) \rho_0(X) \nabla_{\mathbf{x}} \frac{\partial F}{\partial \rho} \right) d\mathbf{x} \cdot \delta \mathbf{q}(X) dX \\
&\quad + \int_{\Omega_0} \int_{\Omega} \left(\delta(\mathbf{x} - \mathbf{q}(X)) \mathbf{p} \nabla_{\mathbf{x}} \frac{\partial F}{\partial \mathbf{m}} \right) \cdot \delta \mathbf{q} + \frac{\partial F}{\partial \mathbf{m}} \delta(\mathbf{x} - \mathbf{q}(X)) \delta \mathbf{p} d\mathbf{x} dX \\
&\quad - \int_{\Omega_0} \left[\frac{\partial}{\partial X^k} \left(\frac{\partial F}{\partial c^{\alpha j}} \frac{\partial q^j}{\partial X^\ell} C^{k\ell} J \right) + \frac{\partial}{\partial X^\ell} \left(\frac{\partial F}{\partial c^{i\alpha}} \frac{\partial q^i}{\partial X^k} C^{k\ell} J \right) \right] \cdot \delta q^\alpha dX
\end{aligned}$$

Thus,

$$\begin{aligned}
\frac{\delta \mathcal{F}}{\delta \mathbf{q}} &= \int_{\Omega} \delta(\mathbf{x} - \mathbf{q}(X)) \left[\rho_0(X) \left(\nabla_{\mathbf{x}} \frac{\partial F}{\partial \rho} \right) + \mathbf{p} \left(\nabla_{\mathbf{x}} \frac{\partial F}{\partial \mathbf{m}} \right) \right] d\mathbf{x} \\
&\quad - \frac{\partial}{\partial X^k} \left(\frac{\partial F}{\partial c^{\alpha j}} \frac{\partial q^j}{\partial X^\ell} C^{k\ell} J + \frac{\partial F}{\partial c^{i\alpha}} \frac{\partial q^i}{\partial X^\ell} C^{\ell k} J \right) \\
\frac{\delta \mathcal{F}}{\delta \mathbf{p}} &= \int_{\Omega} \frac{\partial F}{\partial \mathbf{m}} \delta(\mathbf{x} - \mathbf{q}(X)) d\mathbf{x} = \frac{\partial F}{\partial \mathbf{m}} \Big|_{\mathbf{x}=\mathbf{q}(X)}
\end{aligned}$$

3. The inner product

$$\begin{aligned}
\int_{\Omega_0} \frac{\delta \mathcal{F}}{\delta \mathbf{q}} \frac{\delta \mathcal{G}}{\delta \mathbf{p}} dX &= \int_{\Omega_0} \left[\int_{\Omega} \delta(\mathbf{x} - \mathbf{q}(X)) \left(\rho_0(X) \nabla_{\mathbf{x}} \frac{\partial F}{\partial \rho} + \mathbf{p} \nabla_{\mathbf{x}} \frac{\partial F}{\partial \mathbf{m}} \right) d\mathbf{x} \right] \cdot \frac{\partial G}{\partial \mathbf{m}} dX \\
&\quad - \int_{\Omega_0} \frac{\partial}{\partial X^k} \left(\frac{\partial F}{\partial c^{\alpha j}} \frac{\partial q^j}{\partial X^\ell} C^{k\ell} J + \frac{\partial F}{\partial c^{i\alpha}} \frac{\partial q^i}{\partial X^\ell} C^{\ell k} J \right) \cdot \frac{\partial G}{\partial \mathbf{m}^\alpha} dX \\
&= \int_{\Omega} \left(\rho \nabla_{\mathbf{x}} \frac{\partial F}{\partial \rho} + \mathbf{m} \nabla_{\mathbf{x}} \frac{\partial F}{\partial \mathbf{m}} \right) \frac{\partial G}{\partial \mathbf{m}} d\mathbf{x} \\
&\quad - \int_{\Omega} \frac{\partial}{\partial x^i} \left(\frac{\partial F}{\partial c^{\alpha j}} c^{ij} + \frac{\partial F}{\partial c^{j\alpha}} c^{ji} \right) \cdot \frac{\partial G}{\partial \mathbf{m}^\alpha} d\mathbf{x}
\end{aligned}$$

In the last step, we use the following lemma

Lemma 14.9.

$$J\nabla_{\mathbf{x}}\sigma = \nabla_X P,$$

where

$$\sigma = J^{-1}PF^T, \quad \sigma_{\alpha}^i = J^{-1}P_{\alpha}^k F_k^i.$$

By setting

$$P_{\alpha}^k := \frac{\partial F}{\partial c^{\alpha j}} \frac{\partial q^j}{\partial X^{\ell}} C^{k\ell} J,$$

we get

$$\sigma_{\alpha}^i = \frac{\partial F}{\partial c^{\alpha j}} F_{\ell}^j F_k^i C^{k\ell} = \frac{\partial F}{\partial c^{\alpha j}} c^{ij}$$

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

$$\begin{aligned} \{\mathcal{F}, \mathcal{G}\} &= \int_{\Omega} \left(\rho \nabla_{\mathbf{x}} \frac{\partial F}{\partial \rho} + \mathbf{m} \nabla_{\mathbf{x}} \frac{\partial F}{\partial \mathbf{m}} \right) \frac{\partial G}{\partial \mathbf{m}} d\mathbf{x} - \int_{\Omega} \frac{\partial}{\partial x^i} \left(\frac{\partial F}{\partial c^{\alpha j}} c^{ij} + \frac{\partial F}{\partial c^{j\alpha}} c^{ji} \right) \cdot \frac{\partial G}{\partial \mathbf{m}^{\alpha}} d\mathbf{x} \\ &\quad - \int_{\Omega} \left(\rho \nabla_{\mathbf{x}} \frac{\partial G}{\partial \rho} + \mathbf{m} \nabla_{\mathbf{x}} \frac{\partial G}{\partial \mathbf{m}} \right) \frac{\partial F}{\partial \mathbf{m}} d\mathbf{x} + \int_{\Omega} \frac{\partial}{\partial x^i} \left(\frac{\partial G}{\partial c^{\alpha j}} c^{ij} + \frac{\partial G}{\partial c^{j\alpha}} c^{ji} \right) \cdot \frac{\partial F}{\partial \mathbf{m}^{\alpha}} d\mathbf{x} \end{aligned}$$

Incomplete, some terms are missing.

Chapter 15

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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15.1 Linear Elasticity

15.1.1 Dynamics of linear elasticity

In simple elasticity, as assuming the strain $\mathbf{e} = \frac{1}{2}(\nabla_X \mathbf{u} + (\nabla_X \mathbf{u})^T)$ being small, the equation of motion can be approximated by

$$\rho_0 \ddot{u}^i = \sum_{jkl} a_{ijkl} \frac{\partial^2 u^k}{\partial X^j \partial X^l}, \quad i = 1, 2, 3, \quad X \in \Omega_0, \quad (15.1)$$

where the coefficients

$$a_{ijkl} := \frac{\partial^2 W(I)}{\partial F_j^i \partial F_l^k} \quad (15.2)$$

satisfies

$$a_{ijkl} = a_{ijlk} = a_{klij} = a_{jikl}. \quad (15.3)$$

The first equality is due to $C = F^T F$ being symmetric. The second equality is from $\frac{\partial^2 W(I)}{\partial F_j^i \partial F_l^k} = \frac{\partial^2 W(I)}{\partial F_l^k \partial F_j^i}$. The third equality is a consequence of the first two equalities.

15.1.2 Hyperbolicity of linear elasticity

We look for plane wave solution for equation (15.1). We plug the ansatz $\mathbf{u} = \xi e^{i(\eta \cdot X - \lambda t)}$ into (15.1) to get

$$\rho_0 \lambda^2 \xi_i = \sum_{j,k,l=1}^3 a_{ijkl} \xi_k \eta_j \eta_l. \quad (15.4)$$

Thus, equation (15.1) supports plane wave solution in direction η if the 3×3 matrix

$$A(\eta)_{ik} := \left(\sum_{j,l=1}^3 a_{ijkl} \eta_j \eta_l \right)$$

has positive eigenvalue $\rho_0 \lambda^2$ with eigenvector ξ .

Lemma 15.10. *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 15.6 (Strong ellipticity). *The 4-tensor (a_{ijkl}) with symmetry property (15.3) is said to satisfy strong ellipticity condition if there exists a positive constant α such that for any $\xi \in \mathbb{R}^3$, $\eta \in \mathbb{R}^3$,*

$$\sum_{ijkl} a_{ijkl} \xi_i \xi_k \eta_j \eta_l \geq \alpha |\xi|^2 |\eta|^2. \quad (15.5)$$

From the above discussion, we have the following proposition.

Proposition 15.14. *Strong ellipticity for the 4-tensor (a_{ijkl}) is equivalent to the hyperbolicity of system (15.1).*

Remarks

- Condition (15.5) is also called Legendre-Hadamard condition in Calculus of Variations.
- Let \mathbb{M}_n be the space of $n \times n$ matrices. Let $W : \mathbb{M}_n \rightarrow \mathbb{R}$. 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

$$\mathbf{F}, \mathbf{G} \in \mathbb{M}_n, \quad \text{rank}(\mathbf{F} - \mathbf{G}) \leq 1.$$

The matrix $(\xi_i \eta_j) := \xi \eta^T$ is a rank-1 matrix. Indeed, all rank-1 matrix has this form.

- $W(F) := a_{ijkl} F_j^i F_l^k$ is rank-1 convex $\Leftrightarrow a_{ijkl}$ is strongly elliptic.

15.1.3 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

$$\rho_0 \ddot{\mathbf{u}} = \frac{1}{2} \nabla_{\mathbf{x}} \cdot [A (\nabla_{\mathbf{x}} \mathbf{u} + (\nabla_{\mathbf{x}} \mathbf{u})^T)] = \nabla_{\mathbf{x}} \cdot \mathbf{Ae}. \quad (15.6)$$

By multiplying (15.6) by $\dot{\mathbf{u}}$ then integrating in X , we get

$$\begin{aligned} \frac{d}{dt} \int_{\Omega_0} \left(\frac{1}{2} \rho_0 |\dot{\mathbf{u}}|^2 \right) dX &= \int_{\Omega_0} \frac{1}{2} \nabla_{\mathbf{x}} \cdot [A (\nabla_X \mathbf{u} + (\nabla_X \mathbf{u})^T)] \cdot \dot{\mathbf{u}} dX \\ &= - \int_{\Omega_0} \frac{1}{2} [A (\nabla_X \mathbf{u} + (\nabla_X \mathbf{u})^T)] \cdot \nabla_X \dot{\mathbf{u}} dX \end{aligned}$$

Note from $a_{ijkl} = a_{jikl}$ we obtain

$$\begin{aligned} \frac{1}{2} \sum_{ijkl} a_{ijkl} \left(\frac{\partial u_l}{\partial X^k} + \frac{\partial u_k}{\partial X^l} \right) \frac{\partial \dot{u}_i}{\partial X^j} &= \frac{1}{4} \sum_{ijkl} a_{ijkl} \left(\frac{\partial u_l}{\partial X^k} + \frac{\partial u_k}{\partial X^l} \right) \left(\frac{\partial \dot{u}_i}{\partial X^j} + \frac{\partial \dot{u}_j}{\partial X^i} \right) \\ &= \int \sum_{ijkl} a_{ijkl} e_{kl} \dot{e}_{ij} = \langle \mathbf{Ae}, \dot{\mathbf{e}} \rangle = \frac{d}{dt} \left(\frac{1}{2} \langle \mathbf{Ae}, \mathbf{e} \rangle \right) \end{aligned}$$

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

$$W(\mathbf{e}) := \frac{1}{2} \langle \mathbf{Ae}, \mathbf{e} \rangle.$$

15.1.4 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

$$\rho_0 \dot{u}^i = \sum_{jkl} a_{ijkl} \frac{\partial^2 u^k}{\partial X^j \partial X^l}, \quad i = 1, 2, 3, \quad X \in \Omega_0. \quad (15.7)$$

The boundary conditions are

$$\begin{cases} \mathbf{u}(X) = \mathbf{h}(X) \text{ on } \partial\Gamma_0^D \\ \sum_{j,k,l=1}^3 a_{ijkl} \frac{\partial u^k}{\partial X^l} N^j = t^i(X), i = 1, 2, 3, \text{ on } \partial\Gamma_0^N \end{cases} \quad (15.8)$$

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

$$\mathbf{u}(0, X) = \mathbf{u}_0(X), \quad \partial_t \mathbf{u}(0, X) = \mathbf{u}_1(X), \quad X \in \Omega_0. \quad (15.9)$$

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

$$\frac{d}{dt} \begin{bmatrix} u \\ \dot{u} \end{bmatrix} = \begin{bmatrix} 0 & I \\ \mathcal{A} & 0 \end{bmatrix} \begin{bmatrix} u \\ \dot{u} \end{bmatrix}, \quad (\mathcal{A}u)^i := \sum_{jkl} a_{ijkl} \frac{\partial^2 u^k}{\partial X^j \partial X^l}.$$

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.

15.1.5 Steady state problem for linear elasticity**Outline**

- The steady state problem is the boundary value problem of

$$-\sum_{jkl} a_{ijkl} \frac{\partial^2 u^k}{\partial X^j \partial X^l} = \rho_0(X) b_i(\mathbf{x}(X)), \quad i = 1, 2, 3, \quad X \in \Omega_0,$$

with boundary condition (15.8). 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. Ciale

Definition 15.7 (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*

$$\sum_{ijkl} a_{ijkl} e_{ij} e_{kl} \geq \tilde{\alpha} \sum_{kl} e_{kl}^2. \quad (15.10)$$

Proposition 15.15. *Assuming a_{ijkl} satisfies*

$$a_{ijkl} = a_{klij} = a_{ijlk}$$

then we have

$$\text{Stability} \Rightarrow \text{Strong Ellipticity.}$$

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

$$\begin{aligned} \sum_{ij} |e_{ij}|^2 &= \frac{1}{4} \sum_{ij} (\xi_i \eta_j + \xi_j \eta_i)^2 \\ &= \frac{1}{4} \sum_{ij} (\xi_i^2 \eta_j^2 + \xi_j^2 \eta_i^2 + 2\xi_i \eta_i \xi_j \eta_j) \\ &= \frac{1}{2} (|\xi|^2 |\eta|^2 + (\xi \cdot \eta)^2) \\ &\geq \frac{1}{2} |\xi|^2 |\eta|^2. \end{aligned}$$

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. \square

Remark The stability condition (15.10) 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 15.12 (Korn's inequality). *Let $u : \Omega \rightarrow \mathbb{R}^3$ and $e = \frac{1}{2}(\partial \mathbf{u} / \partial X + (\partial \mathbf{u} / \partial X)^T)$. It holds that*

$$\int_{\Omega} \sum_{ij} \left(\frac{\partial u_i}{\partial X^j} \right)^2 dx \leq 2 \int_{\Omega} \sum_{ij} e_{ij}^2 dx \text{ for all } u \in H_0^1(\Omega).$$

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

$$\begin{aligned}\frac{\partial u_i}{\partial X^j} \frac{\partial u_j}{\partial X^i} &= \frac{\partial}{\partial X^j} \left(u_i \frac{\partial u_j}{\partial X^i} \right) - u_i \frac{\partial^2 u_j}{\partial X^i \partial X^j} \\ \frac{\partial u_i}{\partial X^i} \frac{\partial u_j}{\partial X^j} &= \frac{\partial}{\partial X^i} \left(u_i \frac{\partial u_j}{\partial X^j} \right) - u_i \frac{\partial^2 u_j}{\partial X^i \partial X^j}, \text{ we get}\end{aligned}$$

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 $u \in H_0^1(\Omega)$. 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.

15.2 Linear isotropic elasticity

15.2.1 Characteristic wave modes

For linear isotropic material

$$a_{ijkl} = \lambda \delta_{ij} \delta_{kl} + \mu (\delta_{ik} \delta_{jl} + \delta_{il} \delta_{jk}), \quad (15.11)$$

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

$$\boxed{\rho_0 \ddot{u}^i = \mu \Delta u^i + (\lambda + \mu) \partial_i (\partial_k u^k)}. \quad (15.12)$$

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 eigenvector is 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

$$\rho_0 \lambda_i^2 = \mu, i = 1, 2, \quad \rho_0 \lambda_3^2 = \lambda + 2\mu. \quad (15.13)$$

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 15.16. 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

$$\lambda + 2\mu > 0, \quad \mu > 0. \quad (15.14)$$

In terms of the Young modulus E and Poisson ratio ν , we have

$$(\lambda > 0, \mu > 0) \Leftrightarrow (0 < \nu < \frac{1}{2}, E > 0) \Rightarrow (\lambda + 2\mu > 0, \mu > 0). \quad (15.15)$$

Proof. 1. (15.14) follows from (15.13).

2. (15.15) follows from (10.40).

□

15.2.2 Dynamics of linear isotropic elasticity

Equation (15.12) in vector form reads

$$\rho_0 \partial_t^2 \mathbf{u} = \mu \Delta \mathbf{u} + (\lambda + \mu) \nabla (\nabla \cdot \mathbf{u}).$$

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

$$\rho_0 \partial_t^2 (\nabla \phi + \mathbf{w}) = \mu \Delta (\nabla \phi + \mathbf{w}) + (\lambda + \mu) \nabla (\nabla \cdot \nabla \phi) = \mu \Delta (\nabla \phi + \mathbf{w}) + (\lambda + \mu) \nabla \Delta \phi.$$

We get

$$\rho_0 \partial_t^2 (\mathbf{v} + \mathbf{w}) = (\lambda + 2\mu) \Delta \mathbf{v} + \mu \Delta \mathbf{w}.$$

Note that the Hodge decomposition is preserved under the operations Δ and ∂_t^2 . Thus, we obtain

$$\boxed{\rho_0 \partial_t^2 \mathbf{v} = (\lambda + 2\mu) \Delta \mathbf{v}, \quad \rho_0 \partial_t^2 \mathbf{w} = \mu \Delta \mathbf{w}.} \quad (15.16)$$

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 (15.11),

$$\langle A\mathbf{e}, \mathbf{e} \rangle = \lambda (Tr \mathbf{e})^2 + \mu \mathbf{e} : \mathbf{e}$$

The stability condition in the off-diagonal component is

$$\mu e_{ij}^2 \geq \tilde{\alpha} e_{ij}^2.$$

¹When 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. $\Delta \mathbf{h} = 0$.

The stability condition for the diagonal part is

$$\lambda(e_{11} + e_{22} + e_{33})^2 + 2\mu e_{kk}^2 \geq \tilde{\alpha} e_{kk}^2, k = 1, 2, 3,$$

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} . This is equivalent to

$$3\lambda + 2\mu > 0.$$

Thus, the *stability condition* for linear isotropic material is

$$\boxed{3\lambda + 2\mu > 0, \quad \mu > 0.} \quad (15.17)$$

In terms of shear modulus μ and bulk modulus $K = \lambda + \frac{2}{3}\mu$, stability condition reads

$$\mu > 0, \quad K > 0. \quad (15.18)$$

Let us summarize the stability and hyperbolicity conditions for linear isotropic materials

- Hyperbolicity: $(\lambda + 2\mu > 0, \mu > 0) \Leftrightarrow \mu, K \Leftrightarrow E, \nu$.

15.2.3 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

$$\begin{cases} -\nabla_X P(X, \mathbf{x}(X)) = \rho_0(X) \mathbf{b}(\mathbf{x}(X)), & X \in \Omega_0, \\ \mathbf{x}(X) = \mathbf{x}_0(X), & X \in \Gamma_D, \\ P(X, \mathbf{x}(X)) \cdot N(X) = \mathbf{t}_0(X, \mathbf{x}(X)), & X \in \Gamma_N. \end{cases} \quad (15.19)$$

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. Cialek pp. 295

Theorem 15.13. *Consider the boundary value problem for a linear isotropic material with $W(\mathbf{e}) = \lambda \text{Tr}(\mathbf{e})^2 + 2\mu \mathbf{e} : \mathbf{e}$. We assume*

$$\mu > 0, \quad \lambda > 0. \quad (15.20)$$

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

$$V = \{\mathbf{v} \in H^1(\Omega_0) : \mathbf{v} = 0 \text{ on } \Gamma_D\}$$

15.3 Hyperbolic System of Nonlinear Elasticity in Lagrangian Coordinate

15.4 Steady State Solutions of Nonlinear Elasticity

15.4.1 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

$$\begin{cases} -\nabla_X P(X, \mathbf{x}(X)) = \rho_0(X) \mathbf{b}(\mathbf{x}(X)), & X \in \Omega_0, \\ \mathbf{x}(X) = \mathbf{x}_0(X), & X \in \Gamma_D, \\ P(X, \mathbf{x}(X)) \cdot N(X) = \mathbf{t}_0(X, \mathbf{x}(X)), & X \in \Gamma_N. \end{cases} \quad (15.21)$$

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 Ciale, Chapter 5.

15.4.2 Nonuniqueness

Ref. Ciale, Chapter 5.8.

- F. John's example [John 1964]:
- Noll [1978]
- Buckling of a rod

15.4.3 Polyconvexity and uniqueness of steady state problems

Definition 15.8. Let \mathcal{M}_n be the space of all $n \times n$ matrices. A function $W : \mathcal{M}_n \rightarrow \mathbb{R}$ is called polyconvex if $W(F)$ can be expressed as a convex function of the determinants of the submatrices of F .

Theorem 15.14 (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 15.15. 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.

15.5 Stability of steady-state solution

TOBE CONTINUED

15.6 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 $u^i = \xi^i e^{i(X \cdot \eta - \lambda t)}$, $p = \pi e^{i(X \cdot \eta - \lambda t)}$. Plug these into the equations, we obtain

$$\begin{cases} A(\eta) \xi = \rho_0 \lambda^2 \xi - i \pi \eta \\ \xi \cdot \eta = 0. \end{cases}$$

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 (ξ_p, λ_p) , $p = 1, 2$. The corresponding $\pi = 0$.
- Longitudinal wave goes to infinity.

TOBE CONTINUED

Chapter 16

Membrane and Shell

16.1 Membrane

16.1.1 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,

$$\langle d\mathbf{x}, d\mathbf{x} \rangle = (F dX, F dX) = (F^T F dX, dX) = \sum_{jk} C_{\alpha\beta} dX^\alpha dX^\beta.$$

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 $dS_t = J dS_0$.

16.1.2 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 $(F^T F)_{2 \times 2}$:

$$\bar{W}(C) := W(F) = W(\Lambda), \quad C = F^T F.$$

4. The energy W can be expressed in terms of principal invariants of $F^T F$: We define

$$\bar{W}(I_1, I_2) = \bar{W}(C) = W(F)$$

where

$$I_k := \iota_k(C), \quad \iota_1(C) := \text{tr}(C), \quad \iota_2(C) := \det(C).$$

Examples

- Hookean law:

$$W(F) = \bar{W}(I_1, I_2) := \frac{H}{2} I_1 = \frac{H}{2} \text{tr}(F^T F) = \frac{H}{2} \sum_{\alpha=1}^2 \sum_{i=1}^3 |F_{\alpha}^i|^2,$$

where $H > 0$ is a constant. The corresponding Piola stress is

$$P_{\alpha}^i = \frac{\partial W}{\partial F_{\alpha}^i} = H F_{\alpha}^i, \quad \alpha = 1, 2, \quad i = 1, 2, 3.$$

- Minimal surface

$$W(F) := \sigma I_2 = \sigma \sqrt{\det(C)} = \sigma \sqrt{\det(F^T F)} = \sigma J.$$

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:

$$W(F) := a(I_1 - 2)^2 + b(\sqrt{I_2} - 1)^2 = a(\text{tr}(F^T F) - 2)^2 + b(\sqrt{\det(F^T F)} - 1)^2.$$

Note that when $F = I$ (i.e. the membrane is at rest), we have $\text{tr}(I) = 2$ and $\det I = 1$. Another fabric model is to decompose $C = F^T F$ into a trace part and a trace-free part. That is,

$$C = \frac{1}{2} \text{tr}(C) I + \left(C - \frac{1}{2} \text{tr}(C) I \right)$$

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

$$W(F) = a(\text{tr}(C) - 2)^2 + b \left\| C - \frac{1}{2} \text{tr}(C) I \right\|_F^2. \quad (16.1)$$

The norm here is the Frobenius norm.¹

Exercise Express (16.1) in terms of I_1 and I_2 .

Piola stress $P_\alpha^i = \frac{\partial P}{\partial F_\alpha^i}$, $i = 1, 2, 3$, $\alpha = 1, 2$.

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.

¹For membrane model, a reference book is: Statistical Mechanics of Membranes and Surfaces, 2nd edition, edited by D. Nelson, T. Piran and S. Weinberg (2004).

16.1.3 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 respect 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

$$\begin{cases} \rho_0(X) \dot{v}^i(t, X) &= \frac{\partial}{\partial X^\alpha} P_\alpha^i(F) \\ \dot{F}_\alpha^i &= \frac{\partial v^i}{\partial X^\alpha} \end{cases}$$

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 $\sigma \cdot N = 0$.

16.2 Shells

In membrane or fabric, the internal energy is only a function of F , which involves only the first fundamental 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

$$\begin{aligned} \tilde{\varphi}_t(X_1, X_2, X_3) &:= \tilde{\mathbf{x}}(X_1, X_2, X_3) := \mathbf{x}(X_1, X_2) + X_3 N(X_1, X_2), \\ N(X_1, X_2) &= \frac{\frac{\partial \mathbf{x}}{\partial X_1} \times \frac{\partial \mathbf{x}}{\partial X_2}}{\left\| \frac{\partial \mathbf{x}}{\partial X_1} \times \frac{\partial \mathbf{x}}{\partial X_2} \right\|}. \end{aligned}$$

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

$$\tilde{I}_k = I_k(F^T F) + X_3 I_k(S).$$

The energy can be decoupled into

$$W(\tilde{F}) = W_m(I_1(F^T F), I_2(F^T F)) + W_b(I_1(S), I_2(S)).$$

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 intrinsic property of surfaces, involves the derivative of F .

Part III

Complex Fluids

Chapter 17

Viscoelasticity

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17.1 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.

17.1.1 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 $\varepsilon(t)$. 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*. 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.

17.2 Spring-dashpot models

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

- Elastic part: $\sigma = G\varepsilon$
- Viscous part: $\sigma = \eta\dot{\varepsilon}$,

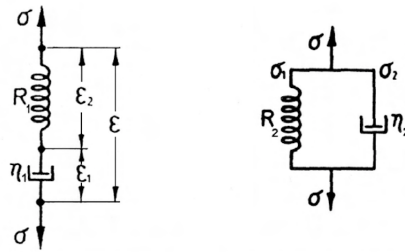


Figure 17.1: Spring-Dashpot models. Maxwell model (left), Kelvin model (right). Copied from https://www.researchgate.net/figure/Simple-two-element-spring-and-dashpot-models-of-linear-viscoelastic-solids-fig1_234027378

where 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 former leads to the Maxwell model. The latter gives the Kelvin-Voigt model. Below, let the subscript s and d stand for spring and dashpot, respectively.

Maxwell Model The Maxwell model is a series connection of spring and dashpot. Thus,

$$\varepsilon = \varepsilon_s + \varepsilon_d, \quad \sigma = \sigma_s = \sigma_d.$$

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-Voigt model The Kelvin-Voigt model is a parallel connection of spring and dashpot. Thus,

$$\varepsilon = \varepsilon_s = \varepsilon_d, \quad \sigma = \sigma_s + \sigma_d.$$

This gives

$$\sigma = G\varepsilon + \eta\dot{\varepsilon}.$$

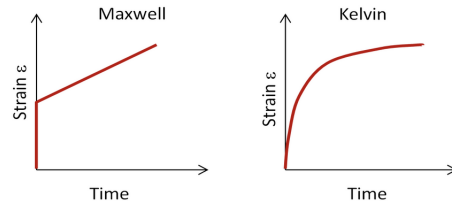


Figure 17.2: Spring-Dashpot models. Copied from <https://polymerdatabase.com/polymer%20physics/Maxwell-Kelvin.html>

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*.

17.3 Dumbbell Model

1

17.3.1 Model set up

1. In general, 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. 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} represents a relative position vector inside the box $\mathbf{x} + d\mathbf{x}$ with respect to \mathbf{x} . We call the configuration space of \mathbf{r} at \mathbf{x} a Fibre space $F_{\mathbf{x}}$. In the present case, $F_{\mathbf{x}} = \mathbb{R}^3$.
3. We assume the microscopic fluid inside the box follows the macroscopic fluid. Thus, the fluid velocity at \mathbf{r} in $F_{\mathbf{x}}$ is

$$\mathbf{v}(t, \mathbf{x}) + \nabla \mathbf{v}(t, \mathbf{x}) \mathbf{r} = \mathbf{v} + \mathbf{L} \mathbf{r}.$$

¹This part of note is mainly from Chapter 6 of Yn-Hwang Lin with some corrections, Polymer Viscoelasticity, 2nd ed. Another nice reference is the book of Doi and Edwards.

4. 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

$$-\frac{\partial \Phi}{\partial \mathbf{r}_1} = \mathbf{F}, \quad -\frac{\partial \Phi}{\partial \mathbf{r}_2} = -\mathbf{F}.$$

5. 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.
6. 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} .

17.3.2 Smoluchowski equation

1. Dynamics of the dumbbell. From the above two forces, the beads satisfy the Langevin equations:

$$m(\dot{\mathbf{r}}_i - \mathbf{v}_i) + \zeta(\dot{\mathbf{r}}_i - \mathbf{v}_i) = -\nabla_{\mathbf{r}_i} \Phi + \alpha \frac{dB_i}{dt}, i = 1, 2.$$

Here, $\mathbf{v}_i = \mathbf{v}(t, \mathbf{x}) + \mathbf{L}\mathbf{r}_i$ are the background flow velocity of the beads. Assuming small inertia, we thus neglect the inertia term and get the equation, called the damped Langevin equation

$$\zeta(\dot{\mathbf{r}}_i - \mathbf{v}_i) = -\nabla_{\mathbf{r}_i} \Phi + \alpha \frac{dB_i}{dt}, i = 1, 2. \quad (17.1)$$

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. 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 two equations are equivalent to

$$\begin{cases} \dot{\mathbf{r}} = \mathbf{L}\mathbf{r} + \frac{\mathbf{F}}{\zeta} + \sqrt{\frac{2k_B T}{\zeta}} \frac{dB}{dt}, \\ \dot{\mathbf{r}}_c = \mathbf{v} + \mathbf{L}\mathbf{r}_c + \sqrt{\frac{2k_B T}{\zeta}} \frac{dB_c}{dt}, \end{cases} \quad (17.2)$$

where B and B_c are two independent Brownian motions. 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. With the diffusion term in (17.2), the polymer particles will diffuse from higher concentration region to lower concentration region. According to Fick's law, the diffusion velocity is ²

$$-\frac{k_B T}{\zeta} \frac{\nabla f}{f}.$$

Thus, the *flux velocities* of \mathbf{r}_c and \mathbf{r} are

$$\begin{cases} \dot{\mathbf{r}}_{c,f} = \mathbf{v} + \mathbf{L}\mathbf{r}_c - \frac{k_B T}{\zeta} \frac{\nabla_{\mathbf{r}_c} \phi}{\phi}, \\ \dot{\mathbf{r}}_f = \mathbf{L}\mathbf{r} - \frac{1}{\zeta} \nabla_{\mathbf{r}} \Phi - \frac{k_B T}{\zeta} \frac{\nabla_{\mathbf{r}} f}{f}. \end{cases} \quad (17.3)$$

4. 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

$$\begin{aligned} \dot{\Xi} &= -\partial_{\mathbf{r}_1} \cdot (\dot{\mathbf{r}}_{1,f} \Xi) - \partial_{\mathbf{r}_2} \cdot (\dot{\mathbf{r}}_{2,f} \Xi) \\ &= -\partial_{\mathbf{r}_c} \cdot (\dot{\mathbf{r}}_{c,f} \Xi) - \partial_{\mathbf{r}} \cdot (\dot{\mathbf{r}}_f \Xi). \end{aligned}$$

Recall Ξ is separable: $\Xi = \phi(t, \mathbf{x}, \mathbf{r}_c) f(t, \mathbf{x}, \mathbf{r})$. We obtain

$$\begin{aligned} (\phi(\mathbf{r}_c) f(\mathbf{r}))' &= -\partial_{\mathbf{r}_c} \cdot (\dot{\mathbf{r}}_{c,f} \phi(\mathbf{r}_c) f(\mathbf{r})) - \partial_{\mathbf{r}} \cdot (\dot{\mathbf{r}}_f \phi(\mathbf{r}_c) f(\mathbf{r})) \\ &\Rightarrow \dot{\phi} f + \phi \dot{f} = -\partial_{\mathbf{r}_c} \cdot (\dot{\mathbf{r}}_{c,f} \phi) f - \partial_{\mathbf{r}} \cdot (\dot{\mathbf{r}}_f f) \phi. \\ &\Rightarrow (\dot{\phi} + \partial_{\mathbf{r}_c} \cdot (\dot{\mathbf{r}}_{c,f} \phi)) f + (\dot{f} + \partial_{\mathbf{r}} \cdot (\dot{\mathbf{r}}_f f)) \phi = 0. \end{aligned}$$

By separating the variables \mathbf{r}_c and \mathbf{r} , we get

$$\begin{cases} \dot{\phi} + \partial_{\mathbf{r}_c} \cdot (\dot{\mathbf{r}}_{c,f} \phi) = 0, \\ \dot{f} + \partial_{\mathbf{r}} \cdot (\dot{\mathbf{r}}_f f) = 0. \end{cases} \quad (17.4)$$

²The diffusion coefficient $D = k_B T / \zeta$ can also be obtained from equilibrium state where the drift and diffusion are balanced and the distribution f obey the Gibbs distribution.

5. To derive the equation for ϕ , we plug (17.3) into the conservation laws (17.4) to get

$$\begin{aligned}\partial_{\mathbf{r}_c} \cdot (\dot{\mathbf{r}}_{c,f} \phi) &= \partial_{\mathbf{r}_c} \cdot \left(\left(\mathbf{v} + \mathbf{L} \mathbf{r}_c - \frac{k_B T}{\zeta} \frac{\partial_{\mathbf{r}_c} \phi}{\phi} \right) \phi \right) \\ &= (\nabla_{\mathbf{x}} \cdot \mathbf{v}) \phi - \frac{k_B T}{\zeta} \partial_{\mathbf{r}_c}^2 \phi.\end{aligned}$$

Thus, from (17.4), the equation for ϕ is

$$\boxed{(\partial_t + \mathbf{v} \cdot \nabla_{\mathbf{x}}) \phi + (\nabla_{\mathbf{x}} \cdot \mathbf{v}) \phi - \frac{k_B T}{\zeta} \partial_{\mathbf{r}_c}^2 \phi = 0.} \quad (17.5)$$

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 $n(t, \mathbf{x}, \mathbf{r}_c)$ 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 $\rho := mn(t, \mathbf{x}, \mathbf{r})$.

6. To derive an equation for $f(t, \mathbf{x}, \mathbf{r})$, using (17.3), 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 (17.4), we arrive at

$$\boxed{\partial_t f + \mathbf{v} \cdot \partial_{\mathbf{x}} f + \partial_{\mathbf{r}} \cdot (\mathbf{L} \mathbf{r} f) = \partial_{\mathbf{r}} \cdot \left(-\frac{\mathbf{F}}{\zeta} f + \frac{kT}{\zeta} \partial_{\mathbf{r}} f \right).} \quad (17.6)$$

This is called the *Smoluchowski equation* for \mathbf{r} .³

17.3.3 Constitutive relation – Kramers formula

Constitutive Equation We shall derive a stress formula for the dumbbell model.

³If we define $\mathbf{r} = \mathbf{r}_2 - \mathbf{r}_1$, then we should get

$$\partial_t f + \mathbf{v} \cdot \partial_{\mathbf{x}} f + \partial_{\mathbf{r}} \cdot (\mathbf{L} \mathbf{r} f) = \partial_{\mathbf{r}} \cdot \left(-\frac{2\mathbf{F}}{\zeta} f + \frac{2kT}{\zeta} \partial_{\mathbf{r}} f \right).$$

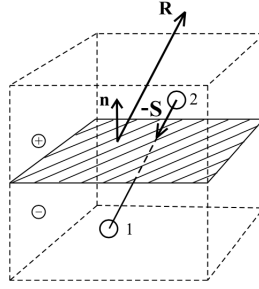


Figure 17.3: Copied from the book by Yn-Hwang Lin, Polymer Viscoelasticity.

1. We consider a plane $dA \subset F_{\mathbf{x}}$ through \mathbf{x} with normal \mathbf{v} pointing from $-$ side to $+$ side. The polymer stress σ_p contains two parts:
 - $\sigma_p^c \cdot \mathbf{v}$: the tensile force from spring-connector;
 - $\sigma_p^b \cdot \mathbf{v}$: 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.⁴ 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

$$\frac{\text{Projection of } \mathbf{r} \text{ along } \mathbf{v}}{\text{side length}} = \frac{|\mathbf{v} \cdot \mathbf{r}|}{n^{-1/3}}.$$

If the distribution of configuration \mathbf{r} is $f(t, \mathbf{x}, \mathbf{r})$, then the above probability should be

$$\frac{|\mathbf{v} \cdot \mathbf{r}|}{n^{-1/3}} f(t, \mathbf{x}, \mathbf{r}) d\mathbf{r}.$$

Now, suppose bead 2 is on $(+)$ side. That is, \mathbf{r} is on the same side of \mathbf{v} . In this case, $|\mathbf{v} \cdot \mathbf{r}| = \mathbf{v} \cdot \mathbf{r}$. 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 \mathbf{v} . In this case, $|\mathbf{v} \cdot \mathbf{r}| = -\mathbf{v} \cdot \mathbf{r}$. The force on bead 1 is \mathbf{F} . Thus, the force exerted on the $(+)$ side from the spring is $-\mathbf{F}$. In both cases, the force exerted on the $(+)$ side from dumbbell connectors is

$$n^{1/3} \int \mathbf{v} \cdot \mathbf{r} \mathbf{F} f(t, \mathbf{r}) d\mathbf{r}.$$

⁴This 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.

Dividing this by the area $dA = n^{-2/3}$, we get the tensile force per unit area is

$$n\mathbf{v} \cdot \int \mathbf{r}\mathbf{F}f(t, \mathbf{r}) d\mathbf{r} = n\langle \mathbf{r}\mathbf{F} \rangle.$$

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 \mathbf{v} per unit time and per unit area is

$$n(\dot{\mathbf{r}}_1 - \mathbf{v}_1) \cdot \mathbf{v}$$

The momenta that bead 1 carries is

$$n[(\dot{\mathbf{r}}_1 - \mathbf{v}_1) \cdot \mathbf{v}]m(\dot{\mathbf{r}}_1 - \mathbf{v}_1).$$

The probability distribution of $\dot{\mathbf{r}}_1 - \mathbf{v}_1$ is a Gaussian

$$\Xi(\xi_1) = \frac{\exp(-m|\xi_1|^2/2kT)}{\iint \exp(-m|\xi_1|^2/2kT)}, \quad \xi_1 := \dot{\mathbf{r}}_1 - \mathbf{v}_1.$$

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

$$nm \int [(\dot{\mathbf{r}}_1 - \mathbf{v}_1)(\dot{\mathbf{r}}_1 - \mathbf{v}_1) \cdot \mathbf{v}] \Xi(\dot{\mathbf{r}}_1) d\dot{\mathbf{r}}_1.$$

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. **Kramers formula for polymeric stress:** Combining the formulae of σ_p^c and σ_p^b , we get

$$\boxed{\sigma_p = -2nkTI + n\langle \mathbf{r}\mathbf{F} \rangle.} \quad (17.7)$$

This is called the Kramers formula for the stress.

5. **Remark.** In the next section, we shall derive the Kramers formula from micro dynamics. There, the Kramers 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 $F_{\mathbf{x}}$, and thus neglect the contribution of randomness of the center \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 Kramers formula (17.7) 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 (17.6) by $M := \mathbf{rr}$, then integrate it in \mathbf{r} :

$$\int \mathbf{rr} [\partial_t f + \mathbf{v} \cdot \nabla_{\mathbf{x}} f + \partial_{\mathbf{r}} \cdot (\mathbf{Lr}f)] d\mathbf{r} = \int \mathbf{rr} \left[\partial_{\mathbf{r}} \cdot \left(-\frac{\mathbf{F}}{\zeta} f + \frac{kT}{\zeta} \partial_{\mathbf{r}} f \right) \right] d\mathbf{r} \quad (17.8)$$

We use the following calculations:

$$\begin{aligned} \int \mathbf{rr} \partial_t f d\mathbf{r} &= \partial_t \langle \mathbf{rr} \rangle \\ \int \mathbf{rr} (\mathbf{v} \cdot \nabla_{\mathbf{x}} f) d\mathbf{r} &= \mathbf{v} \cdot \nabla_{\mathbf{x}} \langle \mathbf{rr} \rangle \\ \int \mathbf{rr} \nabla_{\mathbf{r}} \cdot (\mathbf{Lr}f) d\mathbf{r} &= -\mathbf{L} \langle \mathbf{rr} \rangle - \langle \mathbf{rr} \rangle \mathbf{L}^T \\ \int \mathbf{rr} \nabla_{\mathbf{r}} \cdot \left(\frac{1}{\zeta} \nabla_{\mathbf{r}} \Phi f \right) d\mathbf{r} &= -\frac{2}{\zeta} \langle (\nabla_{\mathbf{r}} \Phi) \mathbf{r} \rangle \\ \int \mathbf{rr} \nabla_{\mathbf{r}} \cdot \left(\frac{k_B T}{\zeta} \nabla_{\mathbf{r}} f \right) d\mathbf{r} &= \frac{2k_B T}{\zeta} I, \end{aligned}$$

where the third equation in component form is

$$\begin{aligned} \int r_i r_j \partial_{r_k} (L_i^k r_l f) dr &= - \int \left(\delta_{ik} r_j L_i^k r_l f + \delta_{kj} r_i L_i^k r_l f \right) dr \\ &= - \int \left(L_i^i r_l r_j f + L_i^j r_i r_l f \right) dr \end{aligned}$$

Finally, equation (17.8) reads

$$\partial_t \langle \mathbf{r}\mathbf{r} \rangle + \mathbf{v} \cdot \partial_{\mathbf{x}} \langle \mathbf{r}\mathbf{r} \rangle - (\nabla \mathbf{v}) \cdot \langle \mathbf{r}\mathbf{r} \rangle - \langle \mathbf{r}\mathbf{r} \rangle \cdot (\nabla \mathbf{v})^T = \frac{2kT}{\zeta} \left(I - \frac{3}{R^2} \langle \mathbf{r}\mathbf{r} \rangle \right).$$

In terms of the conformation tensor, it is

$$\boxed{\mathbf{c}_{(1)} := \partial_t \mathbf{c} + \mathbf{v} \cdot \partial_{\mathbf{x}} \mathbf{c} - (\nabla \mathbf{v}) \cdot \mathbf{c} - \mathbf{c} \cdot (\nabla \mathbf{v})^T = \frac{2kT}{\zeta} \left(I - \frac{3}{R^2} \mathbf{c} \right).} \quad (17.9)$$

Here, we abbreviate the left-hand side of (17.9) 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} . 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 $\frac{4kT}{\zeta} I$ as $t \rightarrow \infty$, due to the damping, spring forcing and random forcing.

3. Kramers formula in terms of \mathbf{c} . From (17.7), we can express σ_p in terms of \mathbf{c} :

$$\boxed{\sigma_p = -2nkTI + \frac{3nkT}{R^2} \mathbf{c}.} \quad (17.10)$$

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.⁵

⁵It 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

$$\mathbf{c}_{eq} = \frac{R^2}{3} I. \quad (17.11)$$

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

$$\tau_p = \sigma_p + p_p I = -nkTI + \frac{3nkT}{R^2} \mathbf{c}. \quad (17.12)$$

This is the Kramers formula for the extra stress.

Evolution equation for the extra stress Let us take the upper convected derivative on (17.12) to get

$$\tau_{p(1)} = \frac{3nkT}{R^2} \mathbf{c}_{(1)} - nkTI_{(1)} \quad (17.13)$$

Note that

$$-I_{(1)} = (\partial_t + \mathbf{v} \cdot \nabla)(-I) + (\nabla \mathbf{v})I + I(\nabla \mathbf{v})^T = \nabla \mathbf{v} + (\nabla \mathbf{v})^T := \dot{\boldsymbol{\epsilon}}.$$

By eliminating $\mathbf{c}_{(1)}$ from (17.13) and (17.9), we get

$$\boxed{s\tau_{p(1)} + \tau_p = \eta_p \dot{\boldsymbol{\epsilon}}}, \quad (17.14)$$

where

$$s = \frac{\zeta R^2}{12kT}, \quad \eta_p = nkTs. \quad (17.15)$$

It means that the stress will relax to the strain rate $\dot{\boldsymbol{\epsilon}}$ with relaxation time s . Here, η_p is the polymer viscosity.

17.4 Micro Model

Fibre space We introduce a fibre space \mathbf{F}_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 $\cup_{\mathbf{x} \in \Omega} \mathbf{F}_x$ forms the configuration space.

Fibre Dynamics We associate \mathbf{r} a potential function $\Phi(\mathbf{r})$, representing interaction potential of polymers. For instance,

$$\Phi(\mathbf{r}) = \frac{3k_B T}{2R^2} |\mathbf{r}|^2$$

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. According to the fluctuation-dissipation theorem, the strength of 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. In the small inertia limit (i.e. $m\ddot{\mathbf{r}}$ is small), this equation is reduced to the damped Langevin equation:

$$d\mathbf{r} = -\frac{1}{\zeta} \nabla_{\mathbf{r}}\Phi(\mathbf{r})dt + \sqrt{\frac{2k_B T}{\zeta}} dB. \quad (17.16)$$

This stochastic differential equation models the fiber dynamics.

Microscopic pdf and its dynamics The microscopic state is described by a probability distribution function (pdf) $f(t, \mathbf{r})$ of the random variable $\mathbf{r}(t)$ of (17.16).⁶ By applying Ito's formula to (17.16), the pdf f satisfies the Fokker-Planck equation:

$$\dot{f} + \nabla_{\mathbf{r}} \cdot \left[-\frac{1}{\zeta} (\nabla_{\mathbf{r}}\Phi) f \right] = \frac{k_B T}{\zeta} \Delta_{\mathbf{r}} f. \quad (17.17)$$

⁶ $f(t, \mathbf{r}) d\mathbf{r}$ is the probability that $\mathbf{r}(t)$ of (17.16) lies in $\mathbf{r} d\mathbf{r}$.

This is also known as the Kolmogorov forward equation. Its derivation is shown in the Appendix. Note that $\int f d\mathbf{r} = \text{const}$. We also note that this equation can be written as the following conservative transport equation

$$\dot{f} + \nabla_{\mathbf{r}} \cdot (\mathbf{v}_f f) = 0, \quad (17.18)$$

where

$$\mathbf{v}_f := -\frac{1}{\zeta} \left(\nabla_{\mathbf{r}} \Phi + k_B T \frac{\nabla_{\mathbf{r}} f}{f} \right) = -\frac{1}{\zeta} \nabla_{\mathbf{r}} (\Phi + k_B T \ln f). \quad (17.19)$$

The first term $-\nabla_{\mathbf{r}} \Phi$ is called the drift velocity, while the second term $-k_B T \frac{\nabla_{\mathbf{r}} f}{f}$ is called the diffusion velocity. The dynamics of the particle is a competition between the drift and the diffusion.

Free energy Let us define the Helmholtz free energy density

$$A(f) := \Phi f + k_B T f \ln f,$$

the specific Helmholtz energy (per unit mass)

$$\mathcal{A}(f) = \int A(f) d\mathbf{r},$$

and the chemical potential

$$\mu := \frac{\delta \mathcal{A}}{\delta f} = A_f = k_B T (\ln f + 1) + \Phi.$$

Then the flux velocity \mathbf{v}_f is

$$\mathbf{v}_f := -\frac{1}{\zeta} \nabla_{\mathbf{r}} \mu = -\frac{1}{\zeta} \nabla_{\mathbf{r}} A_f. \quad (17.20)$$

Dissipation of free energy By multiplying the Fokker-Planck equation (17.18) (17.20) by A_f

$$A_f \cdot \left(\dot{f} - \nabla_{\mathbf{r}} \cdot \left(f \frac{1}{\zeta} \nabla_{\mathbf{r}} A_f \right) \right) = 0$$

then integrating in \mathbf{r} over the fibre space,

$$\int A_f \dot{f} - \frac{1}{\zeta} A_f \nabla_{\mathbf{r}} \cdot (f \nabla_{\mathbf{r}} A_f) d\mathbf{r} = 0.$$

Using integration-by-part, one can show that the dynamics (17.17) 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 $t \rightarrow \infty$. As $t \rightarrow \infty$, $f \rightarrow f_{eq}$. The state f_{eq} is called an equilibrium state.

Equilibrium distribution At equilibrium, $A(f_{eq}) = 0$, 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} :

$$f_{eq}(\mathbf{r}) = C^{-1} \exp(-\Phi(\mathbf{r})/k_B T).$$

where C is a normalization constant. $C = \int \exp(-\Phi(\mathbf{r})/k_B T) d\mathbf{r}$.

Theorem 17.16. *When Φ is strictly convex and $\Phi(\mathbf{r}) \rightarrow \infty$ as $\mathbf{r} \rightarrow \infty$, then $f(t) \rightarrow f_{eq}$ as $t \rightarrow \infty$ 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.

17.5 Micro-Macro model

17.5.1 Smoluchowski equation

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 and by R at time 0.

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,

$$\mathbf{r} = FR = \frac{\partial \mathbf{x}^i}{\partial X^\alpha}(t, X) R^\alpha. \quad (17.21)$$

Here, R is the Lagrangian coordinate of the micro state variable. The volume form of the microscopic space satisfies

$$d\mathbf{r} = JdR.$$

Probability distribution function The dynamics of the micro structure is described by (17.16).

$$\dot{\mathbf{r}} = \mathbf{L}\mathbf{r} - \frac{1}{\zeta} \nabla_{\mathbf{r}} \Phi(\mathbf{r}) + \sqrt{\frac{2k_B T}{\zeta}} \frac{dB}{dt}. \quad (17.22)$$

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 (17.22) in the background flow $\mathbf{v}(t, \mathbf{x})$ is modified from (17.17). It is

$$\partial_t f + \mathbf{v} \cdot \nabla_{\mathbf{x}} f + \nabla_{\mathbf{r}} \cdot (\mathbf{L}\mathbf{r}f) = \nabla_{\mathbf{r}} \cdot \frac{1}{\zeta} [(\nabla_{\mathbf{r}}\Phi)f + k_B T \nabla_{\mathbf{r}} f]. \quad (17.23)$$

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 variational approach below.

17.5.2 Derivation of stress from kinetic dynamics – 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

$$\begin{aligned} \mathcal{S}[\mathbf{x}] &= \mathcal{K}[\mathbf{x}] - \mathcal{U}[\mathbf{x}], \\ \mathcal{K}[\mathbf{x}] &:= \int_0^t \int \rho(t, \mathbf{x}) \frac{1}{2} |\mathbf{v}(t, \mathbf{x})|^2 d\mathbf{x} dt \\ \mathcal{A}[\mathbf{x}] &:= \int_0^t \iint \rho(t, \mathbf{x}) A(f(t, \mathbf{x}, \mathbf{r})) d\mathbf{r} d\mathbf{x} dt, \\ \mathcal{U}[\mathbf{x}] &:= TS[\mathbf{x}] + \mathcal{A}[\mathbf{x}] \end{aligned}$$

- Note that we assume the system is adiabatic. That is, $S[\mathbf{x}(t, X)]$ is constant along a flow path. In the variation velow, the term TS makes no contribution. Thus, the variation of $\mathcal{T} - \mathcal{U}$ is the same as that of $\mathcal{T} - \mathcal{A}$.
- Another case is that if we consider the isothermal case. In this case, we use Helmholtz free energy. The temperature of fluid parcel remains constant during fluid motion.

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

$$\rho(\partial_t \mathbf{v} + \mathbf{v} \cdot \nabla \mathbf{v}) = \nabla_{\mathbf{x}} \cdot \boldsymbol{\sigma}, \quad (17.24)$$

where σ is given by

$$\sigma^{ij} = \rho \int \mathbf{r}^j (\partial_{\mathbf{r}^i} A_f) f d\mathbf{r} \quad (17.25)$$

We show this result in the following calculations.

1. We denote the variation of the flow map \mathbf{x} by $\dot{\mathbf{x}}$.⁷ The variation of kinetic energy with respect to the flow path \mathbf{x} is

$$\delta \mathcal{K}[\mathbf{x}] = - \int_0^T \int \rho_0(X) \dot{\mathbf{x}}(X, t) \cdot \dot{\mathbf{x}} dX dt.$$

Here, we have taken integration by part for the t -integration and used $\dot{\mathbf{x}}(0) = \dot{\mathbf{x}}(T) = 0$.

2. Next, we compute \dot{f} . Note that the variation of F is \dot{F} , which is $\frac{\partial \dot{\mathbf{x}}}{\partial X}$. From $\mathbf{r} = FR$, we get the variation of dynamic variable $\mathbf{r}(t)$ satisfying

$$\dot{\mathbf{r}} = \dot{F}R = \dot{F}F^{-1}\mathbf{r}.$$

Conservation of micro particles reads

$$\dot{f} + \nabla_{\mathbf{r}} \cdot (\dot{\mathbf{r}}f) = 0. \quad (17.26)$$

Combine these two formulae, the variation of f satisfies

$$\dot{f} = -\nabla_{\mathbf{r}} \cdot (\dot{F}F^{-1}\mathbf{r}f).$$

3. Let us compute the variation of the Helmholtz energy

$$\begin{aligned} \mathcal{A}[\mathbf{x}] &= \int_0^T \int_{\Omega} \int_{\mathbb{R}^3} \rho(t, \mathbf{x}) A(f(t, \mathbf{x}, \mathbf{r})) d\mathbf{r} d\mathbf{x} dt \\ &= \int_0^T \int_{\Omega_0} \rho_0(X) \int_{\mathbb{R}^3} A(f(t, \mathbf{x}(t, X), \mathbf{r})) d\mathbf{r} dX dt. \end{aligned}$$

Here, we have used $d\mathbf{x} = JdX$ and $\rho J = \rho_0$. We take variation of \mathcal{A} with respect to

⁷Suppose $\mathbf{x}(\cdot)$ is perturbed by an one-parameter family of path $\mathbf{x}^\varepsilon(t)$. Then $\dot{\mathbf{x}}$ denotes the time derivative, while $\dot{\mathbf{x}}$ denotes the derivative with respect to ε . In our earlier notation, $\dot{\mathbf{x}}(t) = \delta\mathbf{x}(t)$.

the flow map $\mathbf{x}(\cdot)$:

$$\begin{aligned}
\delta \mathcal{A}[\mathbf{x}] &= \iint \rho_0(X) \delta \int A(f) d\mathbf{r} dX dt \\
&= \iint \rho_0(X) \left(\int A_f \dot{f} d\mathbf{r} \right) dX dt \\
&= - \iint \rho_0(X) \left(\int A_f \nabla_{\mathbf{r}} \cdot (\dot{F} F^{-1} \mathbf{r} f) d\mathbf{r} \right) dX dt \\
&= \iint \rho_0(X) \left(\int (\nabla_{\mathbf{r}} A_f) \cdot (\dot{F} F^{-1} \mathbf{r} f) d\mathbf{r} \right) dX dt \\
&= \iint \rho_0(X) \left(\int (\nabla_{\mathbf{r}} A_f) \cdot \left(\frac{\partial \dot{\mathbf{x}}}{\partial X} F^{-1} \mathbf{r} f \right) d\mathbf{r} \right) dX dt \\
&= - \iint \left[\nabla_X \cdot \left(\rho_0(X) \int (\nabla_{\mathbf{r}} A_f) (F^{-1} \mathbf{r} f) d\mathbf{r} \right) \right] \cdot \dot{\mathbf{x}} dX dt
\end{aligned}$$

Thus,

$$\frac{\delta \mathcal{A}}{\delta \mathbf{x}} = -\nabla_X \cdot P,$$

where

$$\begin{aligned}
P(t, X) &:= \rho_0(X) \int (\nabla_{\mathbf{r}} A_f) F^{-1} \mathbf{r} f d\mathbf{r} = \rho_0(X) \int (\nabla_{\mathbf{r}} A_f) R f J dR, \\
P_{\beta}^i &= \rho_0 \int \partial_{\mathbf{r}^i} A_f R^{\beta} f J dR,
\end{aligned}$$

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

$$\begin{aligned}
\rho_0(X) \ddot{\mathbf{x}} - \nabla_X \cdot P &= 0 \quad (\text{in Lagrangian coordinate}) \\
\rho \dot{\mathbf{v}} - \nabla_{\mathbf{x}} \cdot \boldsymbol{\sigma} &= 0 \quad (\text{in Eulerian coordinate})
\end{aligned}$$

where

$$\begin{aligned}
\boldsymbol{\sigma} &:= J^{-1} P F^T = J^{-1} P_{\beta}^i F_{\beta}^j \\
&= J^{-1} \rho_0 \int (\partial_{\mathbf{r}^i} A_f) R^{\beta} f J dR F_{\beta}^j \\
&= \rho \int (\partial_{\mathbf{r}^i} A_f) F_{\beta}^j R^{\beta} f J dR \\
&= \rho \int (\partial_{\mathbf{r}^i} A_f) \mathbf{r}^j f d\mathbf{r}.
\end{aligned}$$

$$\sigma^{ij} = \rho \int \mathbf{r}^j (\partial_{\mathbf{r}^i} A_f) f d\mathbf{r} \quad (17.27)$$

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

$$\begin{aligned} \sigma^{ij} &= \rho \int \mathbf{r}^j \partial_{\mathbf{r}^i} [\Phi(\mathbf{r}) + T k_B (\ln f + 1)] f d\mathbf{r} \\ &= \rho \int (\mathbf{r}^j \Phi_{\mathbf{r}^i} f + T k_B \mathbf{r}^j f_{\mathbf{r}^i}) d\mathbf{r} \\ &= \rho \int (\mathbf{r}^j \Phi_{\mathbf{r}^i} f - T k_B \delta^{ij} f) d\mathbf{r} \\ &= \rho \langle (\partial_{\mathbf{r}^i} \Phi) \mathbf{r}^j \rangle - \rho T k_B \delta^{ij} \end{aligned}$$

Thus,

$$\sigma = \rho \langle (\nabla_{\mathbf{r}} \Phi) \otimes \mathbf{r} \rangle - \rho k_B T I, \quad (17.28)$$

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 (17.23) 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.

17.5.3 Derivation of stress from kinetic dynamics – 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 $\mathbf{x}(t, X)$, which is the integral curve of the vector field $\mathbf{v}(t, \mathbf{x})$, and given a pseudo-velocity field $\mathbf{w}(t, \mathbf{x})$, we consider the following one-parameter family of flow maps $\mathbf{x}^s(t, X)$ satisfying

$$\partial_s \mathbf{x}^s(t, X) = \mathbf{w}(s, \mathbf{x}^s(t, X)), \quad \mathbf{x}^0(t, X) = \mathbf{x}(t, X).$$

This is a perturbation of $\mathbf{x}(t, X)$ in direction $\mathbf{w}(t, X)$.

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

$$\partial_s \rho^s + \nabla_{\mathbf{x}} \cdot (\mathbf{w} \rho^s) = 0, \quad (17.29)$$

$$\partial_s f^s + \mathbf{w} \cdot \nabla_{\mathbf{x}} f^s + \nabla_{\mathbf{r}} \cdot ((\nabla_{\mathbf{x}} \mathbf{w}) \mathbf{r} f^s) = 0. \quad (17.30)$$

The second equation is from

$$\dot{f} + \nabla_{\mathbf{r}} \cdot (\dot{\mathbf{r}}f) = 0,$$

and $\mathbf{r} = FR$,

$$\dot{\mathbf{r}} = \dot{F}F^{-1}\mathbf{r} = \nabla_{\mathbf{x}}\mathbf{w}\mathbf{r}.$$

The term $\partial_s \rho^s$ and $\partial_s f^s$ are the dynamically accessible variations $\delta\rho$ and δf .

5. Now we take variation of \mathcal{A} with respect to \mathbf{v} in direction \mathbf{w} with ρ and f satisfying the constraints (17.29),(17.30).

$$\delta \int \rho(t, \mathbf{x}) \left(\int A(f(t, \mathbf{x}, \mathbf{r})) d\mathbf{r} \right) d\mathbf{x} = \int (\delta\rho)\bar{A} d\mathbf{x} + \int \rho(\delta\bar{A}) d\mathbf{x} = I + II.$$

$$I = \int \delta\rho\bar{A} d\mathbf{x} = - \int (\nabla_{\mathbf{x}} \cdot (\rho\mathbf{w}))\bar{A} d\mathbf{x} = \int \rho \nabla_{\mathbf{x}}\bar{A} \cdot \mathbf{w} d\mathbf{x}.$$

$$\begin{aligned} II &= \int \rho(\delta\bar{A}) d\mathbf{x} = \int \rho \frac{\delta\bar{A}}{\delta f} \cdot \delta f d\mathbf{x} \\ &= \int \rho \int A_f [-\mathbf{w} \cdot \nabla_{\mathbf{x}}f - \nabla_{\mathbf{r}} \cdot ((\nabla_{\mathbf{x}}\mathbf{w})\mathbf{r}f)] d\mathbf{r} d\mathbf{x} \\ &= \int \rho \left[- \int A_f \nabla_{\mathbf{x}}f d\mathbf{r} \cdot \mathbf{w} + \int (\nabla_{\mathbf{r}}A_f) \cdot (\nabla_{\mathbf{x}}\mathbf{w})\mathbf{r}f d\mathbf{r} \right] d\mathbf{x} \\ &= - \int \rho \nabla_{\mathbf{x}} \left(\int A d\mathbf{r} \right) \cdot \mathbf{w} d\mathbf{x} - \int \nabla_{\mathbf{x}} \left[\rho \int (\nabla_{\mathbf{r}}A_f)\mathbf{r}f d\mathbf{r} \right] \cdot \mathbf{w} d\mathbf{x} \end{aligned}$$

Here,

$$\int d\mathbf{x} \rho \int d\mathbf{r} (-A_f \partial_{\mathbf{r}^i} (\partial_{\mathbf{x}^j} w^i \mathbf{r}^j)) = - \int d\mathbf{x} \partial_{\mathbf{x}^j} \left(\rho \int d\mathbf{r} (\partial_{\mathbf{r}^i} A_f) \mathbf{r}^j w^i \right),$$

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

$$\begin{aligned} \delta \int_{t_0}^{t_1} \int \rho \bar{A}[f] d\mathbf{x} dt &= - \int_{t_0}^{t_1} \int \nabla_{\mathbf{x}} \cdot \left[\rho \int (\nabla_{\mathbf{r}}A_f)\mathbf{r}f d\mathbf{r} \right] \cdot \mathbf{w} d\mathbf{x} dt \\ &= - \int_{t_0}^{t_1} \int \nabla_{\mathbf{x}} \cdot \boldsymbol{\sigma} \cdot \mathbf{w} d\mathbf{x} dt \end{aligned}$$

where

$$\boldsymbol{\sigma} = \rho \int (\nabla_{\mathbf{r}}A_f)\mathbf{r}f d\mathbf{r}. \quad (17.31)$$

6. Thus, the Euler-Lagrange equation is

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

Formula (17.31) is called the Kramers formula, or the Irving-Kirkwood formula, or the virial stress.

17.5.4 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

$$\partial_t \rho + \nabla_{\mathbf{x}} \cdot (\rho \mathbf{v}) = 0. \quad (17.32)$$

$$\rho(\partial_t \mathbf{v} + \mathbf{v} \cdot \nabla_{\mathbf{x}} \mathbf{v}) = \nabla_{\mathbf{x}} \cdot \boldsymbol{\sigma}, \quad (17.33)$$

the microscopic equation

$$\partial_t f + \mathbf{v} \cdot \nabla_{\mathbf{x}} f + \nabla_{\mathbf{r}} \cdot (\nabla_{\mathbf{r}} \mathbf{r} f) = \nabla_{\mathbf{r}} \cdot \frac{1}{\zeta} [(\nabla_{\mathbf{r}} \Phi) f + k_B T \nabla_{\mathbf{r}} f]. \quad (17.34)$$

and the coupling between micro and macro dynamics is through

$$\boldsymbol{\sigma} = -\rho k_B T \mathbf{I} + \rho \langle \mathbf{r} \nabla_{\mathbf{r}} \Phi \rangle, \quad \text{where } \langle (\cdot) \rangle := \int (\cdot) f d\mathbf{r}. \quad (17.35)$$

Incompressible viscoelastic flow ⁸ 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

$$\begin{cases} \rho(\partial_t \mathbf{v} + \mathbf{v} \cdot \nabla \mathbf{v}) + \nabla p = \eta \Delta \mathbf{v} + \nabla \cdot \boldsymbol{\tau} \\ \nabla \cdot \mathbf{v} = 0 \\ \boldsymbol{\tau} = n_p (-k_B T \mathbf{I} + \mathbb{E}[\mathbf{r}_t \otimes \mathbf{F}(\mathbf{r}_t)]) \\ d\mathbf{r}_t + \mathbf{v} \cdot \nabla_{\mathbf{x}} \mathbf{r}_t dt = \left((\nabla_{\mathbf{x}} \mathbf{v}) \mathbf{r}_t - \frac{2}{\zeta} \mathbf{F}(\mathbf{r}_t) \right) dt + \sqrt{\frac{4k_B T}{\zeta}} dW_t \end{cases} \quad (17.36)$$

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.

⁸Ref. C. Le Bris, T. Lelièvre, Micro-macro models for viscoelastic fluids: modelling, mathematics and numerics.

The non-dimensional model is

$$\begin{cases} Re(\partial_t \mathbf{v} + \mathbf{v} \cdot \nabla \mathbf{v}) + \nabla p = (1 - \varepsilon) \Delta \mathbf{v} + \nabla \cdot \boldsymbol{\tau} \\ \nabla \cdot \mathbf{v} = 0 \\ \boldsymbol{\tau} = \frac{\varepsilon}{We} (-kTI + \mathbb{E}[\mathbf{r}_t \otimes \mathbf{F}(\mathbf{r}_t)]) \\ d\mathbf{r}_t + \mathbf{v} \cdot \nabla_{\mathbf{x}} \mathbf{r}_t dt = ((\nabla_{\mathbf{x}} \mathbf{v}) \mathbf{r}_t - \frac{1}{2We} \mathbf{F}(\mathbf{r}_t)) dt + \frac{1}{\sqrt{We}} dW_t \end{cases} \quad (17.37)$$

The parameters are

$$Re = \frac{\rho UL}{\eta}, \quad We = \frac{\lambda U}{L}, \quad \varepsilon = \frac{\eta_p}{\eta}$$

where Re is the Reynolds number and We is the Weissenberg 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

$$\begin{cases} Re(\partial_t \mathbf{v} + \mathbf{v} \cdot \nabla \mathbf{v}) + \nabla p = (1 - \varepsilon) \Delta \mathbf{v} + \nabla \cdot \boldsymbol{\tau} \\ \nabla \cdot \mathbf{v} = 0 \\ \boldsymbol{\tau} = \frac{\varepsilon}{We} (-I + \int (\mathbf{r}_t \otimes \mathbf{F}(\mathbf{r}_t)) f d\mathbf{r}) \\ \partial_t f + \mathbf{v} \cdot \nabla_{\mathbf{x}} f + \nabla_{\mathbf{r}} \cdot ((\nabla_{\mathbf{x}} \mathbf{v}) \mathbf{r} f) = \nabla_{\mathbf{r}} \cdot \left(\frac{1}{2We} \mathbf{F}(\mathbf{r}) f \right) + \frac{1}{2We} \Delta_{\mathbf{r}} f. \end{cases} \quad (17.38)$$

Energy dissipation The dissipation of energy is

$$\begin{aligned} \frac{d}{dt} \int_{\Omega} \left[\frac{1}{2} \rho \mathbf{v}^2 + \left(\int_{\mathbb{R}^3} \frac{\sigma^2}{2} f \ln f + \Phi f d\mathbf{r} \right) \right] d\mathbf{x} \\ = - \int_{\Omega} \int_{\mathbb{R}^3} f |\nabla_{\mathbf{r}} \mu|^2 d\mathbf{r} d\mathbf{x} \leq 0. \end{aligned}$$

17.6 Macro models – 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 $\langle \mathbf{r}\mathbf{r} \rangle$, 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.⁹

Conformation tensor Let us define the conformation tensor as

$$\mathbf{c} := \int \mathbf{r}\mathbf{r} f(t, \mathbf{x}, \mathbf{r}) d\mathbf{r} := \langle \mathbf{r}\mathbf{r} \rangle.$$

It represents the second moment of the micro configuration of the polymeric structure. By Taking $\int \mathbf{r}\mathbf{r} (17.23) d\mathbf{r}$, we obtain

$$\mathbf{c}_t + \mathbf{v} \cdot \nabla_{\mathbf{x}} \mathbf{c} - (\nabla \mathbf{v}) \cdot \mathbf{c} - \mathbf{c} \cdot (\nabla \mathbf{v})^T = \frac{1}{\zeta} [2k_B T I - 2\langle (\nabla_{\mathbf{r}} \Phi) \mathbf{r} \rangle]. \quad (17.39)$$

In the above formula, we have used the following calculations:

$$\begin{aligned} \int \mathbf{r}\mathbf{r} \partial_t f d\mathbf{r} &= \partial_t \langle \mathbf{r}\mathbf{r} \rangle \\ \int \mathbf{r}\mathbf{r} (\mathbf{v} \cdot \nabla_{\mathbf{x}} f) d\mathbf{r} &= \mathbf{v} \cdot \nabla_{\mathbf{x}} \langle \mathbf{r}\mathbf{r} \rangle \\ \int \mathbf{r}\mathbf{r} \nabla_{\mathbf{r}} \cdot (\nabla_{\mathbf{x}} \mathbf{v} f) d\mathbf{r} &= -\nabla_{\mathbf{x}} \mathbf{v} \cdot \langle \mathbf{r}\mathbf{r} \rangle - \langle \mathbf{r}\mathbf{r} \rangle \cdot (\nabla_{\mathbf{x}} \mathbf{v})^T \\ \int \mathbf{r}\mathbf{r} \nabla_{\mathbf{r}} \cdot \left(\frac{1}{\zeta} \nabla_{\mathbf{r}} \Phi f \right) d\mathbf{r} &= -\frac{2}{\zeta} \langle (\nabla_{\mathbf{r}} \Phi) \mathbf{r} \rangle \\ \int \mathbf{r}\mathbf{r} \nabla_{\mathbf{r}} \cdot \left(\frac{k_B T}{\zeta} \nabla_{\mathbf{r}} f \right) d\mathbf{r} &= \frac{2k_B T}{\zeta} I. \end{aligned}$$

In component form, the third equation is

$$\begin{aligned} \int r_i r_j \partial_{r_k} (L_i^k r_l f) d\mathbf{r} &= - \int \left(\delta_{ik} r_j L_i^k r_l f + \delta_{kj} r_i L_i^k r_l f \right) d\mathbf{r} \\ &= - \int \left(L_i^i r_l r_j f + L_i^j r_i r_l f \right) d\mathbf{r} \\ &= -L\mathbf{c} - \mathbf{c}L^T. \end{aligned}$$

⁹Wiki, 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 (17.39) by

$$\mathbf{c}_{(1)} = \frac{2k_B T}{\zeta} I - \frac{2}{\zeta} \langle (\nabla_{\mathbf{r}} \Phi) \mathbf{r} \rangle. \quad (17.40)$$

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 $\Phi(\mathbf{r}) = 3k_B T |\mathbf{r}|^2 / 2R^2$, we obtain

$$\langle (\nabla_{\mathbf{r}} \Phi) \mathbf{r} \rangle = \frac{3k_B T}{R^2} \mathbf{c}.$$

Plug this into (17.40) and (17.35), we obtain the evolution equation of the conformation tensor \mathbf{c} :

$$\mathbf{c}_{(1)} = \frac{2k_B T}{\zeta} \left(I - \frac{3}{R^2} \mathbf{c} \right). \quad (17.41)$$

The Kramers formula for the Hookean potential is

$$\boldsymbol{\sigma} = -\rho k_B T I + \rho \frac{3k_B T}{R^2} \mathbf{c}. \quad (17.42)$$

We can eliminate \mathbf{c} to get an evolution equation for $\boldsymbol{\sigma}$:

$$\begin{aligned} \boldsymbol{\sigma}_{(1)} &= -\rho k_B T I_{(1)} + \rho \frac{3k_B T}{R^2} \mathbf{c}_{(1)} \\ &= \rho k_B T (\nabla \mathbf{v} + (\nabla \mathbf{v})^T) + \rho \frac{3k_B T}{R^2} \frac{2k_B T}{\zeta} \left(I - \frac{3}{R^2} \mathbf{c} \right) \\ &= \rho k_B T (\nabla \mathbf{v} + (\nabla \mathbf{v})^T) - \frac{6k_B T}{R^2 \zeta} \boldsymbol{\sigma}. \end{aligned}$$

This is the evolution equation for $\boldsymbol{\sigma}$. It is precisely the Maxwell model.

17.7 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 18

Two Phase Flows

18.1 Two-fluid model

18.1.1 Inviscid flows

Consider two simple fluids occupied region Ω_i , $i = 1, 2$ connected by an 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 ρ_i are constants. On the boundary Γ_t , the divergence free condition ($\nabla \cdot \mathbf{v}_i = 0$) leads to

$$[\mathbf{v}] \cdot \boldsymbol{\nu} = 0 \quad \text{on } \Gamma_t,$$

where $[\mathbf{v}] := \mathbf{v}_2 - \mathbf{v}_1$ and $\boldsymbol{\nu}$ is the normal of Γ_t . This implies that the motion of the interface, which can be characterized by its normal velocity $v_n = v_n \boldsymbol{\nu}$, satisfies

$$v_n = \mathbf{v}_1 \cdot \boldsymbol{\nu} = \mathbf{v}_2 \cdot \boldsymbol{\nu}.$$

For force balance on the interface, we have

$$[p] \boldsymbol{\nu} = \boldsymbol{\sigma} \cdot \boldsymbol{\nu}$$

where $\boldsymbol{\sigma}$ is the stress on the surface. If the surface is infinitesimal thin, then $\boldsymbol{\sigma} = \boldsymbol{\sigma} H \boldsymbol{\nu} \otimes \boldsymbol{\nu}$. Here, H is the mean curvature of the surface.

Given v_n , we can solve (\mathbf{v}_i, p_i) on domains Ω_i with boundary conditions: $\mathbf{v}_i \cdot \boldsymbol{\nu} = v_n$ on the boundary $\partial\Omega_i$. On the interface Γ_t , we need two conditions to move the interface. The interface normal velocity v_n in turn, is determined by the other interface condition: $[p] = \boldsymbol{\sigma} H$.

18.1.2 Viscous flows

Now we consider two viscous flows occupy two domains Ω_i and is connected by an interface Γ_t . The governed equations in each region Ω_i are the Navier-Stokes equation:

$$\begin{cases} \nabla \cdot \mathbf{v}_i = 0 \\ \rho_i(\partial_t \mathbf{v}_i + \mathbf{v}_i \cdot \nabla \mathbf{v}_i) + \nabla p_i = \nabla \cdot \mu_i \nabla \mathbf{v}_i. \end{cases} \quad \text{in } \Omega_i$$

On the boundary Γ_t , due to viscosity, we should impose the condition

$$[\mathbf{v}] = 0.$$

This leads to

$$\mathbf{v}_1 = \mathbf{v}_2 = \mathbf{v},$$

where \mathbf{v} is the surface velocity. From momentum equation, the surface force due to an elastic material on Γ_t is $\sigma H \mathbf{v}$ (assume the elastic material is inviscid), σ is the surface tension and H is the mean curvature of the surface. Let $\boldsymbol{\tau}_i := \mu_i \nabla \mathbf{v}_i - p_i \mathbf{I}$ be the stress tensor of the fluid i in region Ω_i . Then the force balance law on the interface is

$$[\boldsymbol{\tau}] \cdot \mathbf{v} = \sigma H \mathbf{v}.$$

If \mathbf{v} is given, then the condition $\mathbf{v}_i = \mathbf{v}$ and N-S equation can determine the flow in Ω_i . On the other hand, there are three conditions in $[\boldsymbol{\tau}] \cdot \mathbf{v} = \sigma H \mathbf{v}$ to determine the interfacial velocity \mathbf{v} .

18.2 Phase field models based on labeled order parameter – Allan-Cahn Model

18.2.1 Order parameter and free energy

In fluid system, we may encounter two different kinds of fluids in a fluid system. For example, oil and water, water and gas, or even have more compositions. We may use a label function to indicate which material it is at a position \mathbf{x} . Such a label function is called order parameter in physics literature. 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:** ϕ is a phase label of the fluids. In this case, ϕ convects with the fluid flow. 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 mass, concentration, etc. In this case, ϕ satisfies

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

which yields

$$\phi(t, \mathbf{x}(t, X))J(t, X) = \phi_0(X).$$

Free energy One can associate ϕ with a free energy \mathcal{F} defined by

$$\mathcal{F}[\phi] = \int_{\Omega} f(\phi, \nabla\phi) d\mathbf{x} = \int_{\Omega} \frac{1}{2\varepsilon} |\nabla\phi|^2 + \frac{1}{\varepsilon} W(\phi) d\mathbf{x}$$

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 the surface energy. It means that same phase material likes to group together. It costs some energy by putting materials with different phase together. 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 $\mathcal{F}[\phi]$ measures surface energy.

Chemical potential The variation of free energy \mathcal{F} w.r.t. ϕ is called the chemical potential

$$\mu := \frac{\delta \mathcal{F}}{\delta \phi} = -\nabla \cdot \frac{\partial f}{\partial \nabla \phi} + \frac{\partial f}{\partial \phi}. \quad (18.1)$$

18.2.2 Variation of free energy w.r.t. flow motion

Dynamically accessible variations Given a flow map $\mathbf{x}(t, X)$ and an arbitrarily vector field $\mathbf{w}(\mathbf{x})$:

$$\mathbf{w} : M \rightarrow TM$$

We define a perturbation of \mathbf{x} in the direction \mathbf{w} as the following flow maps

$$\frac{\partial}{\partial s} \mathbf{x}^s(t, X) = \mathbf{w}(\mathbf{x}^s(t, X)), \quad \mathbf{x}^0(t, X) = \mathbf{x}(t, X). \quad (18.2)$$

The quantity

$$\delta \mathbf{x}(t, X) := \left. \frac{\partial \mathbf{x}^s(t, X)}{\partial s} \right|_{s=0} = \mathbf{w}(\mathbf{x}(t, X))$$

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

$$\delta \phi := \left. \frac{\partial}{\partial s} \right|_{t, X} \phi^s(t, \mathbf{x}^s(t, X)) \text{ at } s = 0,$$

is called a dynamically accessible variation of ϕ . It satisfies

$$\partial_s \phi + \mathbf{w} \cdot \nabla \phi = 0.$$

Variation of free energy \mathcal{F} w.r.t. flow motion The variation of \mathcal{F} at a flow map \mathbf{x} along the tangent direction \mathbf{w} is a Frechet derivative of \mathcal{F} along \mathbf{x}^s :

$$\begin{aligned} \delta \mathcal{F} \cdot \mathbf{w} &= \frac{\delta \mathcal{F}}{\delta \phi^s} \frac{\partial \phi^s}{\partial s} \\ &= \mu(-\mathbf{w} \cdot \nabla \phi) \\ &= -\mu \nabla \phi \cdot \mathbf{w} \end{aligned}$$

Equation of Motion The action is defined to be

$$\mathbb{S}[\mathbf{x}] = \int_0^T \int_{\Omega_0} \frac{1}{2} \rho_0(X) |\dot{\mathbf{x}}(t, X)|^2 - f(\phi, \nabla \phi)(t, \mathbf{x}(t, X)) J(t, X) dX dt.$$

The potential energy is indeed the functional

$$\mathcal{F}(\phi) = \int_{\Omega_t} f(\phi(t, \mathbf{x}), \nabla \phi(t, \mathbf{x})) d\mathbf{x}.$$

The variation of action w.r.t. flow motion gives

$$\rho \frac{D\mathbf{v}}{Dt} = \mu \nabla \phi, \quad \mu := \frac{\delta \mathcal{F}}{\delta \phi} = -\nabla \cdot \frac{\partial f}{\partial \nabla \phi} + \frac{\partial f}{\partial \phi}.$$

This together with

$$\begin{aligned} \partial_t \phi + \mathbf{v} \cdot \nabla \phi &= 0, \\ \partial_t \rho + \nabla \cdot (\rho \mathbf{v}) &= 0, \end{aligned}$$

give the set of equations for (ρ, ϕ, \mathbf{v}) .

Conservation of energy We multiply momentum equation by \mathbf{v} then integrate in X and in t to get

$$\frac{d}{dt} \int \frac{1}{2} \rho |\mathbf{v}|^2 dx = \int \mu \mathbf{v} \cdot \nabla \phi dx = - \int \mu \partial_t \phi dx = - \int \frac{\delta \mathcal{F}}{\delta \phi} \cdot \partial_t \phi dx = - \frac{d\mathcal{F}}{dt}$$

That is

$$\frac{d}{dt} \mathcal{E} = \frac{d}{dt} \left(\int \frac{1}{2} \rho |\mathbf{v}|^2 dx + \int f(\phi, \nabla \phi) dx \right) = 0.$$

This is the conservation of total energy. It also shows that the force $\mu \nabla \phi$ is the opposite force of the convection of ϕ .

Dissipation of the velocity One can add dissipation term in the momentum equation:

$$\rho \frac{D\mathbf{v}}{Dt} = \mu \nabla \phi + \nabla \cdot \boldsymbol{\tau}$$

where

$$\boldsymbol{\tau} = \nu \left(\nabla \mathbf{v} + (\nabla \mathbf{v})^T - \frac{2}{3} \nabla \cdot \mathbf{v} I \right) + \lambda \nabla \cdot \mathbf{v} I,$$

is the viscous stress. It will dissipate the kinetic energy.

Dissipation of order parameter The order parameter has a tendency to move from high potential energy to low potential energy. For Allan-Cahn model, it is simply defined by

$$\partial_t \phi + \mathbf{v} \cdot \nabla \phi = - \frac{\delta \mathcal{F}}{\delta \phi} = -\mu.$$

The dissipation of energy can be obtained by multiplying momentum equation by \mathbf{v} , multiplying advection equation by μ , then adding them together:

$$\left(\rho \frac{D\mathbf{v}}{Dt} \cdot \mathbf{v} - \mu \nabla \phi \cdot \mathbf{v} \right) + \left(\mu \partial_t \phi + \mu \mathbf{v} \cdot \nabla \phi \right) = \mathbf{v} \cdot \nabla \cdot \boldsymbol{\sigma} - \mu^2.$$

This gives

$$\frac{d\mathcal{E}}{dt} = -\boldsymbol{\sigma} \cdot \nabla \mathbf{v} - \mu^2.$$

The viscous dissipation becomes

$$-\boldsymbol{\sigma} \cdot \nabla \mathbf{v} = -\nu |\nabla \mathbf{v} + (\nabla \mathbf{v})^T|^2 - \lambda |\nabla \cdot \mathbf{v}|^2.$$

18.3 Phase field models based on conservative order parameter – Cahn-Hilliard model

18.3.1 Variation of free energy w.r.t. predomain

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 \mathcal{F} w.r.t. \mathbf{x}^s is

$$\begin{aligned} \delta \mathcal{F} \cdot \mathbf{w} &= \frac{\delta \mathcal{F}}{\delta \phi^s} \frac{\partial \phi^s}{\partial s} \\ &= \int \mu (-\nabla \cdot (\phi \mathbf{w})) d\mathbf{x} \\ &= \int \phi \nabla \mu \cdot \mathbf{w} d\mathbf{x} \end{aligned}$$

Conserved order parameter In the case

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

The force from the convection becomes

$$\rho \frac{D\mathbf{v}}{Dt} = -\phi \nabla \mu.$$

This together with

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

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

give a set of equations for (ρ, ϕ, \mathbf{v}) .

Conservation of energy For the energy equation, we multiply the above equation by \mathbf{v} , take integration by part:

$$\begin{aligned} \frac{d}{dt} \int \frac{1}{2} \rho |\mathbf{v}|^2 dx &= - \int \phi \nabla \mu \cdot \mathbf{v} dx = \int \mu \nabla \cdot (\phi \mathbf{v}) dx \\ &= - \int \mu \partial_t \phi dx = - \int \frac{\delta \mathcal{F}}{\delta \phi} \cdot \partial_t \phi dx = - \frac{d\mathcal{F}}{dt} \end{aligned}$$

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

$$\frac{d\mathcal{E}}{dt} = -\tau \cdot \nabla \mathbf{v} - m |\nabla \mu|^2.$$

18.4 Interface structure

18.4.1 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.

$$\mathcal{F}[\phi] = \int f(\nabla \phi, \phi) dx$$

1. Let

$$f(\nabla \phi, \phi) = \frac{\varepsilon}{2} |\nabla \phi|^2 + \frac{1}{\varepsilon} W(\phi) dx$$

where W is a double well potential. As $\varepsilon \rightarrow 0$, $\phi \rightarrow \pm 1$. The interface energy tends to

$$\mathcal{F}[\phi] \rightarrow \sigma_0 |\Gamma(t)|.$$

where σ_0 is a constant.

2. Mean curvature:

$$\int_{\Omega(t)} \frac{\eta}{2} \left(\Delta \phi - \frac{1}{\eta^2} W'(\phi) \right)^2 d\mathbf{x} \approx \int_{\Gamma(t)} H^2 dS.$$

3. Gaussian curvature:

$$\int_{\Omega(t)} \left(\eta \Delta \phi - \frac{1}{\eta} W'(\phi) \right) W'(\phi) d\mathbf{x} \approx \int_{\Gamma(t)} K dS.$$

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. $\varepsilon \Delta V = n - p$.

18.4.2 Structure of one dimensional interface

Allen-Cahn interface The order parameter satisfies

$$\phi_t = -\frac{\delta \mathcal{F}}{\delta \phi} = \Delta \phi - W'(\phi)$$

where

$$\mathcal{F} = \int \frac{1}{2} |\nabla \phi|^2 + W(\phi) d\mathbf{x}$$

$$W(\phi) = \frac{1}{4} (\phi^2 - 1)^2.$$

The interface is assumed to be steady, so $\phi_t = 0$. Thus, we want to solve

$$\Delta \phi - W'(\phi) = 0.$$

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:

$$\phi' = \sqrt{2W} \quad (18.3)$$

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

$$\mathcal{F}^\varepsilon[\phi^\varepsilon] = \int \frac{\varepsilon}{2} |\nabla \phi^\varepsilon|^2 + \frac{1}{\varepsilon} W(\phi^\varepsilon) dx$$

This gives the traveling wave equation

$$\varepsilon \Delta \phi^\varepsilon - \frac{1}{\varepsilon} W'(\phi^\varepsilon) = 0.$$

Taking $\phi^\varepsilon(x) = \phi(x/\varepsilon)$, we get the rescaled equation. Notice that in \mathcal{F} , the energy for the traveling wave solution ϕ^ε is

$$\mathcal{F}^\varepsilon[\phi^\varepsilon] = \mathcal{F}[\phi] = \sigma_0.$$

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 $\delta \mathcal{F} / \delta \phi = 0$, we get

$$-c\phi' - \Delta\phi + W'(\phi) = 0.$$

Cahn-Hilliard interface The Cahn-Hilliard equation is

$$\phi_t = -\nabla \cdot (m \nabla \mu), \quad \mu = -\frac{\delta \mathcal{F}}{\delta \phi}.$$

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,

$$\phi' = \pm (W(\phi) - W(1) - \mu_0(\phi - 1))^{1/2}.$$

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 equilibria of the double well potential W . Thus, the only admissible chemical potential connecting two equilibria 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

$$u_t = \Delta u + f(u)$$

where $f(u)$ has two equilibria 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
- $(F^{-1}) = \frac{\partial X}{\partial \mathbf{x}}$: inverse deformation gradient (for the use in Eulerian coordinate)
- $B = F F^T$: Right Cauchy-Green strain
- $E = \frac{1}{2} (F + F^T) - I$: Green-St. Venant strain.
- $\varepsilon = \frac{1}{2} \left(\frac{\partial u^i}{\partial x^j} + \frac{\partial u^j}{\partial x^i} \right)$: strain
- $(e_{kl}) = \frac{1}{2} \left(\frac{\partial u^k}{\partial X^l} + \frac{\partial u^l}{\partial X^k} \right)$: Infinitesimal strain

Strain-rate

- $D = \frac{1}{2} (\nabla \mathbf{v} + (\nabla \mathbf{v})^T)$: rate-of-strain, strain-rate tensor
- $\dot{\gamma} = 2D = \dot{\epsilon}$: rate-of-strain
- $S = \frac{1}{2} (\nabla \mathbf{v} - (\nabla \mathbf{v})^T)$: 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 $F_\alpha^i = \partial x^i / \partial X^\alpha$ 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

$$w^i = F_\alpha^i v^\alpha.$$

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 $\{X(t) | 0 \leq t \leq 1\}$ 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 spanned 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

$$N = \frac{\frac{\partial \mathbf{x}}{\partial X^1} \times \frac{\partial \mathbf{x}}{\partial X^2}}{\left\| \frac{\partial \mathbf{x}}{\partial X^1} \times \frac{\partial \mathbf{x}}{\partial X^2} \right\|}$$

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,

$$\begin{aligned} II(X'(0)) &:= -L_{\alpha\beta} X'^\alpha(0) X'^\beta(0) \\ &= - \left(\frac{\partial N}{\partial X^\alpha} X'^\alpha(0), \frac{\partial \mathbf{x}}{\partial X^\beta} X'^\beta(0) \right) \\ &= -(N'(0), \mathbf{x}'(0)) = (N(0), \mathbf{x}''(0)) = (N, kn) = k_n. \end{aligned}$$

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 II w.r.t. the first fundamental form g is called the principal curvature of the surface. If we define

$$W := g^{-1} II,$$

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
- 2.

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

$$w^i = F_\alpha^i v^\alpha.$$

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

$$F_\beta^i w^i = F_\beta^i F_\alpha^i v^\alpha$$

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 $dX^\alpha(\partial / \partial X^\beta) = \delta_\beta^\alpha$. 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

$$\omega_i \frac{\partial x^i}{\partial X^\alpha} dX^\alpha = \omega_i F_\alpha^i dX^\alpha$$

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 $v_i dx^j dx^k$, the vector (v_i) is also treated as a covector. Therefore, we can pull back them by $F^T \mathbf{v}$.

If \mathbf{v} is a unit covector in Σ and \mathbf{n} be the normalized pull back of \mathbf{v} under F , then

$$\mathbf{n} = J^{-1} F^T \mathbf{v}.$$

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 $\mathbf{v} \in T^*\Sigma$, then $n = J^{-1}F^T\mathbf{v}$. Let T be the tensor which maps a co-vector \mathbf{v} to a vector in $T\Sigma$. $T\mathbf{v}$ can be represented as $T^{ij}n_j\partial/\partial x_i$. If

$$T\mathbf{v} = P\mathbf{n},$$

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, $\hat{P} = W'(F^T F)$.

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 $(dX^\alpha, \partial/\partial X^\beta) = \delta_\beta^\alpha$. We can also define the gradient $\nabla_{\mathbf{x}}\phi$ to be

$$d\phi(\mathbf{w}) = (\nabla_{\mathbf{x}}\phi, \mathbf{w})$$

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

C.1 Some tensor notations

We shall use 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 \mathbf{v} , \mathbf{n} .
- A rank 2 tensor is a matrix, for example, the stress tensor $\boldsymbol{\sigma}$, \mathbf{I} .
- Tensor product $\mathbf{vw} := v^i w^j$.
- Scalar product $\mathbf{v} \cdot \mathbf{w} = v^i w^i$, $\boldsymbol{\sigma} \cdot \mathbf{v} = \sigma_j^i v^j$, $\mathbf{A} \cdot \mathbf{B} = A_j^i B_k^j$.
- Scalar product of rank 2 tensors $\mathbf{A} : \mathbf{B} = A_{ij} B_{ij}$.
- Nabla operator ∇ :

$$(\nabla \mathbf{v})_j^i := \frac{\partial v^i}{\partial x^j}$$

$$\nabla \cdot \mathbf{v} := \frac{\partial v^j}{\partial x^j},$$

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 use $\mathbf{v} \otimes \nabla$ to stand for $\partial_{x^i} v^j$. (e.g. Vlado A. Lubarda). We will only use $\nabla \mathbf{v}$ to stand for $\partial_{x^i} v^j$ and $\nabla \cdot \mathcal{F} = \partial_{x^i} \mathcal{F}_j$.

Theorem 3.17 (Divergence theorem). *Let $\mathcal{F} : \Omega(\subset \mathbb{R}^3) \rightarrow \mathbb{R}^m \times \mathbb{R}^3$ be a vector field. Then*

$$\int_{\partial\Omega} \mathcal{F} \cdot \mathbf{v} dS = \int_{\Omega} \nabla \cdot \mathcal{F} d\mathbf{x}.$$

Here, $\partial\Omega$ denotes for the boundary of Ω , dS is the surface element, and \mathbf{v} is the outer normal of $\partial\Omega$.

C.2 Tensors in Euler and Lagrange coordinates

C.2.1 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 $\varphi_t : \hat{M} \rightarrow M$. 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)	$e^i, e^i \cdot e_j = \delta_j^i$	$dx^i, (dx^i, \partial / \partial x^j) = \delta_j^i$
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	$v^i = g^{ij} v_j$	$\mathbf{v} = \mathbf{v}^\flat = \mathbf{v}^\sharp$
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	$\bar{g}^\alpha \cdot \bar{g}_\beta = \delta_\beta^\alpha$	$(dX^\alpha, \partial / \partial X^\beta) = \delta_\beta^\alpha$
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	$q^\alpha = g^{\alpha\beta} q_\beta$	$\bar{q} = \bar{q}^\flat = \bar{q}^\sharp$
Tensor product	$\bar{q}_1 \bar{q}_2$	$\bar{q}_1 \otimes \bar{q}_2$

C.2.2 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:

$$\bar{g}_\alpha := \frac{\partial x^i}{\partial X^\alpha} e_i = F_\alpha^i e_i.$$

In DG,

$$\bar{g}_\alpha = \frac{\partial}{\partial X^\alpha}.$$

The inner product of \bar{g}_α and \bar{g}_β is induced by the Euclidean space TM . Thus

$$\bar{g}_\alpha \cdot \bar{g}_\beta := \sum_k F_\alpha^k F_\beta^\ell e_k \cdot e_\ell = \sum_k F_\alpha^k F_\beta^k := g_{\alpha\beta}.$$

- Similarly, in T^*M , the corresponding Lagrangian frame is

$$\bar{g}^\beta = (F^{-1})^\beta_\ell e^\ell.$$

Since $F_\beta^i = \frac{\partial x^i}{\partial X^\beta}$, we get

$$(F^{-1})^\beta_\ell = \frac{\partial X^\beta}{\partial x^\ell}.$$

We have

$$\bar{g}_\alpha \cdot \bar{g}^\beta = \delta_\alpha^\beta$$

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:

$$\begin{aligned} (F)_\alpha^i &= F_\alpha^i = \frac{\partial x^i}{\partial X^\alpha} & (F^{-1})_i^\alpha &= \frac{\partial X^\alpha}{\partial x^i} \\ (F^T)_i^\alpha &= F_\alpha^i = \frac{\partial x^i}{\partial X^\alpha} & (F^{-T})_i^\alpha &= (F^{-1})_i^\alpha \end{aligned}$$

$$(F^T F)_{\alpha\beta} = (F^T)_k^\alpha F_\beta^k = F_\alpha^k F_\beta^k = \bar{g}_\alpha \cdot \bar{g}_\beta.$$

$$(F F^T)^{ij} = F_\alpha^i (F^T)_j^\alpha = F_\alpha^i F_\alpha^j$$

C.2.3 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 $\bar{\mathbf{v}}$. It is still the same vector, but in different coordinate system. Thus,

$$\mathbf{v} = v_i dx^i = v_i \frac{\partial x^i}{\partial X^k} dX^k = v_i F_k^i dX^k.$$

or its pull-back (same vector, but represented in Lagrange coordinate system)

$$\bar{p} = p_k \bar{g}^k$$

Thus,

$$p_k = v_i F_k^i.$$

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

$$p^i = g^{ij} p_j, \quad p_i = g_{ij} p^j.$$

- 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

$$\begin{aligned} e_i \cdot e^j &= e_i \cdot e_j = e^i \cdot e^j = \delta_i^j \\ \bar{g}_i \cdot \bar{g}_j &= g_{ij}, \quad \bar{g}^i \cdot \bar{g}^j = g^{ij}, \quad \bar{g}_i \cdot \bar{g}^j = \delta_i^j. \end{aligned}$$

C.2.4 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

$$T = T^{ij} e_i e_j = T_{ij} e^i e^j = T_j^i e_i e^j = T_i^j e^i e_j, \quad T_{ij} = T^{ij} = T_j^i = T_i^j.$$

Its pullback Q in the Lagrange coordinate system can be represented as

$$Q = Q_{ij} \bar{g}^i \bar{g}^j = Q^{ij} \bar{g}_i \bar{g}_j = Q_j^i \bar{g}_i \bar{g}^j = Q_i^j \bar{g}^i \bar{g}_j.$$

The transformation of the coefficients is, for example,

$$T^{kl} = Q^{ij} F_i^k F_j^l$$

obtained by using $\bar{g}_i = F_i^k e_k$.

One can also check that

$$Q_{ij} = Q^{k\ell} g_{ik} g_{j\ell} = Q_j^k g_{ik} = Q_i^k g^{kj}.$$

The transpose of Q the above tensor Q is defined as

$$\begin{aligned} Q^T &= Q_{ji} \bar{g}^i \bar{g}^j = Q^{ji} \bar{g}_i \bar{g}_j = Q_i^j \bar{g}_i \bar{g}^j = Q_j^i \bar{g}^i \bar{g}_j \\ &= Q_{ij} \bar{g}^j \bar{g}^i = Q^{ij} \bar{g}^i \bar{g}^j = Q_j^i \bar{g}_j \bar{g}^i = Q_i^j \bar{g}^j \bar{g}_i. \end{aligned}$$

- 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

$$Q \cdot \bar{q} = Q_i^j \bar{g}^j \bar{g}_j \cdot q_k \bar{g}^k = Q_i^k q_k \bar{g}^i.$$

One can check that

$$Q \cdot \bar{q} = \bar{q} \cdot Q^T \quad \text{and} \quad (P \cdot Q)^T = Q^T \cdot P^T.$$

For the first one, we have

$$\begin{aligned} Q \cdot \bar{q} &= Q_{ij} \bar{g}^i \bar{g}^j \cdot q^k \bar{g}_k = Q_{ik} q^k \bar{g}^i, \\ \bar{q} \cdot Q^T &= q^k \bar{g}_k \cdot Q_{ij} \bar{g}^j \bar{g}^i = q^k Q_{ik} \bar{g}^i = Q \cdot \bar{q}. \end{aligned}$$

For the second one,

$$\begin{aligned} P \cdot Q &= P_{ij} \bar{g}^i \bar{g}^j \cdot Q_{\ell}^k \bar{g}_k \bar{g}^{\ell} = P_{ik} Q_{\ell}^k \bar{g}^i \bar{g}^{\ell}, \\ Q^T P^T &= Q_{\ell}^k \bar{g}^{\ell} \bar{g}_k P_{ij} \bar{g}^j \bar{g}^i = Q_{\ell}^k P_{ik} \bar{g}^{\ell} \bar{g}^i = (P \cdot Q)^T. \end{aligned}$$

One can also define

$$Q^2 := Q \cdot Q, \quad Q^3 := Q \cdot Q^2 = Q^2 \cdot Q, \text{ etc.}$$

- Convolution

$$P : Q = P_{ij} \bar{g}^i \bar{g}^j Q^{k\ell} \bar{g}_k \bar{g}_\ell := P_{ij} Q^{ij}.$$

- 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 $Q_{i_1, \dots, i_n} e^{i_1} \dots e^{i_n}$ is called isotropic if

$$Q = Q_{i_1, \dots, i_n} (Re^{i_1}) \dots (Re^{i_n})$$

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

$$\begin{aligned} \nabla f &= \frac{\partial f}{\partial x^i} e^i = \frac{\partial f}{\partial x^i} \delta^{ij} e_j = \frac{\partial f}{\partial x^i} e_i. \\ \nabla f &= \frac{\partial f}{\partial X^i} \bar{g}^i = \left(\frac{\partial f}{\partial X^i} g^{ij} \right) \bar{g}_j. \end{aligned}$$

- 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

$$\frac{\partial \bar{g}^k}{\partial X^i} = -\Gamma_{ij}^k \bar{g}^j.$$

Here, the coefficients Γ_{ij}^k are called the Christoffel symbol of second kind. We denote

$$\nabla_{X^i} \bar{q} := \frac{\partial}{\partial X^i} \bar{q} := \left(\frac{\partial q_j}{\partial X^i} - q_k \Gamma_{ij}^k \right) \bar{g}^j.$$

Thus,

$$\begin{aligned} \nabla \bar{q} &= \bar{g}^i \frac{\partial \bar{q}}{\partial X^i} = \left(\frac{\partial q_j}{\partial X^i} - q_k \Gamma_{ij}^k \right) \bar{g}^i \bar{g}^j. \\ d\mathbf{x} &= dx^i e_i = dX^j \frac{\partial x^i}{\partial X^j} e_i = dX^j \bar{g}_j. \end{aligned}$$

Hence

$$d\mathbf{x} \cdot \nabla \bar{q} = dX^k \bar{g}_k \cdot \left(\bar{g}_i \frac{\partial \bar{q}}{\partial X^i} \right) = dX^k \frac{\partial \bar{q}}{\partial X^k} = d\bar{q}$$

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

$$\nabla \cdot \mathbf{w} = e^i \frac{\partial}{\partial x^i} \cdot w^j e_j = \frac{\partial w^i}{\partial x^i}.$$

$$\nabla \cdot \bar{q} = \bar{g}^i \frac{\partial}{\partial X^i} \cdot (q^j \bar{g}_j) = \frac{\partial q^i}{\partial X^i} + q^\ell \Gamma_{\ell i}^i.$$

For a tensor Q ,

$$\nabla \cdot Q = \frac{\partial Q_{ij}}{\partial x^i} e^j.$$

- Properties of ∇ :

$$\begin{aligned} \nabla(f_1 f_2) &= (\nabla f_1) f_2 + f_1 (\nabla f_2). \\ \nabla(\bar{q}_1 \cdot \bar{q}_2) &= (\nabla \bar{q}_1) \cdot \bar{q}_2 + \bar{q}_1 \cdot (\nabla \bar{q}_2). \\ \nabla \cdot (Q \cdot \bar{q}) &= (\nabla \cdot Q) \cdot \bar{q} + Q : (\nabla \bar{q})^T. \end{aligned}$$

For a symmetric tensor Q , we have

$$\nabla \cdot (Q \cdot \bar{q}) = (\nabla \cdot Q) \cdot \bar{q} + Q : \varepsilon(\bar{q}), \quad \varepsilon(\bar{q}) := \frac{1}{2} (\nabla \bar{q} + (\nabla \bar{q})^T).$$

For any tensor P and Q ,

$$\nabla \cdot (P \cdot Q) = Q^T \cdot (\nabla \cdot P) + P^T : \nabla Q.$$

C.2.5 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.2.6 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

$$\bar{q}^\nabla := \frac{\partial}{\partial t} \bar{q} - \bar{q} \cdot \nabla \mathbf{v}.$$

Then \bar{q}^∇ 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

$$\begin{aligned}
Q' \cdot \nabla' \mathbf{v}' &= O^T \cdot Q \cdot (O^T \cdot \nabla \mathbf{v} \cdot O - \Omega) \\
\nabla' \mathbf{v}'^T \cdot Q' &= (O^T \cdot \nabla \mathbf{v}^T \cdot O + \Omega) \cdot Q
\end{aligned}$$

Here, we have used $\Omega^T = -\Omega$. Putting the above calculations together, we get

$$\begin{aligned}
Q'^\nabla &= \dot{Q}' - Q' \cdot \nabla' \mathbf{v}' - \nabla' \mathbf{v}'^T \cdot Q' \\
&= O^T \cdot (\dot{Q} - Q \cdot \nabla \mathbf{v} - \nabla \mathbf{v}^T \cdot Q) \cdot O \\
&= O^T \cdot Q^\nabla \cdot O.
\end{aligned}$$

□

- 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 $\{e_i | i = 1, \dots, n\}$. 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} for the basis in the initial tangent space $T\hat{M}$.
- A vector field is a map $\mathbf{v} : M \rightarrow TM$ 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 $\varphi_t : \hat{M} \rightarrow M_t$ is a diffeomorphism with $\varphi_t(X) := \mathbf{x}(t, X)$. The flow map φ_t satisfies

- It is 1-1 and onto;
- 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

$$\mathbf{v}(t, \mathbf{x}) = \partial_t \varphi_t(X), \quad \text{for } \mathbf{x} = \varphi_t(X).$$

- 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 $a_\alpha^j(\star dX^\alpha)$, we want to find the coefficient a_α^j . 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

$$\begin{aligned} J \hat{\mu} \delta_j^i &= \varphi_t^* \mu \delta_j^i \\ &= \varphi_t^*(dx^i \wedge (\star dx^j)) \\ &= \varphi_t^*(dx^i) \wedge \varphi_t^*(\star dx^j) \\ &= F_\alpha^j dX^\alpha \wedge a_\beta^j (\star dX^\beta) \\ &= F_\alpha^i a_\alpha^j \hat{\mu}. \end{aligned}$$

Thus,

$$F_\alpha^i a_\alpha^j = J \delta_j^i.$$

This leads to

$$a = J F^{-T}, \quad a_\alpha^i = J (F^{-T})_\alpha^i = J \frac{\partial X^\alpha}{\partial x^i}.$$

We obtain

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

The general definition of pullback of a differential k -form α by a map φ is

$$\varphi^*(\alpha)(v_1, \dots, v_k) := \alpha(d\varphi(v_1), \dots, d\varphi(v_k)). \quad (4.1)$$

It is 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 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 by

$$\varphi_{t*} \left(\frac{\partial}{\partial X^\alpha} \right) := \frac{\partial x^k}{\partial X^\alpha} \frac{\partial}{\partial x^k}.$$

Note that

$$\left\langle \varphi_{t*} \frac{\partial}{\partial X^\alpha}, dx^\ell \right\rangle = \left\langle \frac{\partial x^k}{\partial X^\alpha} \frac{\partial}{\partial x^k}, dx^\ell \right\rangle = \frac{\partial x^\ell}{\partial X^\alpha}$$

On the other hand,

$$\left\langle \frac{\partial}{\partial X^\alpha}, \varphi_t^* dx^\ell \right\rangle = \left\langle \frac{\partial}{\partial X^\alpha}, \frac{\partial x^\ell}{\partial X^\beta} dX^\beta \right\rangle = \frac{\partial x^\ell}{\partial X^\alpha}$$

We get that

$$\left\langle \varphi_{t*} \frac{\partial}{\partial X^\alpha}, dx^\ell \right\rangle = \left\langle \frac{\partial}{\partial X^\alpha}, \varphi_t^* dx^\ell \right\rangle$$

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 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

Let us use the notations

$$\frac{d}{dt} := d_t := \left(\frac{\partial}{\partial t} \right)_X, \quad \partial_t := \left(\frac{\partial}{\partial t} \right)_x.$$

The Lie derivative is nothing but 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 :

$$\begin{aligned} \frac{d}{dt} \int_{C(0)} \eta_i(t, \mathbf{x}(t, X)) \frac{\partial x^i}{\partial X^\alpha} dX^\alpha &= \int_{C(0)} \frac{d}{dt} \left(\eta_i(t, \mathbf{x}(t, X)) \frac{\partial x^i(t, X)}{\partial X^\alpha} \right) dX^\alpha \\ &= \int_{C(0)} \left[(\partial_t + \mathbf{v} \cdot \nabla) \eta_i \frac{\partial x^i}{\partial X^\alpha} + \eta_i \frac{\partial v^i}{\partial X^\alpha} \right] dX^\alpha = \int_{C(t)} (\partial_t + \mathbf{v} \cdot \nabla) \eta_i dx^i + \eta_i \frac{\partial v^i}{\partial x^k} dx^k \\ &=: \int_{C(t)} (\partial_t + \mathcal{L}_{\mathbf{v}_t}) \eta \end{aligned}$$

The notation \mathbf{v}_t simply stands for a vector field in M_t with t fixed. The Lie derivative 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,

$$\boxed{d_t \varphi_t^*(\alpha) = \varphi_t^*(\partial_t + \mathcal{L}_{\mathbf{v}_t})\alpha.} \quad (4.2)$$

If both α and \mathbf{v} are independent of t , then the Lie derivative $\mathcal{L}_{\mathbf{v}}\alpha$ is defined as

$$\varphi_t^*(\mathcal{L}_{\mathbf{v}}\alpha) := d_t \varphi_t^*(\alpha).$$

We remark that in the time-dependent case, the Lie derivative $\mathcal{L}_{\mathbf{v}_t}$ only involves $v(t, \mathbf{x})$ with t fixed, although we use the flow map φ_t in its definition. Thus, $\mathcal{L}_{\mathbf{v}_t}$ is the Lie derivative of \mathbf{v}_t with t fixed.

List of Lie derivatives for differential forms

- Lie derivative for scalar function:

$$\begin{aligned} d_t(\varphi_t^* f)(t, X) &= \frac{d}{dt} f(t, \mathbf{x}(t, X)) = \partial_t f + \frac{\partial f}{\partial x^i} \dot{x}^i \\ &= (\partial_t + \mathbf{v} \cdot \nabla) f = (\partial_t + \mathcal{L}_{\mathbf{v}_t}) f. \end{aligned}$$

Therefore, $\mathcal{L}_{\mathbf{v}_t} f = \mathbf{v} \cdot \nabla f$.

- Lie derivative for dx^i

$$\begin{aligned}\mathcal{L}_{\mathbf{v}}(dx^i) &:= d_t(\varphi_t^*(dx^i))(t, X) \\ &= \frac{d}{dt} \frac{\partial x^i(t, X)}{\partial X^\alpha} dX^\alpha = \frac{\partial v^i}{\partial X^\alpha} dX^\alpha \\ &= \frac{\partial v^i}{\partial X^\alpha} \frac{\partial X^\alpha}{\partial x^k} dx^k = \frac{\partial v^i}{\partial x^k} dx^k.\end{aligned}$$

- For 1-form $\eta = \eta_i dx^i$, we have

$$\begin{aligned}d_t \varphi_t^*(\eta) &= [d_t \varphi_t^*(\eta_i)] dx^i + \eta_i [d_t \varphi_t^*(dx^i)] \\ &= (\partial_t \eta_k + v^j \partial_{x^j} \eta_k) dx^k + \eta_j \frac{\partial v^j}{\partial x^k} dx^k \\ &= (\partial_t \eta + \mathbf{v} \cdot \nabla \eta + \eta \cdot (\nabla \mathbf{v})^T) \cdot d\mathbf{x} \\ &= \varphi^*(\partial_t + \mathcal{L}_{\mathbf{v}_t}) \eta.\end{aligned}$$

- For volume form $dx^1 \wedge \cdots \wedge dx^n$, we have

$$\begin{aligned}d_t \varphi_t^*(dx^1 \wedge \cdots \wedge dx^n) &= \sum_i dx^1 \wedge \cdots (d_t \varphi_t^*(dx^i)) \cdots \wedge dx^n \\ &= \sum_i dx^1 \wedge \cdots \left(\frac{\partial v^i}{\partial x^i} dx^i \right) \cdots \wedge dx^n \\ &= (\nabla \cdot \mathbf{v}) (dx^1 \wedge \cdots \wedge dx^n)\end{aligned}$$

- For n -form $\rho dx^1 \wedge \cdots \wedge dx^n$:

$$d_t \varphi_t^*(\rho dx^1 \wedge \cdots \wedge dx^n) = (\partial_t \rho + (\nabla \cdot \mathbf{v}) \rho) dx^1 \wedge \cdots \wedge dx^n = (\partial_t + \mathcal{L}_{\mathbf{v}_t})(\rho dx^1 \wedge \cdots \wedge dx^n)$$

- 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

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

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.

- Let

$$\sigma := \sigma_j^i (\star dx^i) \otimes dx^j$$

Then

$$d_t \varphi_t^* \sigma = (\partial_t + \mathcal{L}_{\mathbf{v}}) (\sigma_j^i (\star dx^i) \otimes dx^j)$$

where

$$\mathcal{L}_{\mathbf{v}} \sigma = \left(v^k \partial_{x^k} \sigma_j^i + \sigma_j^i \frac{\partial v^k}{\partial x^k} - \frac{\partial v^i}{\partial x^k} \sigma_j^k + \sigma_\ell^i \frac{\partial v^\ell}{\partial x^j} \right) (\star dx^i \otimes dx^j)$$

D.4 Lie derivatives for vectors and tensors

- Lie derivative for $\frac{\partial}{\partial x^i}$

$$\begin{aligned}
 \mathcal{L}_v \frac{\partial}{\partial x^i} &:= d_t(\varphi_t^*(\frac{\partial}{\partial x^i}))(t, X) \\
 &= d_t \left(\frac{\partial X^\alpha}{\partial x^i} \frac{\partial}{\partial X^\alpha} \right) \\
 &= d_t (F^{-T})_\alpha^i \frac{\partial}{\partial X^\alpha} \\
 &= -(F^{-T} \dot{F}^T F^{-T})_\alpha^i \frac{\partial}{\partial X^\alpha} \\
 &= -(F^{-T})_\beta^i (\dot{F}^T)_\ell^\beta (F^{-T})_\alpha^\ell \frac{\partial}{\partial X^\alpha} \\
 &= -\frac{\partial X^\beta}{\partial x^i} \frac{\partial v^\ell}{\partial X^\beta} \frac{\partial X^\alpha}{\partial x^\ell} \frac{\partial}{\partial X^\alpha} \\
 &= -\frac{\partial v^\ell}{\partial x^i} \frac{\partial}{\partial x^\ell}
 \end{aligned}$$

Alternatively, we can use

$$\mathcal{L}_v \langle dx^i, \frac{\partial}{\partial x^j} \rangle = \langle \mathcal{L}_v(dx^i), \frac{\partial}{\partial x^j} \rangle + \langle dx^i, \mathcal{L}_v \frac{\partial}{\partial x^j} \rangle$$

to obtain

$$\langle \mathcal{L}_v \frac{\partial}{\partial x^j}, dx^i \rangle = -\langle \frac{\partial}{\partial x^j}, \mathcal{L}_v(dx^i) \rangle = -\langle \frac{\partial}{\partial x^j}, \frac{\partial v^i}{\partial x^k} dx^k \rangle = -\frac{\partial v^i}{\partial x^j}.$$

Hence,

$$\mathcal{L}_v \frac{\partial}{\partial x^j} = -\frac{\partial v^i}{\partial x^j} \frac{\partial}{\partial x^i}.$$

- Lie derivative for vector field $A = A^i \frac{\partial}{\partial x^i}$.

$$\begin{aligned}
 \mathcal{L}_v A &= (\mathcal{L}_v A^i) \frac{\partial}{\partial x^i} + A^k \mathcal{L}_v \left(\frac{\partial}{\partial x^k} \right) \\
 &= \left(\partial_t A^i + v^k \partial_{x^k} A^i - A^k \frac{\partial v^i}{\partial x^k} \right) \frac{\partial}{\partial x^i}
 \end{aligned}$$

- The deformation gradient

$$F := F_\alpha^i dX^\alpha \otimes \frac{\partial}{\partial x^i}$$

is a 2-point tensor. Its Lie derivative w.r.t. for the second argument $\frac{\partial}{\partial x^i}$ is

$$\mathcal{L}_v F = \left(\partial_t F_\alpha^i + v^k \partial_{x^k} F_\alpha^i - F_\alpha^k \frac{\partial v^i}{\partial x^k} \right) dX^\alpha \otimes \frac{\partial}{\partial x^i}$$

- The inverse deformation gradient

$$(F^{-1}) = (F^{-1})_i^\alpha \frac{\partial}{\partial X^\alpha} \otimes dx^i.$$

is a two-point tensor. Its Lie derivative w.r.t. the second argument is

$$\mathcal{L}_v (F^{-1}) = \left(\partial_t (F^{-1})_i^\alpha + v^k \partial_{x^k} (F^{-1})_i^\alpha + (F^{-1})_k^\alpha \frac{\partial v^i}{\partial x^k} \right) \frac{\partial}{\partial X^\alpha} \otimes dx^i$$

- 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

$$\begin{aligned} \mathcal{L}_v A &= (\mathcal{L}_v A^{ij}) \frac{\partial}{\partial x^i} \otimes \frac{\partial}{\partial x^j} + A^{kj} \mathcal{L}_v \left(\frac{\partial}{\partial x^k} \right) \otimes \frac{\partial}{\partial x^j} + A^{il} \frac{\partial}{\partial x^i} \otimes \mathcal{L}_v \left(\frac{\partial}{\partial x^l} \right) \\ &= \left(\partial_t A^{ij} + v^k \partial_{x^k} A^{ij} - A^{kj} \frac{\partial v^i}{\partial x^k} - A^{il} \frac{\partial v^j}{\partial x^l} \right) \frac{\partial}{\partial x^i} \otimes \frac{\partial}{\partial x^j} \end{aligned}$$

This is also known as the upper-convected derivative of the tensor A .

- Lie derivative for tensor of type (1, 1). Let

$$B = B_j^i \partial_{x^i} \otimes dx^j.$$

Then

$$\begin{aligned} \mathcal{L}_v B &= (\mathcal{L}_v B_j^i) \partial_{x^i} \otimes dx^j + B_j^k \mathcal{L}_v (\partial_{x^k}) \otimes dx^j + B_j^i \partial_{x^i} \otimes \mathcal{L}_v (dx^j) \\ &= \left(\partial_t B_j^i + v^k \partial_{x^k} B_j^i - B_j^k \partial_{x^k} v^i + B_j^i \partial_{x^j} v^k \right) \partial_{x^i} \otimes dx^j. \end{aligned}$$

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

$$\Sigma_{\mathbf{v}}(t_1, t_2) := \cup_{t_1 \leq t \leq t_2} \varphi_t(\Sigma_0)$$

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:

$$\boxed{\frac{d}{dt} \int_{\Sigma(t)} f(t, \mathbf{x}) d^n \mathbf{x} = \int_{\Sigma(t)} \frac{\partial}{\partial t} f(t, \mathbf{x}) d^n \mathbf{x} + \int_{\partial \Sigma(t)} f(t, \mathbf{x}) \mathbf{v} \cdot \mathbf{n} d\mathbf{x}} \quad (4.3)$$

This result is called the Reynolds transportation theorem.

- When Σ_0 is a k -dimensional submanifold, α is a k -form.

$$\begin{aligned} \frac{d}{dt} \int_{\Sigma(t)} \alpha &= \int_{\Sigma(t)} \frac{\partial}{\partial t} \alpha + \mathcal{L}_{\mathbf{v}} \alpha \\ &= \int_{\Sigma(t)} \frac{\partial}{\partial t} \alpha + i_{\mathbf{v}} d\alpha + \int_{\partial \Sigma(t)} i_{\mathbf{v}} \alpha \\ &= \int_{\Sigma(t)} \frac{\partial}{\partial t} \alpha + i_{\mathbf{v}} d\alpha + d i_{\mathbf{v}} \alpha. \end{aligned}$$

This shows Cartan's magic formula

$$\boxed{\mathcal{L}_{\mathbf{v}} = i_{\mathbf{v}} \circ d + d \circ i_{\mathbf{v}}.}$$