Continuum Mechanics

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Contents

Chapter 1

Fluid Mechanics

1.1 Thermodynamics

The equations of gas dynamics are derived based on conservation of mass, momentum and energy. Before we derive these equations, let us review some thermodynamics. First, the basic thermo variables are pressure (p), specific volume (τ), called state variables. The internal energy (e) is a function of p and τ. Such a relation is called a constitutive equation. The basic assumption are

$$\left.\frac{\partial e}{\partial p}\right|_{\tau} > 0, \ \left.\frac{\partial e}{\partial \tau}\right|_{p} > 0$$

Sometimes, it is convinient to express p as a function of (τ, e).

In an adiabetic process (no heat enters or losses), the first law of thermodynamics (conservation of energy) reads

$$de + pd\tau = 0. \tag{1.1}$$

This is called a Pfaffian equation mathematically. A function $\sigma(e, \tau)$ is called an integral of (1.1) if there exists a function $\mu(e, \tau)$ such that

$$d\sigma = \mu \cdot (de + pd\tau).$$

Thus, $\sigma =$ constant represents a specific adiabetic process. For Pfaffian equation with only two independent variables, one can always find its integral. First, one can derive equation for μ: from

$$\sigma_e = \mu \text{ and } \sigma_\tau = \mu p$$

and using $\sigma_{e\tau} = \sigma_{\tau e}$, we obtain the equation for μ:

$$\mu_\tau = (\mu p)_e.$$

This is a linear first-order equation for μ. It can be solved by the method of characteristics in the region $\tau > 0$ and $e > 0$. The solutions of μ and σ are not unique. If σ is a solution, so does $\bar{\sigma}$ with $d\bar{\sigma} = \nu(\sigma)d\sigma$ for any function $\nu(\sigma)$. We can choose μ such that if two systems are in thermo-equilibrium, then they have the same value μ.

In other words, μ is only a function of emperical temperature. We shall denote it by $1/T$. Such T is called the absolute temperature. The corresponding σ is called the physical entropy S. The relation $d\sigma = \mu(de + pd\tau)$ is re-expressed as

$$de = TdS - pd\tau. \tag{1.2}$$

For ideal gas, which satisfies the laws of Boyle and Gay-Lussac:

$$p\tau = RT, \tag{1.3}$$

where R is the universal gas constant. From this and (1.2), treating S and τ as independent variables, one obtains

$$Re_S(S,\tau) + \tau e_\tau(S,\tau) = 0.$$

We can solve this linear first-order equation by the method of characteristics. We rewrite this equation as a directional differentiation:

$$\left(R\frac{\partial}{\partial S} + \tau\frac{\partial}{\partial \tau}\right) e = 0.$$

This means that e is constant along the characteristic curves

$$R\frac{d\tau}{dS} = \tau.$$

These characteristics can be integrated as

$$\tau e^{-S/R} = \phi.$$

Here ϕ is a positive constant. The energy $e(\tau, S)$ is constant when $\tau e^{-S/R}$ is a constant. That is, $e = h(\phi)$ for some function h. We notice that $h' < 0$ because $p = -(\frac{\partial e}{\partial \tau})_S = -e^{-S/R}h'(\tau H) > 0$. From $T = (\frac{\partial e}{\partial S})_\tau = -\frac{1}{R}h'(\phi)\cdot\phi$, we see that T is a function of ϕ. In most cases, T is a decreasing function of ϕ. We shall make this as an assumption. With this, we can invert the relation between T and ϕ and treat ϕ as a decreasing function of T. Thus, we can also view e as a function of T, say $e(T)$, and $e(T)$ is now an increasing function. Now, we have five thermo variables p, τ, e, S, T, and three relations:

$$\begin{aligned} p\tau &= RT \\ e &= e(T) \\ de &= TdS - pd\tau \end{aligned}$$

Hence, we can choose two of as independent thermo variables and treat the rest three as dependent variables.

For instance, e is a linear function of T, i.e. $e = c_v T$, where c_v is a constant called specfic heat at constant volume. Such a gas is called polytropic gas. We can obtain

$$p\tau = RT \text{ and } e = c_v T = \frac{p\tau}{\gamma - 1} \tag{1.4}$$

or in terms of entropy,

$$\begin{aligned} p &= A(S)\tau^{-\gamma} \\ T &= \frac{A(S)}{R}\tau^{-\gamma+1} \\ e &= \frac{c_v A(S)}{R}\tau^{-\gamma+1} \end{aligned}$$

where

$$\begin{aligned} A(S) &= (\gamma-1)\exp((S-S_0)/c_v) \\ \gamma &= 1 + R/c_v \end{aligned}$$

If we define $dQ = TdS$, it is easy to see that c_v and c_p are the specific heat at constant volume and constant pressure, respectively.

$$\begin{aligned} c_v &= \left(\frac{\partial Q}{\partial T}\right)_\tau = \left(\frac{\partial e}{\partial T}\right)_\tau, \\ c_p &:= \left(\frac{\partial Q}{\partial T}\right)_p = ((\frac{\partial e}{\partial \tau})_p + p)/(\frac{\partial T}{\partial \tau})_p \\ &= \left(\frac{\partial e}{\partial T}\right)_p + p\left(\frac{\partial \tau}{\partial T}\right)_p \end{aligned}$$

In general, $c_p > c_v$. Because c_p is the amount of heat added to a system per unit mass at constant pressure. In order to maintain constant pressure, the volume has to expand (otherwise, pressure will increase), the extra amount of work due to expansion is supplied by the extra amount of heat $c_p - c_v$.

1.2 Compressible Euler Equations

Next, we derive the equations of gas dynamics. Let us consider an arbitrary domain $\Omega \subset R^3$. The mass flux from outside to inside per unit time per unit area dS is $-\rho v\cdot$, where n is the outer normal of Ω. Thus, the conservation of mass can be read as

$$\begin{aligned} \frac{d}{dt}\int_\Omega \rho\, dx &= \int_{\partial\Omega}[-\rho v\cdot n]dS \\ &= -\int_\Omega \text{div }(\rho\, v)\, dx \end{aligned}$$

This holds for arbitrary Ω, hence we have

$$\rho_t + \text{ div}(\rho\, v) = 0. \tag{1.5}$$

This is called the continuity equation.

Now, we derive momentum equation. Let us suppose the only surface force is from pressure (no viscous force). Then the momentum change in Ω is due to (i) the momentum carried in through boundary, (ii) the pressure force exerted on the surface, (iii) the body force. The first term is $-\rho v v \cdot n$, the second term is $-pn$. Thus, we have

$$\begin{aligned} \frac{d}{dt}\int_\Omega \rho v \, dx &= \int_{\partial\Omega} -[\rho v v \cdot n + pn] \, dS + \int F \, dx \\ &= \int_\Omega \operatorname{div}[-\rho v \otimes v - pI] + F \, dx \end{aligned}$$

This yields

$$(\rho v)_t + \operatorname{div}(\rho \, v \otimes v) + \nabla p = F \tag{1.6}$$

Here, the notation $\nabla \cdot \rho v \otimes v$ stands for a vector whoes ith component is $\sum_j \partial_j (\rho v^i v^j)$. The energy per unit volume is $E = \frac{1}{2}\rho \, v^2 + \rho e$. The energy change in Ω per unit time is due to (i) the energy carried in through boundary (ii) the work done by the pressure from boundary, and (iii) the work done by the body force. The first term is $-Ev \cdot n$. The second term is $-pv \cdot n$. The third term is $F \cdot v$. The conservation of energy can be read as

$$\frac{d}{dt}\int_\Omega E \, dx = \int_{\partial\Omega} [-Ev \cdot n - pv \cdot n] \, dS + \int_\Omega F \cdot v \, dx$$

By applying divergence theorem, we obtain the energy equation:

$$E_t + \operatorname{div}[(E+p)v] = \rho F \cdot v. \tag{1.7}$$

In one dimension, the equations are (without body force)

$$\begin{aligned} \rho_t + (\rho u)_x &= 0 \\ (\rho u)_t + (\rho u^2 + p)_x &= 0 \\ (\frac{1}{2}\rho u^2 + e)_t + [(\frac{1}{2}\rho u^2 + e + p)u]_x &= 0. \end{aligned}$$

Here, the unknowns are two thermo variable ρ and e, and one kinetic variable u. Other thermo variable p is given by the constitutive equation $p(\rho, e)$.

1.3 Invariants

1.3.1 Compressible gas dynamics in Lagrangian coordinate

Given velocity field $v(x,t)$, we can define the particle path $x(t,X)$ to be the solution of the ODE

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

The coordinate X is called the Lagrangian coordinate, or the material coordinate, where x is the orginal coordinate in the physical space. It is also called the Eulerian coordinate. The derivative

$$\frac{d}{dt} := \frac{\partial}{\partial t} + v \cdot \nabla$$

is called the material derivative.

We shall rewite the Euler equation in terms of Lagrangian coordinate.

Rate of change of density First, we have

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

This means that

$$\nabla \cdot v = -\frac{\frac{d\rho}{dt}}{\rho} = \frac{\frac{d\tau}{dt}}{\tau} \tag{1.8}$$

is the relative rate of change of volume. A fluid is called incompressible if

$$\frac{d\rho}{dt} = 0.$$

This is indeed equivalent to

$$\nabla \cdot v = 0.$$

Rate of change of velocity The momentum equation is

$$\rho v_t + \rho_t v + \rho v\nabla v + \rho(\nabla v)v + \nabla p = 0.$$

Using the continuity equation, we get

$$\frac{dv}{dt} = -\frac{\nabla p}{\rho}. \tag{1.9}$$

Rate of change of internal energy and entropy We can subtract the kinetic energy from the energy equation to obtain the motion of internal energy:

$$\rho\frac{de}{dt} + p\nabla \cdot v = 0.$$

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

$$de = TdS - pd\tau$$

lead to

$$\frac{dS}{dt} = 0. \tag{1.10}$$

In compressible flows, $dS/dt = 0$ means S is constant along particle path, S may still be different on different path. Indeed, as the particle passes through a shock front, the entropy increases.

When a flow with constant S, it is called an isentropic flow.

1.3.2 Vorticity

The momentum equation can be rewritten as

$$\rho \frac{dv}{dt} + \nabla p = 0.$$

We can rewrite the convection term $v \cdot \nabla v$ in the momentum equation by applying the following identity

$$v \cdot \nabla v = \nabla \left(\frac{1}{2} v^2 \right) - v \times \omega.$$

Here, $\omega := \nabla \times v$ is called the vorticity. This leads to

$$v_t + \omega \times v + \nabla \left(\frac{1}{2} v^2 \right) + \frac{1}{\rho} \nabla p = 0. \tag{1.11}$$

In the case of barotropic flows where p is only a function of ρ, the last term $\nabla p/\rho$ can be expressed as ∇w. This is an important formula. It says that the acceleration is due to (i) rotation ($\omega \times v$) and (ii) conservative force $\nabla(v^2/2 + w)$.

One consequence from this formula is the Bernoulli law: *For barotropic steady flows, the quantity*

$$\frac{1}{2} v^2 + w = constant, \tag{1.12}$$

along stream lines. Here, steady flow means that the solution is independent of time. We take inner product of (1.11) with v. We can get

$$v \cdot \nabla \left(\frac{1}{2} v^2 + w \right) = 0.$$

This means that $\frac{1}{2} v^2 + w$ stay constant along the stream line.

Another important result can be derived from (1.11) is by taking *curl* on both sides, we can eliminate those gradient terms and leave only kinematic variables.

$$\omega_t + v \cdot \nabla \omega = (\omega \cdot \nabla)\, v - \omega\, (\nabla \cdot v) + \frac{1}{\rho^2} \nabla \rho \times \nabla p. \tag{1.13}$$

Here, we have used the identity from vector calculus

$$\nabla \times (\omega \times v) = \omega(\nabla \cdot v) - v(\nabla \cdot \omega) + (v \cdot \nabla)\omega - \omega \cdot \nabla v.$$

Now, we consider the variation of the quantity ω/ρ.

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

This kinematic relation is due to Helmholtz. When p is only a function of ρ, $\nabla\rho\times\nabla p = 0$. Such flows are called barotropic flows. The isothermal flows, isentropic flows are examples of barotropic flows. In this case,

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

We claim this is equivalent to

$$\frac{d}{dt}\left(\frac{\omega}{\rho}\frac{\partial X}{\partial x}\right) = 0. \tag{1.14}$$

To prove this claim, we use Lagrange coordinate

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

We differentiate the identity

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

in t to get

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

Plug this into the above equation, we get

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

This leads to

$$\frac{d}{dt}\left(\frac{\omega}{\rho}\frac{\partial X}{\partial x}\right) = 0. \tag{1.15}$$

We integrate it to obtain

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

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

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

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

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

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

This shows that the vortex line stays as a vortex line as it flows with the fluid.

1.3.3 Irrotational 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,

$$\nabla \times v \equiv 0.$$

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

$$v = \nabla \phi$$

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

$$\nabla \cdot v = 0,$$

we call an incompressible and irrotational flow a *potential flow*. The potential theory can be applied.

Chapter 2

Viscous Fluids

2.1 Viscosity

2.1.1 Source of viscosity

Stress The stress is a surface force due to the impact of particles onto the surface from the other side per unit time. Suppose the small surface has area dA with (outer) normal n. The surface for from particles from outer region is F. The stress is a tensor which maps n to F:

$$\sigma n = F$$

The stress can be decomposed into a pressure part and viscous part:

$$\sigma_{ij} = -p\delta_{ij} + \sigma'_{ij}$$

The pressure is isotropic. It exists even the veclocity is zero or a constant. The viscous part is an internal friction. It can occur only when different fluid particles move at different velocities. If v is a constant, then $\sigma' = 0$. Thus σ' is a function of ∇v. We assume ∇v is small, then it is reasonable to assume σ' as a linear function of ∇v.

The rotation does not contribute any viscous force. For a rigid-body rotation: $\frac{dv}{dt} = \Omega \times v$, Ω is the rotation vector. The corresponding v satisfies $E = 0$. Here, $E = \nabla v + (\nabla v)^T$. From σ' being linear to ∇v, zero when $\nabla v = 0$ or $E = 0$, we get

$$\sigma' = aE + b\,\mathrm{tr}(E)I.$$

Here, a and b are two constants. We can modify it a little so that the first term is divergence free.

$$\sigma' = \eta(\nabla v + (\nabla v)^T - \frac{2}{3}\nabla \cdot vI) + \zeta \nabla \cdot vI. \tag{2.1}$$

The coefficient η is called the shear viscosity, while ζ the bulk viscosity. These two coefficient should satisfy

$$\eta > 0,\ \zeta > 0. \tag{2.2}$$

for energy dissipation requirement in viscous systems, as we shall see later.

The viscous force is

$$\begin{aligned}\nabla \cdot \sigma' &= \eta(\nabla v + (\nabla v)^T - \frac{2}{3}\nabla \cdot vI) + \zeta \nabla \cdot vI \\ &= \eta \nabla^2 v + (\zeta + \frac{1}{3}\eta)\nabla \cdot v.\end{aligned}$$

The momentum equation

$$\rho\left(v_t + \omega \times v + \nabla(\frac{1}{2}v^2)\right) + \nabla p = \nabla \cdot \sigma'$$

Chapter 3

Elasticity

The material of this chapter is mainly from Ciarlet's book, Mathematical Elasticity, Vol. 1, Three dimensional elasticity.

3.1 Strain

Let us imagine an elastic material deforms from a region Ω_0 at time 0 to $\Omega(t)$ at time t. We denote such a *deformation* by $y = y(t, x)$, or $y = \phi^t(x)$. That is, a position with coordinate x is deformed to position y at time t. The coordinate x is called the Lagrange coordinate, while y the Euler coordinate.

The gradient

$$F := \nabla_x y(t, x)$$

is called the *deformation gradient*. It is clear that $F(0, x) = I$. Let us denote $\det F$ by J. We have $J(t) > 0$ for all time from physical consideration. Thus the mapping ϕ^t is invertible. Let us call $u := y - x$ the displacement. Its gradient $\nabla_x u$ the displacement gradient. We have $F = I + \nabla_x u$.

Examples.

1. Rigid body motion: A trivial deformation is the rigid body motion

   $$y = a + Q(t)x$$

   where $Q(t)$ is an orthogonal matrix $QQ^T = 1$.

2. Let us consider

   $$y = D(t)x$$

   where

   $$\dot{D}(t) = \mathrm{diag}(\lambda_1, \lambda_2, \lambda_3)D(t)$$

   and λ_i are constants with $\sum_i \lambda_i = 0$. This gives $y^i = e^{\lambda_i t} x_i$. $i = 1, 2, 3$. If $\lambda_1 > 0$ and $\lambda_2, \lambda_3 < 0$, then the material expands in x_1 direction while squeezs in x_2 and x_3 directions.

3. Shear motion:

4. Expansion

Let us characterize the rigid-body motion without proof.

Theorem 3.1 *Let $\phi^t : \Omega \to \mathbb{R}^3$. Then $\phi^t(x) = a + Q(t)x$ is a rigid-body motion if and only if $F^T F \equiv I$. Here, $F = \nabla_x \phi^t$ and $Q(t)$ is an orthogonal matrix.*

The geometry of deformation Suppose an infinitesimal vector dx at time 0 is deformed to dy at time t. Then

$$dy = \frac{\partial y}{\partial x} dx = F dx.$$

The Euclidean inner product at time t induces a time-dependent Riemannian metric at $t = 0$:

$$(dy, dy) = (Fdx, Fdx) = (dx, F^T F dx).$$

We call $C := F^T F$ the right Cauchy-Green strain tensor. It is also the first fundamental form of the domain $\Omega(t)$. In terms of displacement gradient, C can be expressed as

$$C = (I + \nabla_x u)^T (I + \nabla_x u) = I + \nabla u + (\nabla u)^T + (\nabla u)^T (\nabla u).$$

If the deformation variation is small (i.e. $|\nabla_x u| << 1$), then

$$C \approx I + 2E, \ E = \frac{1}{2} \left(\nabla_x u + (\nabla_x u)^T \right),$$

E is called the Cauchy strain tensor. Its components are

$$e_{ij} = \frac{1}{2} \left(\frac{\partial u^i}{\partial x^j} + \frac{\partial u^j}{\partial x^i} \right).$$

Physical meaning of strain. To understand the physical meaning of e_{11}, let us consider an infinitesimal vector $dx^1 := (d\ell_1, 0, 0)^T$. The vector is deformed to

$$dy^1 = (1 + \frac{\partial u^1}{\partial x^1}, \frac{\partial u^2}{\partial x^1}, \frac{\partial u^3}{\partial x^1})^T d\ell_1.$$

Its length square

$$(d\tilde{\ell}_1)^2 = (dy^1, dy^1) \approx \left(1 + 2\frac{\partial u^1}{\partial x^1} \right) (d\ell_1)^2$$

Here we have neglected the hight order terms. Thus,

$$d\tilde{\ell}_1 \approx \left(1 + \frac{\partial u^1}{\partial x^1} \right) d\ell_1 \tag{3.1}$$

That is

$$e_{11} \approx \frac{d\tilde{\ell}_1 - d\ell_1}{d\ell_1}.$$

Thus, the physical meaning of e_{11} is the relative change of $d\ell$ in the direction e_1. Similarly, to understand the physical meaning of e_{12}, we consider two infinitesimal vectors

$$\begin{aligned} dx^1 &= (d\ell_1, 0, 0)^T \\ dx^2 &= (0, d\ell_2, 0)^T. \end{aligned}$$

The corresponding deformed vectors are

$$\begin{aligned} dy^1 &= (1 + \frac{\partial u^1}{\partial x^1}, \frac{\partial u^2}{\partial x^1}, \frac{\partial u^3}{\partial x^1})^T d\ell_1 \\ dy^2 &= (\frac{\partial u^1}{\partial x^2}, 1 + \frac{\partial u^2}{\partial x^2}, \frac{\partial u^3}{\partial x^2})^T d\ell_2. \end{aligned}$$

The inner product

$$(dy^1, dy^2) \approx \left(\frac{\partial u^1}{\partial x^2} + \frac{\partial u^2}{\partial x^1} \right) d\ell_1 d\ell_2.$$

Hence, we get

$$d\tilde{\ell}_1 d\tilde{\ell}_2 \cos\theta = 2e_{12} d\ell_1 d\ell_2$$

where θ is the angle between dy^1 and dy^2. Using (3.1) 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.

compression and shear.

3.2 Stress

3.2.1 The stress tensor in Euler coordinate

The stress is a surface force. It is due to the molecular force of the elastic material on one side of the surface to the other side. More precisely, the stress $\sigma = \Delta P / \Delta S$, P is the power, i.e. the force per unit time.

The time derivative of the trajectory $\phi^t(x)$, or $y(t, x)$ is the velocity

$$v := \frac{dy(t, x)}{dt}.$$

We notice that the velocity defined here is in Lagrange coordinate system. We may also define $v(t, y) = dy/dt(t, x)$ with $y = y(t, x)$, then this is the velocity in Euler coordinate system, and $y(t, x)$ is the solution of the ODE $\dot{y} = v(t, y)$ with $y(0, x) = x$.

The momentum equation reads

$$\int_{\Omega_t} \rho \frac{dv}{dt} \, dy = \int_{\partial\Omega_t} \sigma \cdot \nu \, dS_y.$$

Here, d/dt means the material derivative (i.e. the partial derivative in t with fixed x)

The stress is indeed a symmetric 2-tensor, which is based on the following three arguments:

- Cauchy stress principle: The stress is assumed to be a function of the Euler coordinate y and the normal of the surface ν.
- From conservation of linear momentum, we can derive that

$$\sigma(y, \nu) = T(y)\nu. \tag{3.2}$$

- From conservation of angular momentum, we can get $T(y)$ is symmetric.

To show (3.2), given ν, we consider a plan with normal ν. The plan intersects the coordinate axes e_1, e_2, e_3 at A_1, A_2, A_3, respectively. Let us consider the perimid $OA_1A_2A_3$, call it ΔG, the surface $A_1A_2A_3$ is called ΔS, and the three sides of the perimid are ΔS_i. The conservation of linear momentum on ΔG reads

$$\int_{\Delta G} \rho \frac{dv}{dt}\, dy = \int_{\Delta S} \sigma(y, \nu)\, dS + \sum_{i=1}^{3} \int_{\Delta S_i} \sigma(y, -e_i)\, dS$$

By dividing both sides by ΔS then take $\Delta S \to 0$, we can get

$$\sigma(y, \nu) = -\sum_{i=1}^{3} \nu_i \sigma(y, -e_i)$$

On the other hand, from Newton's third law, we can get $\sigma(y, -e_i) = -\sigma(y, e_i)$. We conclude that σ is linear in ν.

The conservation of angular momentum reads

$$\int_G \rho \left(y \times \frac{dv}{dt} \right)\, dy = \int_{\partial G} (y \times T\nu) dS$$

In differential form:

$$\rho y \times \frac{dv}{dt} = \nabla_y (y \times T)$$

The last term in coordinate form is

$$\begin{aligned} \partial_l(\epsilon_{ijk} y_j T_{kl}) &= \epsilon_{ijk}\delta_{jl} T_{kl} + \epsilon_{ijk} y_j \partial_l T_{kl} \\ &= \epsilon_{ijk} T_{kj} + \epsilon_{ijk} y_j \partial_l T_{kl} \end{aligned}$$

On the other hand, from linear momentum equation:

$$\rho \frac{dv}{dt} - \nabla_y T = 0$$

we take cross product with y on both sides to get

$$\rho y \times \frac{dv}{dt} = y \times (\nabla_y T).$$

This together with the angular equation, we get

$$\epsilon_{ijk} T_{kj} = 0,$$

That is $T_{ij} = T_{ji}$. Thus, by assuming the conservation of linear momentum, the conservation of angular momentum is equivalent to the symmetry of the stress tensor.

3.2.2 The stress tensor in Lagrangian coordinate–Piola stress

We want to express the linear momentum equation in Lagrangian coordinate. Let G_0 is deformed to G_t, its boundary S_0 to S_t. In Euler coordinate, the linear momentum equation is

$$\int_{G_t} \rho \frac{dv}{dt}\, dy = \int_{S_t} T\nu \, dS_y$$

In Lagrange coordinate, we have

$$\int_{G_0} \rho_0 \frac{dv}{dt}\, dx = \int_{S_0} Pn \, dS_0 \tag{3.3}$$

We want to find the relation between T and P. The tensor P is called the Piola stress tensor.

First, the conservation of mass reads

$$\int_{G_t} \rho \, dy = \int_{G_0} \rho_0 \, dx.$$

The left-hand side is $\int_{G_t} \rho J \, dx$. This leads to

$$\rho J = \rho_0.$$

Using this,

$$\int_{G_t} \rho \frac{dv}{dt}\, dy = \int_{G_0} \rho \frac{dv}{dt} J \, dx = \int_{G_0} \rho_0 \frac{dv}{dt}\, dx.$$

In (3.3), the velocity v at time t is the same vector, the stress σ is also the same vector in the Lagrange coordinate. We now change the surface force term to the Lagrange coordinate. We claim that

$$\nu dS_t = JF^{-T} n \, dS_0 \tag{3.4}$$

With this, then

$$P = JTF^{-T}.$$

Now, we prove (3.4). Let dx^1 and dx^2 are two infinitesimal vectors such that

$$n dS_0 = dx^1 \times dx^2.$$

Suppose dx^i is deformed to dy^i at time t, then

$$\nu dS_t = dy^1 \times dy^2.$$

In coordinate form, we have

$$\begin{aligned} \nu_i dS_t &= \epsilon_{ijk} dy^1_j dy^2_k \\ &= \epsilon_{ijk} y_{j,q} y_{k,r} dx^1_q dx^2_r \end{aligned}$$

Multiplying both sides by $y_{i,p}$ and using

$$J = \epsilon_{pqr} y_{1,p} y_{2,q} y_{3,r},$$

we obtain

$$\nu_i y_{i,p} dS_t = \epsilon_{pqr} J dx^1_q dx^2_r = J n_p dS_0$$

Thus, we get

$$F^T \nu dS_t = J n dS_0.$$

The equation of motion now reads

$$\rho_0 \frac{dv}{dt} = \nabla_x P.$$

From the symmetry of T, we get

$$\Sigma := F^{-1} P = J F^{-1} T F^{-T},$$

called the second Piola stress tensor, which is also symmetric.

3.3 Stress-strain relation

The stress in an elastic material is due to deformation. Therefore we assume the stress tensor T is a function of the deformation gradient F. Such a relation

$$T(y) = \widehat{T}(x, F)$$

is called a constitutive relation and $\widehat{T}$ is called a response function. If $\widehat{T}$ is independent of x, the material is called homogeneous. Below, we will find the physical conditions for a response function.

3.3.1 Frame indifference

First, the stress should be independent of the frame of reference physically. Suppose y is the coordinate in the original frame, and y^* is the coordinate in new frame which is a rotation of the old frame. That is, $y^* = Qy$, and Q is a rotation. Then

$F^* := \partial y^*/\partial x = QF$; the normal and the stress in the old and new frames are related by $\nu^* = Q\nu$, $\sigma^* = Q\sigma$. In terms of the response function, it reads

$$\begin{aligned} \sigma^* &= \widehat{T}(QF)\nu^* = \widehat{T}(QF)Q\nu \\ Q\sigma &= Q\widehat{T}(F)\nu. \end{aligned}$$

Hence,

$$\widehat{T}(QF) = Q\widehat{T}(F)Q^T. \tag{3.5}$$

This condition is called the *axiom of material frame-indifference.*

Next, we will show that $\widehat{T}$ is indeed a function of the Cauchy-Green strain tensor only. Let us write F in polar form

$$F = RU.$$

where R is a rotation and U is positive definite. From the axiom of material frame-indifference, we get

$$\widehat{T}(F) = \widehat{T}(RU) = R\widehat{T}(U)R^T = FU^{-1}\widehat{T}(U)UF^T = F\overline{T}(C)F^T.$$

where $C = U^2 = F^TF$ is the right Cauchy-Green strain tensor.

Similarly, for the Piola tensor P, the frame-indifference reads

$$P(QF) = J\widehat{T}(QF)(QF)^{-T} = J(Q\widehat{T}(F)Q^T)Q^{-T}F^{-T} = QP(F).$$

and

$$P(F) = J\widehat{T}(F)F^{-T} = JF\overline{T}(C) = F\overline{P}(C),$$

where $J^2 = detC$ and $\overline{P}(C) := \sqrt{detC}\,\overline{T}(C)$. For the second Piola tensor it satisfies

$$\Sigma(QF) = (QF)^{-1}P(QF) = (F^{-1}Q^{-1})(QP(F)) = \Sigma(F),$$

and

$$\Sigma(F) := F^{-1}P = \overline{P}(C).$$

3.3.2 Isotropic material

A material is isotropic if its stress tensor is independent of a rotational of the strain. Suppose we have two identical materials. One has material coordinate x, while the other is x^* with $x^* = Qx$ and Q being a rotation. If these two materials deform in the same way and result the same stresses, we call this material isotropic. Mathematically, this means

$$\widehat{T}(FQ) = \widehat{T}(F). \tag{3.6}$$

In terms of Piola stress tensor, it reads

$$P(FQ) = P(F)Q \text{ for all orthogonal matrix } Q \tag{3.7}$$

This follows from

$$P(FQ) = J\widehat{T}(FQ)(FQ)^{-T} = J\widehat{T}(F)F^{-T}Q = P(F)Q.$$

In order to characterize the response function of an isotropic material, we review some spectral properties of a matrix.

3.3.3 Hyper-elastic material

A material is called hyper-elastic material if there exists a potential $W(F)$ such that

$$P(F) = \frac{\partial W}{\partial F}.$$

Notice that such materials satisfy the frame-indifference axiom if and only if

$$W(QF) = W(F) \text{ for all } Q.$$

To see this, we differentiate the above equation in F to get

$$P(F) = \frac{\partial}{\partial F} W(F) = \frac{\partial}{\partial F} W(QF) = Q^T \frac{\partial W(QF)}{\partial (QF)} = Q^T P(QF).$$

This shows $W(F) = W(QF)$ if and only if $P(QF) = QP(F)$ for all Q. Similarly, a hyper-elastic material is isotropic (i.e. $P(FQ) = P(F)Q$) if and only if $W(FQ) = W(F)$ for all Q. This follows from

$$P(F) = \frac{\partial}{\partial F} W(F) = \frac{\partial}{\partial F} W(FQ) = \frac{\partial W(QF)}{\partial (QF)} Q^T = P(QF)Q^T.$$

Thus, for an isotropic hyper-elastic material, its potential energy function W satisfies

$$W(FQ) = W(QF) = W(F) \text{ for all } Q \tag{3.8}$$

Thus, W is only a function of the principal invariants of F, the eigenvalues of $F^T F$.

Two simple examples:

- Hook's law: $W(F) = \frac{1}{2} H |F|^2$, where $|F|^2 = \sum_{ij} |F_{ij}|^2$.
- Linear isotropic elastic material:

$$W = \frac{\lambda}{2} (tr\, E)^2 + \mu\, tr\, (E^2), \text{ where } E = \frac{1}{2}(C - I) \tag{3.9}$$

Chapter 4

Variation Formulation of Fluid Mechnics and Elasticity

4.1 Flow maps

4.1.1 Lagrangian and Eulerian Coordinates

We will derive a unified theory for both fluid and elasticity. We shall use the following notations.

- Let $x(\cdot, X)$ be the particle path of a piece of material (or fluid) with position X initially. X is called the Lagrangian coordinate, whereas x the Eulerian coordinate. It is assumed that the mapping satisfies $x(0, X) = X$.
- Ω_t: the region occupied by the material at time t. Thus, the mapping $x(t, \cdot) : \Omega_0 \to \Omega_t$. Or the mapping

  $$x(\cdot, \cdot) : [0, T] \times \Omega_0 \to \cup_{t\in[0,T]}\Omega_t.$$

  In most of case, we assume the whole region occupied by the material is unchanged. We denote this wholeregion by D. Thus, $x : [0, T] \times D \to D$. We always assume $x(t, \cdot)$ is 1-1 and onto from D to D.
- The deformation matrix $F := \frac{\partial x}{\partial X}$, or $F^i_\alpha(t, X) = \partial x^i(t, X)/\partial X^\alpha$.
- The Jacobian $J := \det F$. We have $dx = JdX$.
- The particle velocity is defined to be $\dot{x}(t, X)$. We shall use dot for the time derivative with the Lagrangian coordinate fixed.
- In Eulerian coordinate, we define

  $$u(t, x(t, X)) = \dot{x}(t, X).$$

  In other words,

  $$\dot{x}(t, X) = \int_D u(t, x)\delta(x - x(t, X))\, dx$$

  where δ is the delta function.

- For a physical quantity, say the density ρ, we denote by ρ_0 the density initially, and the density $\rho(t,x)$ is defined to be

$$\rho(t,x) = \int \rho_0(X)\delta(x - x(t,X))\,dX.$$

Thus, the mass in a region Ω is

$$\begin{aligned}\int_\Omega \rho(t,x)\,dx &= \int_\Omega \int \rho_0(X)\delta(x - x(t,X))\,dX\,dx \\ &= \int_{x(t,X)\in\Omega} \rho_0(X)\,dX\end{aligned}$$

If we take $\Omega = \Omega_t$, then we get

$$\int_{\Omega_t} \rho(t,x)\,dx = \int_{\Omega_0} \rho_0(X)\,dX.$$

Thus, the definition above implicitly assumes *conservation of mass*. By deviding the above equation by $|\Omega_0|$, and use $\lim_{\Omega_0\to 0} \frac{|\Omega_t|}{|\Omega_0|} = J$, we get

$$\rho(t,x(t,X))J(t,X) = \rho_0(X).$$

Alternatively, we take $\Omega = [x^1, x^1+\epsilon) \times [x^2, x^2+\epsilon) \times [x^3, x^3+\epsilon)$. Then

$$\begin{aligned}\int_{x^1}^{x^1+\epsilon}\int_{x^2}^{x^2+\epsilon}\int_{x^3}^{x^3+\epsilon} \rho(t,x)\,dx &= \int_{x^i\le x^i(t,X)<x^i+\epsilon} \rho_0(X)\,dX \\ &= \int_{x^i\le x^i(t,X)<x^i+\epsilon} \rho_0(X)J^{-1}\,dx\end{aligned}$$

By dividing both sides by ϵ^3, we get $\rho(t,x) = \rho_0(X)J^{-1}(t,X)$, where $x = x(t,X)$.

- Internal energy W. The deformation F stores an internal energy W in the material. It is due to the strenching between atoms. This internal energy W is assumed to be a function of F.

Examples

  - Hook's law:
$$W(F) = \frac{k}{2}\sum |F^i_\alpha|^2 = \frac{k}{2} tr(F^T F).$$
  - St. Venant-Kirchhoff: we assume small variation, i.e. $x(t,X) - X$ is small. Let $E = \frac{1}{2}(F^T F - I)$.

$$W(F) = \frac{\lambda}{2}(trE)^2 + \mu tr(E^2).$$

- The stress tensor. The derivative $P = W'(F)$ is called the Piola stress tensor. It is a surface force in Lagrange coordinate system. The stress in Eulerian coordinate system is denoted T, called the Cauchy-Green stress tensor. The surface force on the surface with normal ν is $T\nu$. In Lagrange coordinate, it is Pn, where n is the normal in Ω_0 which is deformed to ν at time t. $T\nu d^2S$ and Pnd^2S_0 represent the same surface force. Thus, $T\nu d^2S = Pnd^2S_0$. Notice that νd^2S is a 2-form in Ω_t, and nd^2S_0 is its pull back by the flow map $x(t, X)$. Thus, the pullback of νd^2S is $J^{-1}F^T\nu d^2S = nd^2S_0$. Thus,

  $$T\nu d^2S = Pnd^2S_0 = PJ^{-1}F^T\nu d^2S,$$

  We then obtain

  $$T = J^{-1}PF^T.$$

4.1.2 Variation of Functionals w.r.t. the flow maps

Functionals Given a flow map $x(\cdot, \cdot)$, we define its kinetic energy, internal energy, action, total energy in the Lagrange coordinate as the follows.

- Kinetic energy: $\int_{\Omega_0} \frac{1}{2}\rho_0(X)|\dot{x}(t, X)|^2\, dX$
- Internal energy: $\int_{\Omega_0} W(F)\, dX$
- Action:

  $$A[x] = \int_0^T \int_{\Omega_0} \frac{1}{2}\rho_0(X)|\dot{x}(t, X)|^2 - W(F)\, dX\, dt$$

- Total energy:

  $$E[x(t)] = \int_{\Omega_0} \frac{1}{2}\rho_0(X)|\dot{x}(t, X)|^2 + W(F)\, dX.$$

Variation w.r.t. flow maps We shall study the variation of these functionals with respect to the flow map $x(\cdot, \cdot)$. Let us perturb the flow map by $x_\epsilon(t, X)$ with $x_0(t, X) = x(t, X)$, the original unperturbed one. We call

$$\delta x(t, X) := \frac{\partial}{\partial \epsilon}|_{\epsilon=0} x_\epsilon(t, X),$$

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

$$\delta I[x] \cdot \delta x := \frac{d}{d\epsilon}|_{\epsilon=0} I[x_\epsilon].$$

Since, for small ϵ, $x_\epsilon(t, \cdot)$ are flow maps, its variation

$$\delta x(t, X) = \lim_{\epsilon \to 0} \frac{x_\epsilon - x_0}{\epsilon}$$

is an infinitesimal variation of position, thus, can be called a pseudo-velocity. Let us thus define the corresponding pseudo-velocity in the Eulerian coordinate as

$$v(t, x(t, X)) = \delta x(t, X).$$

- $\delta F = (\nabla v)F$, where ∇ is the abbreviation of ∇_x. From $\delta x(t, X) = v(t, x(t, X))$, we differentiate in X to get

$$\frac{\partial \delta x_i}{\partial X_j} = \frac{\partial v_i}{\partial x_k}\frac{\partial x_k}{\partial X_j}$$

  Interchange ∂ and δ operators, we get $\delta F = (\nabla v)F$.

- Let $J = \det F$, then

$$\delta J = tr\left((\delta F)F^{-1}\right) J.$$

  This follows from the following lemma.

  Lemma 4.1 *Let $A(\epsilon)$ be a smooth $n \times n$ matrix-valued function. Then*

$$\frac{d}{d\epsilon}\det(A) = tr(\dot{A}A^{-1})\det(A)$$

  Proof. We write $A = (a_{ij})$. First, we recall the expansion formula of $\det A$:

$$\sum_k a_{ik}A_{jk} = (\det A)\delta_{ij}$$

  where A_{ij} is the signed cofactor of A at (i, j). That is, $A(cofA)^T = (\det A)I$. 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 notice that A_{ik} does not involve a_{ij} for all k. Thus,

$$\frac{\partial \det A}{\partial a_{ij}} = A_{ij}.$$

  Next,

$$\begin{aligned}\frac{d}{d\epsilon}\det A &= \sum_{ij}\frac{da_{ij}}{d\epsilon}\frac{\partial \det(A)}{\partial a_{ij}} = \sum_{ij}\dot{a}_{ij}A_{ij} = \sum_{ij}(\dot{A})_{ij}((cofA)^T)_{ij} \\ &= \sum_{ij}(\dot{A})_{ij}(A^{-1})_{ij}\det A = tr(\dot{A}A^{-1})\det A\end{aligned}$$

  ∎

4.2 Inviscid Flows and Elasticity

4.2.1 Equation of Motion

1. Compressible elasticity We shall take variation of action w.r.t. flow map (position). This will give us the equation of motion

Lagrange formulation. We take the variation δx satisfying $\delta x(t, X) = 0$ for $t = 0$ and $t = T$. We can take integration by part for t.

$$\begin{aligned}
\delta A[x] \cdot \delta x &= \int_0^T \int_{\Omega_0} (\rho_0(X)\dot{x}(t,X) \cdot \delta\dot{x} - W'(F)\delta F)\, dX\, dt \\
&= \int_0^T \int_{\Omega_0} \left(-\frac{d}{dt}\rho_0(X)\dot{x}(t,X) \cdot \delta x - W'(F)\frac{\delta\partial x}{\partial X} \right) dX\, dt \\
&= \int_0^T \int_{\Omega_0} \left(-\frac{d}{dt}\rho_0(X)\dot{x}(t,X) \cdot \delta x + \left(\frac{\partial}{\partial X} W'(F) \right) \cdot \delta x \right) dX\, dt
\end{aligned}$$

Here, we also choose $W'(F)\delta x \cdot n = 0$ on the boundary of Ω_0 so that no boundary terms show up in the integration-by-part for the integration in X over Ω_0. This leads to the Euler-Lagrange equation

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

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

$$P^i_\alpha = \frac{\partial W}{\partial X^i_\alpha},\ (\nabla_X \cdot P)^i = \frac{\partial}{\partial X^\alpha} P^i_\alpha.$$

This is the equation of motion for an elastic material in Lagrange coordinate system.

We can also use the variable $u(t, X) := \dot{x}(t, X)$ and $F(t, X) = \frac{\partial x}{\partial X}(t, X)$ as the new unknowns to write the above equations as a first-order system. Notice that the velocity $u(t, X)$ is in Lagrange coordinate in this formulation. The equation of motion is

$$\rho_0(X)\dot{u}(t,X) = \nabla_X \cdot P(F).$$

By differentiate $\dot{x}(t, X) = u(t, X)$, we obtain the equation for F is

$$\dot{F}_{ij} = \frac{\partial u_i}{\partial X_j}(t, X).$$

Two special cases:

1. One dimension: In one dimension, let us call $v = F^1_1 - 1$ and $P(f^1_1) = \sigma(v)$. Then the equation of motion are

$$\begin{aligned}
\rho_0(X)u_t &= \sigma(v)_X \\
v_t &= u_X
\end{aligned}$$

   Such an equation is a 2×2 hyperbolic system. The stress $\sigma(v)$ satisfies $\sigma'(v) > 0$, but is a nonvex function of v in general. A shock wave attached to a rarefaction wave can be found.

2. Linear elasticity: In the Hook's case where $W(F) = \frac{k}{2}|F|^2$, the stress is $P(F) = kF$. The equation of motion becomes

$$\begin{aligned} \rho_0(X)u_t &= k\nabla_X \cdot F \\ F_t &= \nabla_X u \end{aligned}$$

Eliminating F, we get

$$\rho_0(X)u_{tt} = k\nabla_X^2 u$$

This is the wave equation.

Eulerian formulation. In the Eulerian formulation, u is defined as $u(t, x(t, X)) = \dot{x}(t, X)$, the perturbation (or the pseudo-velocity) v is defined as $v(t, x(t, X)) = \delta x(t, x(t, X))$. Let us define the material derivative as

$$\frac{D}{Dt} := \frac{\partial}{\partial t} + u \cdot \nabla.$$

The gradient is with respect to the Eulerian coordinate x. Thus, we have

$$\frac{Du}{Dt}(t, x(t, X)) = \ddot{x}(t, X).$$

We can use delta function to express δx and $\ddot{x}$ in terms of v and Du/Dt as the follows.

$$\begin{aligned} \delta x(t, X) &= \int v(x, t)\delta(x - x(t, X))\, dx \\ \ddot{x}(t, x(t, X)) \cdot \delta x(t, X) &= \int \frac{Du}{Dt} \cdot v(x, t)\delta(x - x(t, X))\, dx \end{aligned}$$

The force from the stress tensor is

$$G(t, X) = \nabla_X \cdot P(t, X)$$

The variation formula

$$\int (\rho_0(X)\ddot{x}(t, X) - G(t, X)) \cdot \delta x(t, X)\, dX$$

can be re-expressed as

$$\int \int \left(\rho_0 \frac{Du}{Dt}(t, x) - G(t, X) \right) \cdot v(t, x)\delta(x - x(X, t))\, dx\, dX$$

Let us define

$$\begin{aligned} \rho(t, x) &= \int \rho_0(X)\delta(x - x(t, X))\, dX \\ g(t, x) &= \int G(t, X)\delta(x - x(t, X))\, dX \end{aligned}$$

This means

$$\rho(t,x) = \lim_{\substack{x\,\in\,\Omega \\ |\Omega|\,\to\,0}} \frac{1}{|\Omega|}\int_{x(t,X)\in\Omega} \rho_0(X)\,dX$$

Then the above variation formula becomes

$$\int_0^T \int \left(\rho(t,x)\frac{Du}{Dt}(t,x) - g(t,x)\right)\cdot v(t,x)\,dx\,dt = 0.$$

This is true for all pseudo-velocity v. We thus obtain the equation of motion in Eulerian coordinate as

$$\rho\frac{Du}{Dt} = g.$$

The stress force

$$\begin{aligned} g(t,x) &= \int G(t,X)\delta(x - x(t,X))\,dX \\ &= \int_{\Omega_0} (\nabla_X \cdot P(t,X))\delta^3(x - x(t,X))\,dX \end{aligned}$$

Here, $\delta^3(x) = \delta(x^1)\delta(x^2)\delta(x^3)$.

$$\begin{aligned} g^i(t,x) &= \int \frac{\partial}{\partial X^\alpha} P^i_\alpha \delta^3(x - x(t,X))\,dX \\ &= \int P^i_\alpha \sum_{k=1}^{3}\prod_{\ell\neq k} \delta(x^\ell - x^\ell(t,X))\delta'(x^k - x^k(t,X))F^k_\alpha\,dX \end{aligned}$$

Now, let write

$$\delta'(x^k - x^k(t,X)) = \lim_{h\to 0}\frac{1}{h}\left(\delta(x^k + h - x^k(t,X)) - \delta(x^k - x^k(t,X))\right)$$

and

$$\begin{aligned} &\int P^i_\alpha F^k_\alpha \textstyle\prod_{\ell\neq k}\delta(x^\ell - x^\ell(t,X))\delta(x^k + h - x^k(t,X)) \\ &= \lim_{\epsilon\to 0}\tfrac{1}{\epsilon^3}\textstyle\int_{x^k+h<x^k(t,X)<x^k+h+\epsilon}\int_{x^\ell<x^\ell(t,X)<x^\ell+\epsilon} P^i_\alpha F^k_\alpha\,dX \\ &= \lim_{\epsilon\to 0}\tfrac{1}{\epsilon^3}\textstyle\int_{x^\ell}^{x^\ell+\epsilon}\int_{x^k+h}^{x^k+h+\epsilon} P^i_\alpha F^k_\alpha J^{-1}\,dx \end{aligned}$$

Similarly, we get

$$\begin{aligned} &\int P^i_\alpha F^k_\alpha \textstyle\prod_{\ell\neq k}\delta(x^\ell - x^\ell(t,X))\delta(x^k - x^k(t,X)) \\ &= \lim_{\epsilon\to 0}\tfrac{1}{\epsilon^3}\textstyle\int_{x^k<x^k(t,X)<x^k+\epsilon}\int_{x^\ell<x^\ell(t,X)<x^\ell+\epsilon} P^i_\alpha F^k_\alpha\,dX \\ &= \lim_{\epsilon\to 0}\tfrac{1}{\epsilon^3}\textstyle\int_{x^\ell}^{x^\ell+\epsilon}\int_{x^k}^{x^k+\epsilon} P^i_\alpha F^k_\alpha J^{-1}\,dx \end{aligned}$$

By taking $\epsilon\to 0$ and $h\to 0$, we obtain

$$g^i(t,x) = \frac{\partial}{\partial x^k}(P^i_\alpha F^k_\alpha J^{-1}),$$

or $g = \nabla_x \cdot T$, where $T = PF^T J^{-1}$.

By differentiating the equality

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

in X, we get the equation for F:

$$\dot{F} = (\nabla u)F.$$

In terms of the Euler coordinate system, it is

$$\frac{DF}{Dt} = (\nabla u)F.$$

Now, ρ is a new unknown. It satisfies $\rho(t, x)J(t, X) = \rho_0(X)$. Differentiate this in t with fixed X, we get

$$\begin{aligned} 0 &= (\rho_t + \nabla_x \rho \cdot \dot{x})\, J + \rho \dot{J} \\ &= (\rho_t + \nabla_x \rho \cdot u)\, J + \rho(\nabla \cdot u)J. \end{aligned}$$

Eliminating J, we get the continuity equation

$$\frac{D\rho}{Dt} + \rho \nabla \cdot u = 0.$$

Thus, the full equations are

$$\left\{ \begin{array}{rcl} \frac{D\rho}{Dt} &=& -\rho \nabla \cdot u \\ \frac{DF}{Dt} &=& (\nabla u)F \\ \rho \frac{Du}{Dt} &=& \nabla \cdot T \end{array} \right.$$

where $T = P(F)F^T J^{-1}$. The unknowns are ρ, F, u. These equations can also be written in conservation form:

$$\left\{ \begin{array}{rcl} \partial_t \rho + \nabla \cdot (\rho u) &=& 0 \\ \frac{DF}{Dt} &=& (\nabla u)F \\ \partial_t(\rho u) + \nabla \cdot (\rho u \otimes u) &=& \nabla \cdot T. \end{array} \right.$$

2. Incompressible elasticity A flow map $x(t, X)$ is called incompressible if

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

This means its volume is unchanged.

Lagrange formulation The constraint is

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

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

$$\delta A[x] + \delta \int_0^T \int p(t, X)(\det F - 1)\, dX\, dt = 0.$$

Here, p is the Lagrange multiplier. The variation

$$\delta(\det F) = tr((\delta F)F^{-1}) \det F = tr((\delta F)F^{-1}).$$

$$((\delta F)F^{-1})^i_j = \frac{\partial \delta x^i}{\partial X^k}(F^{-1})^k_j$$

Thus,

$$tr((\delta F)F^{-1}) = \sum_i \sum_k \frac{\partial \delta x^i}{\partial X^k}(F^{-1})^k_i$$

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

$$\begin{aligned}
\delta \int_0^T \int p(t, X)(\det F - 1)\, dX\, dt &= \int_0^T \int p \sum_k \sum_i \frac{\partial \delta x^i}{\partial X^k}(F^{-1})^k_i\, dX\, dt \\
&= -\int_0^T \int \sum_k \frac{\partial}{\partial X^k} \left(p(F^{-1})^k_i\right) \delta x^i\, dX\, dt \\
&= -\int_0^T \int \nabla_X \cdot \left(p(F^{-1})\right) \cdot \delta x\, dX\, dt
\end{aligned}$$

Thus, we obtain the constraint flow equation

$$\rho_0 \ddot{x} = \nabla_X \cdot (P - pF^{-1}).$$

The full set of equations are

$$\begin{cases}
\rho_0 \dot{u} &= \nabla_X \cdot (P(F) - pF^{-1}) \\
\dot{F} &= \nabla_X u \\
\det F &= 1
\end{cases}$$

The unknowns are (F, u, p).

Eulerian formulation If $u(t, x)$ is the velocity field which generates the flow map $x(t, X)$, that is, $\dot{x}(t, X) = u(t, x(t, X))$, then the incompressibility of $x(t, X)$ is equivalent to $\nabla \cdot u(t, x) = 0$. This comes from the following formula

$$\delta \det(A) = tr\left((\delta A)A^{-1}\right) \det(A).$$

and the formula

$$\frac{\partial \dot{x}}{\partial X} = (\nabla u)\frac{\partial x}{\partial X},$$

we get

$$\dot{J} = tr\left(\dot{F}F^{-1}\right)J = tr(\nabla u)J = (\nabla \cdot u)\, J.$$

Thus,

$$\dot{J} = 0 \text{ if and only if } \nabla \cdot u = 0.$$

Similarly, let $x_\epsilon(t, X)$ be a perturbation of x satisfying volume preserving property. Let $\delta x(t, X) := \frac{\partial}{\partial \epsilon}|_{\epsilon=0} x_\epsilon(t, X)$. Let $v(t, x(t, X)) = \delta x(t, X)$. Let $F_\epsilon = \partial x_\epsilon / \partial X$. $\delta F := \frac{\partial}{\partial \epsilon}|_{\epsilon=0} F_\epsilon$. Then

$$\delta F = (\nabla v)F.$$

Similarly,

$$\delta J = (\nabla \cdot v)J.$$

Thus, the volume preserving of x_ϵ is equivalent to $\delta J = 0$, and is also equivalent to $\nabla \cdot v = 0$.

Now, for the constraint $\nabla \cdot v = 0$, we introduce a Lagrange multiplier p. Then we have the constrained variation

$$\begin{aligned} 0 &= \int_0^T \int (-\rho \frac{Du}{Dt} + \nabla \cdot T) \cdot v + p(\nabla \cdot v)\, dx\, dt \\ &= \int_0^T \int (-\rho \frac{Du}{Dt} + \nabla \cdot T - \nabla p) \cdot v\, dx\, dt \end{aligned}$$

This gives

$$\rho \frac{Du}{Dt} + \nabla p = \nabla \cdot T.$$

Here, $T(F) = W'(F)F^T$. We still need an equation for F. From

$$\dot{F} = \left(\frac{\partial x}{\partial X}\right)_t = \frac{\partial u}{\partial X} = \frac{\partial u}{\partial x}\frac{\partial x}{\partial X} = (\nabla u)F,$$

we get

$$\frac{DF}{Dt} = (\nabla u)F.$$

Thus, the complete set of equations for incompressible inviscid elasticity are

$$\left\{ \begin{array}{rcl} \frac{D\rho}{Dt} &=& 0 \\ \nabla \cdot u &=& 0 \\ \rho \frac{Du}{Dt} &=& -\nabla p + \nabla \cdot T(F) \\ \frac{DF}{Dt} &=& (\nabla u)F. \end{array} \right.$$

with the constitutive equation $T(F) = W'(F)F^T$. The unknowns are (ρ, p, u, F). We notice that these equations can be written in conservation form

$$\left\{ \begin{array}{rcl} \partial_t \rho + \nabla \cdot (\rho u) &=& 0 \\ \nabla \cdot u &=& 0 \\ \partial_t(\rho u) + \nabla \cdot (\rho u \otimes u) &=& -\nabla p + \nabla \cdot T(F) \\ \frac{DF}{Dt} &=& (\nabla u)F. \end{array} \right.$$

3. Incompressible fluid The only difference between fluid and elastic material is the stress term. Consider the ideal fluids, where no stress appears. Then the equation of motion of an ideal fluid in Eulerian coordinate reads

$$\rho \frac{Du}{Dt} + \nabla p = 0.$$

$$\nabla \cdot u = 0.$$

The continuity equation reads

$$\rho_t + \nabla \cdot (\rho u) = 0.$$

Here, we have (ρ, p, u) as our unknowns.

Two special cases.

- $\rho \equiv 1$, we have
$$\frac{Du}{Dt} + \nabla p = 0, \ \nabla \cdot u = 0.$$
- Barotropic flow: the pressure is a function of ρ. In this case, we can find a potential Φ such that $\Phi'(\rho) = p'(\rho)/\rho$. Then the barotropic flow equation becomes
$$\frac{Du}{Dt} + \nabla \Phi = 0, \ \nabla \cdot u = 0.$$

4.2.2 Boundary conditions

1. Compressible invisid elasticity The natural boundary condition can be found through the variation formulation. The natural condition is

$$W_k^i \delta x^i \cdot n^k = 0 \ \text{ for } X \in \partial\Omega_0$$

for all perturbation δx. Here, n is the outer normal of Ω_0. There are many possibilities to achieve such condition.

- Dirichlet boundary condition:

  $$x(t, X) = x_0(X), X \in \partial\Omega_0,$$

  or equivalently,

  $$\dot{x}(t, X) = 0, X \in \partial\Omega_0.$$

  in Lagrange coordinate system. Or

  $$u(t, x) = 0 \, x \in \partial\Omega_t.$$

  in Euler coordinate system.

- In Lagrange coordinate system: $P_k^i n^k = 0$.
  In Euler coordinate system: $T_k^i \nu^k = 0$.

These consist of three conditions on boundary $\partial\Omega_0$.

2. Incompressible invisid elasticity The natural boundary condition is to have

$$(P - pF^{-1}) \cdot n\delta x = 0$$

$$u \cdot \nu = 0, x \in \partial D.$$

There is only one boundary condition on the boundary.

3. Incompressible invisid fluid

$$u \cdot \nu = 0, x \in \partial D.$$

There is only one boundary condition on the boundary.

4.2.3 Energy conservation laws

The energies $E(t)$ defined below are conserved.

- Compressible/incompressible inviscid elasticity

$$E(t) = \int_{\Omega_0} \frac{1}{2}\rho_0(X)|\dot{x}(t,X)|^2 + W(\frac{\partial x}{\partial X})\, dX$$

or

$$E(t) = \int_{\Omega_t} \frac{1}{2}\rho(t,x)|u(t,x)|^2 + WJ^{-1}\, dx.$$

- Incompressible inviscid fluid

$$E(t) = \int_{\Omega_0} \frac{1}{2}\rho_0(X)|\dot{x}(t,X)|^2\, dX$$

or

$$E(t) = \int_{\Omega_t} \frac{1}{2}\rho(t,x)|u(t,x)|^2\, dx.$$

4.3 Visco-elasticity

4.3.1 Equation of Motion

In classical mechanics, if a system has a damping term, then we have

$$\frac{dE(t)}{dt} = -\gamma|\dot{x}|^2 \Leftrightarrow m\ddot{x} + V'(x) = -2\gamma\dot{x}.$$

This is generalized to the following Onsager's maximum dissipation principle:

- **Incompressible viscous fluid** With the incompressibility $\nabla \cdot u = 0$ and continuity equation $D\rho/Dt = 0$, the equation

$$\rho \frac{Du}{dt} + \nabla p = \nabla \cdot (\mu \nabla u).$$

is equivalent to

$$\frac{d}{dt} \int \frac{1}{2} \rho |u|^2 \, dx = - \int \mu |\nabla u|^2 \, dx.$$

- **Incompressible visco-elasticity** With

$$\begin{aligned} \frac{D\rho}{Dt} &= 0 \\ \nabla \cdot u &= 0 \\ \frac{DF}{Dt} &= (\nabla u) F \end{aligned}$$

the momentum equation

$$\rho \frac{Du}{Dt} = -\nabla p + \nabla \cdot T + \nabla \cdot (\mu \nabla u)$$

is equivalent to

$$\frac{d}{dt} \int \frac{1}{2} \rho |u|^2 + W(F) \, dx = - \int \mu |\nabla u|^2 \, dx.$$

4.3.2 Boundary conditions

Due to the viscous term in the momentum equation, it is natural to impose velocity on the boundary to be

$$u(x) = 0, \ x \in \partial D.$$

This consists of three condition because $u \in \mathbb{R}^3$. There are no boundary condition for ρ, F, p for compressible elasticity, and no boundary condition for p for incompressible elasticity.

Chapter 5

Membrane

5.1 Energy law of membrane

5.1.1 Surface geometry

We assume $X = (X_1, X_2)$ be two dimensional and $x = (x_1, x_2, x_3)$ be three dimensional. The deformation matrix $F = \partial x/\partial X$ is a 3×2 matrix. The metrix (dx, dx) induces a metric

$$g_{\alpha\beta} = \frac{\partial x}{\partial X^\alpha} \cdot \frac{\partial x}{\partial X^\beta}$$

on the manifold $\Sigma_t = \{x(t, \cdot)\}$. That is,

$$(dx, dx) = (FdX, FdX) = (F^T F dX, dX) = \sum_{jk} g_{\alpha\beta} dX^\alpha dX^\beta.$$

The matrix $F^T F$ is called the first fundamental form of the surface Σ_t. The area spanned by the vectors $v^\alpha = \partial x/\partial X^\alpha$ and $v^\beta = \partial x/\partial X^\beta$ is

$$\sqrt{(v^\alpha, v^\alpha)\,(v^\beta, v^\beta) - (v^\alpha, v^\beta)^2} = \sqrt{\det(F^T F)}.$$

Thus, we define $J = \sqrt{\det(F^T F)}$. Then $dS_t = J\, dS_0$.

We want to define an energy $W(F)$ on the manifold Σ_t.

The frame indifference condition reads

$$W(QF) = W(F),$$

where Q is any 3×3 orthogonal matrix. Taking the singular value decomposition of F, $F = U\Lambda V^T$, where $U \in O(3)$, $V \in O(2)$ and Λ is a 3×2 matrix

$$\Lambda = \begin{pmatrix} \lambda_1 & 0 \\ 0 & \lambda_2 \\ 0 & 0 \end{pmatrix}$$

we then have

$$W(F) = W(U\Lambda V^T) = W(\Lambda V^T)$$

Isotropic condition reads The isotropy assumption is

$$W(FQ_1) = W(F),$$

where Q_1 is any 2×2 orthogonal matrix. If we represent $F = U\Lambda V^T$, then $W(F) = W(\Lambda)$. That is, The isotropy condition implies that W only depends on the eigenvalues of g.

Two simple examples

- Hook's law:

$$W(F) = \frac{1}{2}tr(F^TF) = \frac{1}{2}\sum_{\alpha=1}^{2} g_{\alpha\alpha} = \frac{1}{2}\sum_{\alpha=1}^{2}\sum_{i=1}^{3}|F_\alpha^i|^2.$$

  The corresponding Piola stress is

$$P_\alpha^i = \frac{\partial W}{\partial F_\alpha^i} = F_\alpha^i, \alpha = 1, 2,\ i = 1, 2, 3.$$

- minimal surface

$$W(F) = \sigma\sqrt{g} = \sigma\sqrt{\det(F^TF)} = \sigma J.$$

  Here, σ is 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:

$$W(F) = a(tr(F^TF) - 2)^2 + b(\sqrt{det(F^TF)} - 1)^2.$$

  Another fabric model is to decompose $g = F^TF$ into a divergence part and a divergence free part. That is,

$$g = \frac{1}{2}tr(g)I + \left(g - \frac{1}{2}tr(g)I\right)$$

  The first part is related to the expansion or shrinking of the surface, while the second is related to the distorsion of the surface. We can design the energy to be

$$W(F) = a(tr(g) - 2)^2 + b\left\|g - \frac{1}{2}tr(g)I\right\|_F^2$$

  The norm here is the Frobenius norm.

- Vesicle model (Canham-Helfrich)

$$W(F) = \frac{\kappa}{2}(H - H_0)^2 + \bar{\kappa}K.$$

  where H is the mean curvature and K the Gaussian curvature. In this formulation, W depends on the second fundamental form of the surface, which, by the intrincit property of surfaces, involves the derivative of F. [1]

[1] For membrane model, a reference book is: Statistical Mechanics of Membranes and Surfaces, 2nd edition, edited by D. Nelson, T. Piran and S. Weinberg (2004).

5.1.2 Isotropic membrane

Let $x(X,t)$ be the flow map with $X \in \Sigma_0$ being two dimensional.

Piola stress $P^i_\alpha = \frac{\partial P}{\partial F^i_\alpha}$.

Relation between Cauchy stress and Piola stress The Piola stress is convinient in the Lagrange coordinate system. In Eulerian coordinate system, the corresponding stress is the Cauchy stress T.

$$T = J^{-1} P F^T.$$

This is to be verified.

5.1.3 Equation of Motion

Lagrange formulation

The action is

$$A[x] = \int_0^T \int_{\Sigma_0} \frac{1}{2}\rho_0(X)|\dot{x}(t,X)|^2 - W\left(\frac{\partial x}{\partial X}\right) dX\, dt$$

The variation of the action with respective to the membrane motion $x(t,X)$ gives the momentum equation. One can see the previous Euler-Lagrange equation is still the same.

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

Let $u(t,X) := \dot{x}(t,X)$. The equation of motion becomes

$$\left\{ \begin{array}{rcl} \rho_0(X)\dot{u}^i(t,X) & = & \frac{\partial}{\partial X^\alpha} P^i_\alpha(F) \\ \dot{F}^i_\alpha & = & \frac{\partial u^i}{\partial X^\alpha} \end{array} \right.$$

Euler formulation

Let Σ_t be the membrane at time t. We assume that there is an 1-1 and onto mapping $x(t,X)$ between Σ_0 and Σ_t. The Jacobian $J \neq 0$. We define the following quantities on Σ_t.

1. Velocity: $u(t,\cdot)$ is defined on Σ_t by $\dot{x}(t,x(t,X))$ if $x = x(t,X)$. The velocity $u(t,x)$ may not lie on $T\Sigma_t(x)$.

2. Pseudo-velocity $v(t,\cdot)$ is defined on Σ_t by $\delta x(t,x(t,X))$ if $x = x(t,X)$. The pseudo-velocity may not lie on $T\Sigma_t(x)$.

3. We define material derivative D/Dt by $\partial/\partial t + u \cdot \nabla_\Sigma$. Here, ∇_Σ is the surface graditent. (This is to be checked.)

4. The volume d^3x can be expressed as $dSd\nu$, where dS is the area element of the surface Σ_t and $d\nu$ is te arc length element in the normal direction. The δ-function in 3-d can be expressed as

$$\delta^3(x - x(t, X))\, d^3x = \delta_S(x - x(t, X))\delta_\nu(x - x(t, X))dS\, d\nu.$$

5. We have

$$\delta x(t, X) = \int_{\Sigma_t} v(t, x)\delta_S(x - x(t, X))\, dS$$

$$\ddot{x}(t, X) \cdot \delta x(t, X) = \int_{\Sigma_t} \frac{Du}{Dt} \cdot v(t, x)\delta_S(x - x(t, X))\, dS$$

6. The Piola stress is pushed forward as the Cauchy-Green stress T by

$$T = J^{-1}PF.$$

7. The density ρ on the surface is defined to be

$$\rho(t, x) = \int \rho_0(X)\delta_S(x - x(t, X))\, dS_0$$

With these, the equation of motion is

$$\rho\frac{Du}{Dt} = \nabla_S \cdot T.$$

This is to be clearified.

5.2 Two-phase Flows

5.2.1 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

$$\begin{cases} \nabla \cdot u_i = 0 \\ \rho_i(u_{i,t} + u_i \cdot \nabla u_i) + \nabla p_i = 0 \end{cases}$$

We assume ρ_i are constants. On the boundary Γ_t, the divergence free $\nabla \cdot u_i = 0$ leads to

$$[u] \cdot \nu = 0,$$

where $[u] = u_2 - u_1$. This implies that the motion of the interface, which can be characterized by its nomal velocity v_n, satifies

$$v_n = u_1 \cdot \nu = u_2 \cdot \nu.$$

For force balance on the interface, we first decompose a vector field V into V_ν and V_S and the divergence is decomposed into $\nabla_\nu V_\nu + \nabla_S V_S$. Similar for a tensor. Now, across an interface

$$[p]\nu = T \cdot \nu$$

where T is the stress on the surface.

Given v_n, it will give the boundary condition $u_i \cdot \nu = v_n$ on the bouundary $\partial\Omega_i$ and will be able to solve the Euler equation. The interface normal velocity v_n in turn, is determined by the other interface condition: $[p] - \sigma u H$.

5.2.2 Viscous flows

Now we consider two viscous flows connected by an interface Γ_t. The governed equations in each region are the Navier Stokes equation:

$$\begin{cases} \nabla \cdot u_i = 0 \\ \rho_i(\partial_t u_i + u_i \cdot \nabla u_i) + \nabla p_i = \nabla \cdot \mu_i \nabla u_i. \end{cases}$$

On the boundary Γ_t, due to viscosity, we should use the condition

$$[u] = 0.$$

This leads to

$$u_1 = u_2 = v,$$

where v is the surface velocity. From momentum equation, the surface force due to an elastic material on Γ_t is $\sigma H \nu$ (assume the elastic material is inviscid). Let $\tau_i := \mu_i \nabla u_i - p_i I$ be the stress tensor of the fluid i in region Ω_i. Then the force balance law on the interface is

$$[\tau] \cdot \nu = \sigma H \nu.$$

If v is given, then the condition $u_i = v$ and N-S equation can determine the flow in Ω_i. On the other hand, there are three conditions in $[\tau] \cdot \nu = \sigma H \nu$ to determine the interfacial velocity v.

Chapter 6

Phase Field Models

6.1 Dynamics of multiphase materials

Order parameter A two-phase fluid model: 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 composition function to indicate which material, which is called order parameter in physics literature. For instance, in a water-oil system, we may use $\phi = 1$ for water and $\phi = -1$ for oil. One can associate a free engrgy W with ϕ by

$$\mathcal{F}[\phi] = \int_\Omega f(\phi, \nabla\phi)\, dx = \int_\Omega \frac{1}{2\epsilon}|\nabla\phi|^2 + \frac{1}{\epsilon}W(\phi)\, dx$$

The energy W is the bulk free energy. A natural choice is a double well potential with minima at -1 and 1, for instance $W(\phi) = \frac{1}{4}(\phi^2 - 1)^2$. 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 the area of the interface.

Chemical potential The variation of $\mathcal{F}$ w.r.t. ϕ is called the chemical corresponding to ϕ.

$$\mu = \frac{\delta\mathcal{F}}{\delta\phi} = -\nabla \cdot \frac{\partial f}{\partial \nabla\phi} + \frac{\partial f}{\partial \phi}.$$

Evolution of order parameter The simplest case is

$$\partial_t\phi + u \cdot \nabla\phi = 0.$$

This is equivalent to

$$\phi(t, x(t, X)) = \phi_0(X).$$

The other possibility is

$$\partial_t\phi + \nabla \cdot (u\phi) = 0,$$

which yields

$$\phi(t, x(t, X))J(t, X) = \phi_0(X).$$

Variation of $\mathcal{F}$ w.r.t. flow motion Let x_s be a one-parameter family of flow maps. $\delta x_s = x_s'$. Let $v_s(t, x(t, X)) = \delta x_s(t, X)$. The order parameter ϕ_s is defined by

$$\phi_s(t, x_s(t, X)) = \phi_0(X).$$

This means that the flow perturbation does not change the phase. Hence, ϕ_s satisfies

$$\partial_s \phi_s + v_s \nabla \phi_s = 0.$$

The variation of $\mathcal{F}$ w.r.t. x^s is

$$\begin{aligned} \delta\mathcal{F} \cdot v &= \frac{\delta \mathcal{F}}{\delta \phi_s} \frac{\partial \phi_s}{\partial s} \\ &= \mu(-v_s \nabla \phi_s) \\ &= -\mu \nabla \phi \cdot v \end{aligned}$$

Variation of $\mathcal{F}$ w.r.t. predomain In this case, we have

$$\phi_s(t, x_s(t, X)) J_s(t, X) = \phi_0(X).$$

This implies

$$\begin{aligned} 0 &= J_s \left(\partial_s \phi_s + v_s \nabla \phi_s\right) + J_s' \phi_s \\ &= J_s \left(\partial_s \phi_s + v_s \nabla \phi_s\right) + (\nabla \cdot v) J_s \phi_s \end{aligned}$$

This gives

$$\partial_s \phi_s + \nabla \cdot (\phi_s v_s) = 0.$$

The variation of $\mathcal{F}$ w.r.t. x^s is

$$\begin{aligned} \delta\mathcal{F} \cdot v &= \frac{\delta \mathcal{F}}{\delta \phi_s} \frac{\partial \phi_s}{\partial s} \\ &= \mu(-\nabla(\phi_s v_s)) \\ &= \phi \nabla \mu \cdot v \end{aligned}$$

Incompressible case In this case,

$$\delta\mathcal{F} \cdot v = \phi \nabla \mu \cdot v = -\mu \nabla \phi \cdot v.$$

6.2 Equation of Motion

The action is defined to be

$$\mathcal{A}[x] = \int_0^T \int_{\Omega_0} \frac{1}{2} \rho_0(X) |\dot{x}(t, X)|^2 - f(\phi, \nabla \phi)(t, x(t, X)) J(t, X) \, dX \, dt.$$

The potential energy is indeed the functional

$$\mathcal{F}(\phi) = \int_{\Omega_t} f(\phi(t, x), \nabla \phi(t, x)) \, dx.$$

The variation of action w.r.t. flow motion gives

$$\rho \frac{Du}{Dt} = \mu \nabla \phi.$$

This together with

$$\partial_t \phi + u \cdot \nabla \phi = 0$$
$$\partial_t \rho + \nabla \cdot (\rho u) = 0,$$

give the set of equations for (ρ, ϕ, u).

Conservation of energy We multiply momentum equation by u then integrate in X and in t to get

$$\begin{aligned} \frac{d}{dt} \int \frac{1}{2} \rho |u|^2 \, dx &= \int \mu u \cdot \nabla \phi \, dx \\ &= -\int \mu \partial_t \phi \, dx \\ &= -\int \frac{\delta \mathcal{F}}{\delta \phi} \partial_t \phi \, dx \\ &= -\int \frac{d\mathcal{F}}{dt} \, dx \end{aligned}$$

This gives the conservation of total energy. It also shows that the force $\mu \nabla \phi$ is the opposite force of the convection of ϕ.

In the case

$$\partial_t \phi + \nabla \cdot (\phi u) = 0,$$

The force from the convection becomes

$$\rho \frac{Du}{Dt} = -\phi \nabla \cdot \mu.$$

We also get same result:

$$\frac{d}{dt} \int \frac{1}{2} \rho |u|^2 + f(\phi, \nabla \phi) \, dx = 0.$$

Dissipation One can add dissipation term in the momentum equation:

$$\rho \frac{Du}{Dt} = \mu \nabla \phi + \nabla \cdot \tau$$

where τ is the viscous stress.

The order parameter has a tendency to move from high potential energy to low potential energy. For the advection equation of ϕ, there are two models. The first one is Allan-Cahn, the second one is Cahn-Hilliard.

- Allan-Cahn:

$$\partial_t \phi + u \nabla \phi = -\frac{\delta \mathcal{F}}{\delta \phi}$$

- Cahn-Hilliard defines the flux to be

$$q = -m\nabla\mu$$

where m is the mobility. The evolution of ϕ satisfies

$$\frac{D\phi}{Dt} = \nabla \cdot (m\nabla\mu).$$

This is the Cahn-Hilliard equation. The total order parameter is conserved.

The dissipation of energy can be obtained by multiplying momentum equation by u, multiplying advection equation by μ, then adding them together:

$$(\rho\frac{Du}{Dt} \cdot u - \mu\nabla\phi \cdot u) + (\mu\partial_t\phi + \mu u\nabla\phi) = u \cdot \nabla \cdot \tau - \mu^2.$$

This gives

$$\frac{d\mathcal{E}}{dt} = -\tau \cdot \nabla u - \mu^2.$$

The stress tensor has the form $\nu(\nabla u + (\nabla u)^T) + \lambda\nabla \cdot u$. The viscous dissipation becomes

$$-\nu|\nabla u + (\nabla u)^T|^2 - \lambda|\nabla \cdot u|^2.$$

For Cahn-Hilliard equation, the energy dissipation is

$$\frac{d\mathcal{E}}{dt} = -\tau \cdot \nabla u - m|\nabla\mu|^2.$$

6.3 Interface structure

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

$$f(\nabla\phi, \phi) = \frac{\epsilon}{2}|\nabla\phi|^2 + \frac{1}{\epsilon}W(\phi)\, dx$$

where W is a double well potential. As $\epsilon \to 0$, $\phi \to \pm 1$. The interface energy tends to

$$\mathcal{F}[\phi] \to \sigma_0|\Gamma(t)|.$$

where σ_0 is a constant.

2. Mean curvature:

$$\int_{\Omega(t)} \frac{\eta}{2}\left(\triangle\phi - \frac{1}{\eta^2}W'(\phi)\right)^2 dx \approx \int_{\Gamma(t)} H^2\, dS.$$

3. Gaussian curvature:

$$\int_{\Omega(t)} \left(\eta \triangle \phi - \frac{1}{\eta} W'(\phi) \right) W'(\phi)\, dx \approx \int_{\Gamma(t)} K\, dS.$$

The bulk energy also has many choices.

1. Binary system: Consider a binary system with two components A and B with constration 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

$$W(p, n) = \int_\Omega p \log p + n \log n + \frac{1}{2}(n - p)V[n - p]\, dx$$

   where $V[n - p]$ is the potential induced by $n - p$, i.e. $\epsilon V = n - p$.

6.3.1 Structure of one dimensional interface

Allen-Cahn interface The order parameter satisfies

$$\phi_t = -\frac{\delta \mathcal{F}}{\delta \phi} = \triangle \phi - W'(\phi)$$

where

$$\mathcal{F} = \int \frac{1}{2} |\nabla \phi|^2 + W(\phi)\, dx$$

$$W(\phi) = \frac{1}{4}(\phi^2 - 1)^2.$$

The interface is assumed to be steady, so $\phi_t = 0$. Thus, we want to solve

$$\triangle \phi - W'(\phi) = 0.$$

Multiplying ϕ on both sides, we get

$$\frac{d}{dx} \left(\frac{1}{2} \phi'^2 - W(\phi) \right) = 0.$$

We look for ϕ which connecting the two equilibria ± 1 at $x = \pm\infty$ and with $\phi'(\pm\infty) = 0$. Thus, the interface we look for satisfies

$$\frac{1}{2} \phi'^2 - W(\phi) = 0.$$

We can solve this ODE:

$$\phi' = \sqrt{2W} \tag{6.1}$$

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

$$\mathcal{F}^\epsilon[\phi^\epsilon] = \int \frac{\epsilon}{2}|\nabla\phi^\epsilon|^2 + \frac{1}{\epsilon}W(\phi^\epsilon)\, dx$$

This gives the traveling wave equation

$$\epsilon \triangle \phi^\epsilon - \frac{1}{\epsilon}W'(\phi^\epsilon) = 0.$$

Taking $\phi^\epsilon(x) = \phi(x/\epsilon)$, we get the rescaled equation. Notice that in $\mathcal{F}$, the energy for the traveling wave solution ϕ^ϵ is

$$\mathcal{F}^\epsilon[\phi^\epsilon] = \mathcal{F}[\phi] = \sigma_0.$$

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 $\phi((x - ct)/\epsilon)$, where c is the speed of the traveling wave. Plug this ansatz into equation $\delta\mathcal{F}/\delta\phi = 0$, we get

$$-c\phi' - \triangle\phi + W'(\phi) = 0.$$

Cahn-Hilliard interface The Cahn-Hilliard equation is

$$\phi_t = -\nabla \cdot (m\nabla\mu),\ \mu = -\frac{\delta \mathcal{F}}{\phi}.$$

Again, we look for steady interface. This leads to

$$m(\phi)\nabla\mu = C,$$

or

$$\nabla\mu = \frac{C}{m(\phi)}$$

We assume for the moment that the mobility is independent of ϕ. Then we get

$$\mu = \mu_0 \text{ for all } x.$$

Or

$$-\phi'' + W'(\phi) = \mu_0.$$

We look for solution with $\phi(\pm\infty) = \pm 1$ and $\phi'(\pm\infty) = 0$. Multiplying this equation by ϕ', we get

$$\frac{d}{dx}\left(-\frac{1}{2}\phi'^2 + W(\phi) - \mu_0\phi\right) = 0.$$

Using the far field condition, we get

$$-\frac{1}{2}\phi'^2 + W(\phi) - \mu_0\phi = W(1) - \mu_0.$$

Or

$$\phi'^2 = 2(W(\phi) - W(1) - \mu_0(\phi - 1)) = F(\phi)$$

Thus,

$$\phi' = \pm\left(W(\phi) - W(1) - \mu_0(\phi - 1)\right)^{1/2}.$$

In order to have $\phi'(\pm\infty) = 0$, we see that $F(1) = 0$, we also need to require $F(-1) = 0$. This leads to

$$W(-1) - W(1) - \mu_0(-1 - 1) = 0,$$

which implies

$$\mu_0 = (W(1) - W(-1))/2 = \frac{W(\phi_a) - W(\phi_b)}{\phi_a - \phi_b}.$$

Here, ϕ_a and ϕ_b are the two equilibra of the double well potential W. Thus, the only addimisible chemical potential connecting two equilibra is the relative energy difference between them. With this choice of chemical potential, we see the interface equation is the same as the Allen-Cahn interface equation. Thus, the structure is the same.

Cahn-Hilliard Traveling wave with nonzero speed Suppose the speed is c, then we look for traveling wave solution $\phi(x - ct)$. In this case, the

Combustion front In reaction-diffusion equation

$$u_t = \triangle u + f(u)$$

where $f(u)$ has two equilibra u_a and u_b.

Appendix A

Stress-Strain relation

A.1 Constitutive relation: Stress-strain relation

The stress in an elastic material is due to deformation. Therefore we assume the stress tensor T is a function of the deformation gradient F. Such a relation

$$T(y) = \widehat{T}(x, F)$$

is called a constitutive relation and $\widehat{T}$ is called a *response function*. If $\widehat{T}$ is independent of x, the material is called homogeneous. Below, we want to find the physical conditions of a response function.

A.1.1 Frame indifference

First, the stress should be independent of the frame of reference physically. Suppose y is the coordinate in the original frame, and y^* is the coordinate in new frame which is a rotation of the old frame. That is, $y^* = Qy$, and Q is a rotation. Then $F^* := \partial y^*/\partial x = QF$; the normal and the stress in the old and new frames are related by $\nu^* = Q\nu$, $\sigma^* = Q\sigma$. In terms of the response function, it reads

$$\begin{aligned} \sigma^* &= \widehat{T}(QF)\nu^* = \widehat{T}(QF)Q\nu \\ Q\sigma &= Q\widehat{T}(F)\nu. \end{aligned}$$

Hence,

$$\widehat{T}(QF) = Q\widehat{T}(F)Q^T. \tag{1.1}$$

Such a condition for $\widehat{T}$ is called the *axiom of material frame-indifference.*

Next, we will show that $\widehat{T}$ is indeed a function of the Cauchy-Green strain tensor only. Let us write F in polar form

$$F = RU.$$

where R is a rotation and U is positive definite. From the axiom of material frame-indifference, we get

$$\widehat{T}(F) = \widehat{T}(RU) = R\widehat{T}(U)R^T = FU^{-1}\widehat{T}(U)UF^T = F\overline{T}(C)F^T.$$

where $C = U^2 = F^T F$ is the right Cauchy-Green strain tensor.

Similarly, for the Piola tensor P, the frame-indifference reads

$$P(QF) = J\widehat{T}(QF)(QF)^{-T} = J(Q\widehat{T}(F)Q^T)Q^{-T}F^{-T} = QP(F).$$

and

$$P(F) = J\widehat{T}(F)F^{-T} = JF\overline{T}(C) = F\overline{P}(C),$$

where $J^2 = detC$ and $\overline{P}(C) := \sqrt{detC}\,\overline{T}(C)$. For the second Piola tensor it satisfies

$$\Sigma(QF) = (QF)^{-1}P(QF) = (F^{-1}Q^{-1})(QP(F)) = \Sigma(F),$$

and

$$\Sigma(F) := F^{-1}P = \overline{P}(C).$$

A.1.2 Isotropic material

A material is isotropic if its stress tensor is independent of a rotation of the strain. Suppose we have two identical materials. One has material coordinate x, while the other is x^* with $x^* = Qx$ and Q being a rotation. If these two materials deform in the same way and result the same stresses, we call this material isotropic. Mathematically, this means

$$\widehat{T}(FQ) = \widehat{T}(F). \tag{1.2}$$

In terms of Piola stress tensor, it reads

$$P(FQ) = P(F)Q \text{ for all } Q \tag{1.3}$$

This follows from

$$P(FQ) = J\widehat{T}(FQ)(FQ)^{-T} = J\widehat{T}(F)F^{-T}Q = P(F)Q.$$

In order to characterize the response function of an isotropic material, we review some spectral properties of a matrix.

- Given a matrix A, the characteric polynomial is

  $$p(\lambda) := det(A - \lambda I) = -\lambda^3 + \iota_1\lambda^2 - \iota_2\lambda + \iota_3.$$

  The coefficients $\iota_1, \iota_2, \iota_3$ are called the principal invariants of A.

- $$\begin{aligned} \iota_1 &= trA = \lambda_1 + \lambda_2 + \lambda_3 \\ \iota_2 &= \frac{1}{2}\left((trA)^2 - tr(A^2)\right) = tr(CofA) = \lambda_1\lambda_2 + \lambda_2\lambda_3 + \lambda_3\lambda_1 \\ \iota_3 &= detA = \lambda_1\lambda_2\lambda_3. \end{aligned}$$

- Caley-Hamilton theorem: $p(A) = 0$.

- The matrix A^p, with $p \in \mathbb{Z}$ and ($p \geq 0$ or $p \leq 1$ if A is invertible) has the 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

$$\beta(B) = \sum_{i=1}^{3} \beta(\lambda_i) p_i p_i^T$$

Theorem 1.1 (Rivlin-Ericksen representation theorem) *A mapping* $\widehat{T} : \mathbb{M}^3_+ \to \mathbb{S}^3$ *satisfies*

$$\widehat{T}(QF) = Q\widehat{T}(F)Q^T \text{ and } \widehat{T}(FQ) = \widehat{T}(F) \text{ for all } F \in \mathbb{M}^3_+, Q \in \mathbb{Q}^3_+, \tag{1.4}$$

if and only if $\widehat{T}(F) = \overline{T}(FF^T)$ *with*

$$\overline{T}(B) = \beta_0(\iota_B)I_0 + \beta_1(\iota_B)B + \beta_2(\iota_B)B^2.$$

Proof.

1. $\widehat{T}(F) = \widehat{T}(VR) = \widehat{T}(V) = \overline{T}(V^2) = \overline{T}(B) = \overline{T}(FF^T)$.

2. $\overline{T}(QBQ^T) = Q\overline{T}(B)Q^T$. This follows from

$$\overline{T}(QBQ^T) = \overline{T}(QV(QV)^T) = \overline{T}(QV) = Q\overline{T}(V)Q^T = Q\overline{T}(B)Q^T.$$

   This means that $\overline{T}(B)$ is only a function of eigenvalues of B.

3. For positive definite matrix B, the function $\overline{T}(B)$ has the representation:

$$\overline{T}(B) = b_0(B)I + b_1(B)B + b_2(B)B^2$$

   where $b_i(B)$ are scalar functions of B. The proof of this claim is divided into three cases: (i) λ_i are distinct, (ii) $\lambda_2 = \lambda_3$, (iii) all eigenvalues are equal.

   (i) We have

$$\begin{aligned} I &= p_1p_1^T + p_2p_2^T + p_3p_3^T \\ B &= \lambda_1p_1p_1^T + \lambda_2p_2p_2^T + \lambda_3p_3p_3^T \\ B^2 &= \lambda_1^2p_1p_1^T + \lambda_2^2p_2p_2^T + \lambda_3^2p_3p_3^T \end{aligned}$$

   and the spectral mapping

$$\overline{T}(B) = \mu_1p_1p_1^T + \mu_2p_2p_2^T + \mu_3p_3p_3^T.$$

   This leads to an inversion from $(p_1p_1^T, p_2p_2^T, p_3p_3^T)$ to I, B, B^2.

(ii) We have

$$\begin{aligned} I &= p_1p_1^T + (p_2p_2^T + p_3p_3^T) \\ B &= \lambda_1 p_1p_1^T + \lambda_2(p_2p_2^T + p_3p_3^T) \end{aligned}$$

and the spectral mapping

$$\overline{T}(B) = \mu_1 p_1p_1^T + \mu_2 p_2p_2^T + \mu_3 p_3p_3^T.$$

From $bT(QBQ^T) = Q\overline{T}Q^T$, we get $\mu_2 = \mu_3$. This leads to

$$\overline{T}(B) = b_0(B)I + b_1(B)B.$$

(iii) In this case, we have $bT(B) = b_0(B)I$.

4. It remains to show that $b_i(B)$ is indeed only functions of its invariants. From the independence of I, B, B^2 and $\overline{T}(QBQ^T) = Q\overline{T}(B)Q^T$, we get $b_i(QBQ^T) = b_i(B)$. This leads to b_i are only functions of the three principal invariants.

∎

Theorem 1.2 *For an isotropic material, its second Piola stress-strain relation has the following representation*

$$\Sigma(C) = \gamma_0(\iota_C)I + \gamma_1(\iota_C)C + \gamma_2(\iota_C)C^2.$$

Proof. (i) From the polar decomposition: $F = RU = VR$ and $C = F^TF = U^2$, $B = FF^T = V^2$, we get $C = R^TBR$. Thus, $\iota_C = \iota_B$, $F^{-1}BF^{-T} = I$ and $F^{-1}B^2F^{-T} = C$.
(ii) Next, from $\Sigma = JF^{-1}TF^{-T}$ and Rivlin-Ericksen theorem, we get

$$\begin{aligned} \Sigma &= JF^{-1}\left(\beta_0(\iota_B)I + \beta_1(\iota_B)B + \beta_2(\iota_B)B^2\right)F^{-T} \\ &= J\left(\beta_0(\iota_C)C^{-1} + \beta_1(\iota_C)I + \beta_2(\iota_C)C\right). \end{aligned}$$

(iii) From Caley-Hamilton theorem, it holds

$$C^3 - \iota_1(C)C^2 + \iota_2(C)C - \iota_3(C)I = 0.$$

Hence,

$$C^{-1} = \iota_3^{-1}\left(\iota_2 I - \iota_1 C + C^2\right).$$

(iv) It holds $J = \iota_3(C)^{1/2}$.
From (ii), (iii) and (iv), we complete the proof of the theorem. ∎

Theorem 1.3 *For an isotropic elastic material, by normalizing $\Sigma(I) = 0$, the Piola stress tensor has the following representation:*

$$\Sigma(C) = \lambda(tr\,E)I + 2\mu E + o(E). \tag{1.5}$$

Here, λ and μ are called the Lamé constants, $E = (C-1)/2$.

Proof. (i) At equilibrium, $y = x$ and $F = I$, $C = I$, $B = I$, the stress is normalized to be $\widehat{T}(I) = 0$ and $\Sigma(I) = 0$. In this case, we have

$$\begin{aligned} \sum_{i=0}^{2} \beta_i(\iota_I) &= 0 \\ \sum_{i=0}^{2} \gamma_i(\iota_I) &= 0. \end{aligned}$$

(ii) We expand the principal invariants about $E = 0$: First, we have

$$\begin{aligned} tr\, C &= 3 + 2tr\, E \\ tr\, C^2 &= 3 + 4tr\, E + o(E) \\ tr\, C^3 &= 3 + 6tr\, E + o(E). \end{aligned}$$

Second, the principal invariants can be expanded as

$$\begin{aligned} \iota_1(C) &= tr\, C \\ \iota_2(C) &= \frac{1}{2}\left((tr\, C)^2 - tr\, C^2\right) = 3 + 4tr\, E + o(E) \\ \iota_3(C) &= \frac{1}{6}(tr\, C)^3 - \frac{1}{2} tr\, C\, tr\, C^2 + \frac{1}{3} tr\, C^3 \\ &= 1 + 2tr\, E + o(E). \end{aligned}$$

(iii) We expand (1.5) in $E = (C - I)/2$ around $E = 0$ and use (i) and (ii). ∎

A.1.3 Hyper-elastic material

A material is called hyper-elastic material if there exists a potential $W(F)$ such that

$$P(F) = \frac{\partial W}{\partial F}.$$

Notice that such materials satisfy the frame-indifference axiom if and only if

$$W(QF) = W(F) \text{ for all } Q.$$

To see this, we differentiate the above equation in F to get

$$P(F) = \frac{\partial}{\partial F} W(F) = \frac{\partial}{\partial F} W(QF) = Q^T \frac{\partial W(QF)}{\partial (QF)} = Q^T P(QF).$$

This shows $W(F) = W(QF)$ if and only if $P(QF) = QP(F)$ for all Q. Similarly, a hyper-elastic material is isotropic (i.e. $P(FQ) = P(F)Q$ if and only if $W(FQ) = W(F)$ for all Q.

$$P(F) = \frac{\partial}{\partial F} W(F) = \frac{\partial}{\partial F} W(FQ) = \frac{\partial W(QF)}{\partial (QF)} Q^T = P(QF)Q^T.$$

Thus, for an isotropic hyper-elastic material, its potential energy function W satisfies

$$W(FQ) = W(QF) = W(F) \text{ for all } Q \tag{1.6}$$

Thus, W is only a function of the principal invariants of F. Two simple examples are

- Hook's law: $W(F) = \frac{1}{2}H|F|^2$, where $|F|^2 = \sum_{ij} |F_{ij}|^2$.
- Neo-Hookean material:

$$W(F) = a|F|^2 + g(\det F), a > 0.$$

- Mooney-Rivlin materials:

$$W(F) = a|F|^2 + b|\text{adj}F|^2 + g(\det F), a, b > 0.$$

- $$W = \frac{\lambda}{2}(tr\, E)^2 + \mu\, tr\,(E^2), \text{ where } E = \frac{1}{2}(C - I) \tag{1.7}$$

A.1.4 Linear elastic material

When there is no deformation, i.e. $F = I$,$C = I$, it is natural to set the corresponding stress $\widehat{T}(I) = 0$. In terms of Piola stress tensor, $\Sigma(I) = \overline{P}(I) = 0$. When $|\nabla_x u| = \epsilon << 1$,

$$C = F^T F = I + \nabla_x u + (\nabla_x u)^T + (\nabla_x u)^T(\nabla u) = I + 2E + o(\epsilon),$$

where

$$E = \frac{1}{2}\left(\nabla_x u + (\nabla_x u)^T\right).$$

We can expand $\overline{P}$ about I in terms of E, or $(C - I)$:

$$\overline{P}(C) = \overline{P}(I) + \frac{1}{2}AE + o(|E|).$$

where $A = (a_{ijkl})$ is a 4-tensor. Then the Piola tensor P has the form:

$$P = F\overline{P}(C) = (I + \nabla u)AE + o(\epsilon) = AE + o(\epsilon).$$

Here, we have absorbed $\nabla u AE$ into $o(\epsilon)$. A material whose Piola tensor has the form $P = AE$ is called a linear elastic material. In coordinate form:

$$P_{ij} = a_{ijkl}e_{kl}.$$

The four-tensor A should satisfy

$$a_{ijkl} = a_{ijlk},$$

because E is symmetric and we can always redefine $\bar{a}_{ijkl} = (a_{ijkl} + a_{ijlk})/2$ so that $\bar{a}_{ijkl}e_{kl} = a_{ijkl}e_{kl}$.

Suppose in addition the material is hyper-elastic, that is, there exists a free energy W such that $P = \partial W/\partial E$. In this case, from $\partial^2 W/\partial e_{ij}\partial e_{kl} = \partial^2 W/\partial e_{kl}\partial e_{ij}$, we get

$$a_{ijkl} = a_{klij}.$$

The equation of motion is

$$\begin{aligned}
\rho_0 \ddot{u}_i &= \sum_j \partial_j \left(\sum_{kl} a_{ijkl} e_{kl} \right) \\
&= \frac{1}{2} \sum_j \sum_{kl} \partial_j \left(\frac{\partial u_k}{\partial x_l} + \frac{\partial u_l}{\partial x_k} \right) \\
&= \sum_{jkl} a_{ijkl} \frac{\partial^2 u_k}{\partial x_j \partial x_l}
\end{aligned}$$

Here, we have used

$$\sum_{kl} a_{ijkl} \frac{\partial u_l}{\partial x_k} = \sum_{kl} a_{ijkl} \frac{\partial u_k}{\partial x_l}$$

Definition 1.1

- *Strong ellipticity: The system is strongly elliptic if there exists a positive constant α such that for any $\xi \in \mathbb{R}^3$, $\eta \in \mathbb{R}^3$,*

$$\sum_{ijkl} a_{ijkl} \xi_i \xi_k \eta_j \eta_l \geq \alpha |\xi|^2 |\eta|^2.$$

- *Stability: The system is stable if there exists a positive constant $\tilde{\alpha}$ such that for any symmetric matrix (e_{ij}), we have*

$$\sum_{ijkl} a_{ijkl} e_{ij} e_{kl} \geq \tilde{\alpha} \sum_{kl} e_{kl}^2.$$

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 notice that

$$\begin{aligned}\sum_{ij}|e_{ij}|^2 &= \frac{1}{4}\sum_{ij}(\xi_i\eta_j+\xi_j\eta_i)^2\\ &= \frac{1}{4}\sum_{ij}\left(\xi_i^2\eta_j^2+\xi_j^2\eta_i^2+2\xi_i\eta_i\xi_j\eta_j\right)\\ &= \frac{1}{2}\left(|\xi|^2|\eta|^2+(\xi\cdot\eta)^2\right)\\ &\geq \frac{1}{2}|\xi|^2|\eta|^2.\end{aligned}$$

Hence, the stability implies strong ellipticity.

Lemma 1.1 (Korn's inequality) *Let $u:\Omega\to\mathbb{R}^3$ and $e=\frac{1}{2}(\partial u/\partial x+(\partial u/\partial x)^T)$. It holds that*

$$\int_\Omega\sum_{ij}\left(\frac{\partial u_i}{\partial x_j}\right)^2 dx\leq 2\int\sum_{ij}e_{ij}^2\,dx \text{ for all } u\in H_0^1(\Omega).$$

Proof. We have that

$$\begin{aligned}\sum_{ij}e_{ij}^2 &= \frac{1}{4}\sum_{ij}\left(\frac{\partial u_i}{\partial x_j}+\frac{\partial u_j}{\partial x_i}\right)^2\\ &= \frac{1}{2}\sum_{ij}\left(\left(\frac{\partial u_i}{\partial x_j}\right)^2+\frac{\partial u_i}{\partial x_j}\frac{\partial u_j}{\partial x_i}\right)\end{aligned}$$

We integrate this equality over Ω, and notice that

$$\int_\Omega\frac{\partial u_i}{\partial x_j}\frac{\partial u_j}{\partial x_i}\,dx=\int_\Omega\frac{\partial u_i}{\partial x_i}\frac{\partial u_j}{\partial x_j}\,dx.$$

Here, we have used $u\in H_0^1(\Omega)$. We then get

$$\begin{aligned}\int_\Omega\sum_{ij}e_{ij}^2\,dx &= \frac{1}{2}\int_\Omega\sum_{ij}\left(\left(\frac{\partial u_i}{\partial x_j}\right)^2+\frac{\partial u_i}{\partial x_i}\frac{\partial u_j}{\partial x_j}\right)dx\\ &= \frac{1}{2}\int_\Omega\left(\frac{\partial u_i}{\partial x_j}\right)^2+\sum_i\left(\frac{\partial u_i}{\partial x_i}\right)^2dx\\ &\geq \frac{1}{2}\int_\Omega\left(\frac{\partial u_i}{\partial x_j}\right)^2dx\end{aligned}$$

∎

Theorem 1.4 (Ball) *If $u^n\rightharpoonup u$ 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 $\partial u/\partial x$.*

The free energy W is called polyconvex in F if it can be expressed as a convex function of the determinants of the submatrices of F.

Theorem 1.5 *If $W(e)=Ae$ is polyconvex, then W is stronly elliptic.*

Appendix B

Surface Theory

B.1 Metric, area and first fundamental form

Deformation and parametrization . Let $X \to x$ be a mapping from $\Sigma_0 \subset \mathbb{R}^2$ to a surface $\Sigma \subset \mathbb{R}^3$. Let $F^i_\alpha = \partial x^i / \partial X^\alpha$ be its differential. For a vector field in $T\Sigma_0$ with $v = v^\alpha \partial/\partial X^\alpha$, the differential F maps it to $w = w^i \frac{\partial}{\partial x^i}$ with

$$w^i = F^i_\alpha v^\alpha.$$

We denote this by $w = Fv$.

First fundamental form . The mapping $x(\cdot)$ induces an inner product on Σ_0. Given any $v_1, v_2 \in \Sigma_0$, we define

$$\langle v_1, v_2 \rangle := (Fv_1, Fv_2) = (F^T F v_1, v_2).$$

Here, $(\cdot, \cdot)$ is the inner product in the Euclidean space. Thus, the Euclidean inner produce in $\mathbb{R}^3$ induces a metric $g_{\alpha\beta}$ on Σ_0 defined by

$$g_{\alpha\beta} = \left(\frac{\partial x}{\partial X^\alpha}, \frac{\partial x}{\partial X^\beta} \right) = (F^T F)_{\alpha\beta}.$$

This metric g is called the first fundamental form for the X-coordinate system for Σ. It can be used to measure the distance, the angle and the area on the surface Σ. The length of a vector v is measured by $\langle v, v \rangle$, the angle between two unit vectors v_1 and v_2 is $\langle v_1, v_2 \rangle$. Thus, a curve $\{X(t) | 0 \le t \le 1\}$ on Σ_0 has length

$$\int_0^1 \sqrt{g_{\alpha\beta} \dot{X}^\alpha \dot{X}^\beta}\, dt.$$

This is indeed the arc length of the curve $x(X(t))$ in $\mathbb{R}^3$.

The area spaned by two vectors v_1 and v_2 is

$$\sqrt{\langle v_1, v_1 \rangle \cdot \langle v_2, v_2 \rangle - \langle v_1, v_2 \rangle^2} = J|u||v|.$$

Here, $J = \sqrt{\det g}$ is the Jacobian. Thus, the area element on Σ under the metric g is

$$dA = J dX_1 dX_2.$$

This is the area element of Σ in $\mathbb{R}^3$.

B.2 Second fundamental form and intrinsic properties

The normal of Σ is

$$N = \frac{\frac{\partial x}{\partial X^1} \times \frac{\partial x}{\partial X^2}}{\| \frac{\partial x}{\partial X^1} \times \frac{\partial x}{\partial X^2} \|}$$

This normal N maps Σ_0 to S^2. Its differential dN maps $T\Sigma_0$ to the tangent of S^2, which can be identified to be $T\Sigma$. This is because

$$0 = d(N, N)(v) = 2(dN(v), N),$$

that is, for $v \in T\Sigma_0$, we have $dN(v) \perp N$. Hence, we can indify $dN(v) \in T\Sigma$. 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

$$L_{\alpha\beta} = -\left(\frac{\partial N}{\partial X^\alpha}, \frac{\partial x}{\partial X^\beta} \right).$$

One can immediately see that

$$L_{\alpha\beta} = \left(N, \frac{\partial^2 x}{\partial X^\alpha \partial X^\beta} \right).$$

Given a curve $C : x(X(t)), -\epsilon < t < \epsilon$ on Σ_0, we parametrize C by its arc length s. We have $(N(s), x'(s)) = 0$. Hence, $(N(s), x''(s)) = -(N'(s), x'(s))$. Therefore,

$$\begin{aligned} II(X'(0)) &:= -L_{\alpha\beta} X'^\alpha(0) X'^\beta(0) \\ &= -\left(\frac{\partial N}{\partial X^\alpha} X'^\alpha(0), \frac{\partial x}{\partial X^\beta} X'^\beta(0) \right) \\ &= -(N'(0), x'(0)) = (N(0), x''(0)) = (N, kn) = k_n. \end{aligned}$$

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.3 Vector, co-vector and tensor fields

Vector A vector on $T\Sigma_0$ has the form $v = v^\alpha \partial/\partial X^\alpha$. Its image under $x(\cdot)$ is $w = w^i \partial/\partial x^i$ with

$$w^i = F^i_\alpha v^\alpha.$$

That is, $w = Fv$.

For any $w \in T\Sigma$, we can find a unique $v \in T\Sigma_0$ such that $Fv = w$. To find v in terms of w, we use

$$F^i_\beta w^i = F^i_\beta F^i_\alpha$$

In matrix form, it is

$$(F^T F)v = F^T w$$

Thus,

$$v = (F^T F)^{-1} F^T w.$$

We denote $F^\dagger = (F^T F)^{-1} F^T$, the pseodo-inverse of F. The mapping $FF^\dagger$ is the projection from $\mathbb{R}^3$ to the tangent plane of $T\Sigma$.

Co-vector On $T^*\Sigma_0$, we define dX^α such that $dX^\alpha(\partial/\partial X^\beta) = \delta^\alpha_\beta$. A co-vector $v^* = v^*_\alpha dX^\alpha$ is defined on $T^*\Sigma$. From Riesz representation theorem, there exists a unique $v \in T\Sigma_0$ such that

$$v^*(\partial/\partial X^\alpha) = \langle v, \partial/\partial X^\alpha \rangle.$$

That is, $v^*_\alpha = g_{\alpha\beta} v^\beta$. This leads to

$$v^\alpha = g^{\alpha\beta} v^*_\beta,$$

where

$$g^{\alpha\beta} := (g^{-1})^{\alpha\beta}.$$

An one-form $\omega = \omega_i dx^i$ in $T^*\Sigma$ can be pull back by

$$\omega_i \frac{\partial x^i}{\partial X^\alpha} dX^\alpha = \omega_i F^i_\alpha dX^\alpha$$

or in matrix form, $F^T \omega$.

Given an one-form $\omega_i dx^i$, the vector $\omega = (\omega_i)$ is a co-vector. In the two form $\nu_i dx^j dx^k$, the vecor (ν_i) is also treated as a covector. Therefore, we can pull back them by $F^T \nu$.

If ν is a unit covector in Σ and n be the normalized pull back of ν under F, then

$$n = J^{-1} F^T \nu.$$

Tensor A tensor P on Σ_0 maps a co-vector $n \in T^*\Sigma_0$ to a vector in $\mathbb{R}^3$. P can be represented as $P^{i\alpha}$ and $Pn = P^{i\alpha}n_\alpha \partial/\partial x^i$ If n is the pullback (with normalization) of a unit co-vector $\nu \in \mathbb{T}^*\Sigma$, then $n = J^{-1}F^T\nu$. Let T be the tensor which maps a co-vector ν to a vector in $T\Sigma$. $T\nu$ can be represented as $T^{ij}n_j\partial/\partial x_i$. If

$$T\nu = Pn,$$

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 whih maps $n \in T^*\Sigma_0$ to $T\Sigma$ and the tensor $P = F\hat{P}$. In this formulation,

$$F\hat{P}F^T = JT$$

In the case of hypermaterial, $\hat{P} = W'(F^TF)$.

B.4 Gradient and Divergence

Scalar field A scalar field ϕ_0 defined on Σ_0 can be push forward to a scalar field defined on Σ by

$$\phi(x) = \phi_0(X) \text{ if } x = x(X).$$

Alternatively, we can use delta function to express ϕ:

$$\phi(x) = \int_{\Sigma_0} \phi_0(X)\delta(x - x(X))\, dX$$

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:

$$d\phi_0(v) = (\nabla_X\phi_0, v).$$

Here, the meaning of $(\cdot,\cdot)$ is the bilinear functional between vector and co-vector, which is defined so that $(dX^\alpha, \partial/\partial X^\beta) = \delta^\alpha_\beta$. We can also define the gradient $\nabla_x\phi$ to be

$$d\phi(w) = (\nabla_x\phi, w)$$

for any vector $w \in T\Sigma$. Since $v = F^\dagger w$, we obtain

$$(\nabla_x\phi, w) = (\nabla_X\phi_0, F^\dagger w) = ({F^\dagger}^T\nabla_X\phi_0, w)$$

Hence,

$$\nabla_x\phi = (F^\dagger)^T\nabla_X\phi_0.$$

This is the definition of $\nabla_x\phi$ on Σ. Since $F^T(F^\dagger)^T = I$, we then get

$$\nabla_X\phi_0 = F^T\nabla_x\phi.$$

Thus, the co-vector $\nabla_X\phi_0$ is the pullback of $\nabla_x\phi$.