PDE and Modelling - inofficial lecture notes

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The lecture will be split in 3 chapters:

Chapter I Basic notions of continuous mechanics

Chapter II PDE techniques for fluid mechanics

Chapter III Solid mechanics $\to$ Calculus of variations

Chapter 1

Basic notions of continuous mechanics

1.1 Modelling a physical system

Point $\rightarrow$ continuous mechanics

Regarding the modelling we have 2 main examples:

a) Flow of a fluid around an obstacle (stone, airplane), or in a pipe

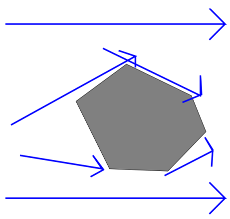

Figure 1.1: Fluid flows around an obstacle

b) Deformations in a solid (ex. a sponge)

Physical description

Microscropic: atosm/molecules, $\sim 10^{26}$ molecules $\Rightarrow$ This is hard!!!
Macroscopic: $\Rightarrow$ See water / sponge as continuous materials! This leads to the concept of continuous mass distribution (has to be defined).

In general, Physics leads to PDE, this means we get a PDE if we translate a physical problem into mathematics.

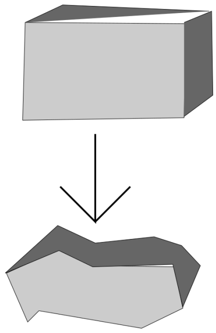

Figure 1.2: Deformation of a sponge

From physics to PDE

1. Identify the mathematical object (what is the size of interest (temperature, pressure, dislocation, ...)?) $\Rightarrow$ This yields a function $u(\vec{x}, t)$, for $\vec{x} \in \mathbb{R}^3$, $t > 0$ and $u \in \mathbb{R}^n$
2. Use physical laws and some assumptions on the material $\Rightarrow$ This shows that the size of interest needs to satisfy a (system of) PDE
3. Boundary conditions tell us, how the sample (domain) interacts with the external world
4. Set initial conditions for the object of interest, i.e. specify $u(\vec{x}, 0)$

Example.
Consider a fluid flowing around an obstacle.

1. *$\vec{u}(\vec{x}, t)$ is the velocity of a small portion of fluid near $\vec{x}$ at time t. The domain K is compact in $\mathbb{R}^3$, so we look for*

$$\begin{aligned} u : \mathbb{R}^3 \setminus K \times (0, \infty) &\to \mathbb{R}^3 \\ (x, t) &\mapsto \vec{u}(x, t) \end{aligned}$$

2. *Use physical laws (conservation laws). Make assumptions on the fluid, i.e. compressible / incompressible. This gives us different PDE.*
   In the incompressible case $\Rightarrow$ ***Navier Stokes equations***

$$\varrho_0[\partial_t \vec{u} + (\vec{u} \cdot \vec{\nabla})\vec{u}] = -\vec{\nabla} p + \eta \Delta \vec{u}$$
$$\operatorname{div} \vec{u} = 0$$

   for $x \in \mathbb{R}^3 \setminus K, t > 0$. Here we used

   - *the mass density $\varrho_0 > 0$*
   - *the dynamical viscosity $\eta > 0$*

- *the pressure* $p : \mathbb{R}^3 \setminus K \times \mathbb{R}_+ \to \mathbb{R}$
- *and the notation*

$$\vec{u} \cdot \vec{\nabla} = \sum_{j=1}^{3} u_j \frac{\partial}{\partial u_j}$$

so

$$[(\vec{u} \cdot \vec{\nabla})\vec{u}]_i = \left[\sum_{j=1}^{3} u_j \frac{\partial}{\partial u_j}\right] u_i,$$

as well as

$$(\vec{\nabla} p)_i = \frac{\partial}{\partial u_i} p$$

and

$$[\Delta \vec{u}]_i = \left[\sum_{j=1}^{3} \left(\frac{\partial}{\partial u_j}\right)^2\right] u_i$$

3. *Impose boundary conditions. We have 2 possible boundaries: either ∂K or the behaviour of our size at interest at infinite distance.*
   For ∂K we have <u>*two*</u> *types of possible boundary conditions:*
   - *Dirichlet B.C. fix the value of our size of interest at ∂K, i.e. fix $u_{|\partial K}$. The homogeneous B.C. $u_{|\partial K}$ is also called no slip (sticky) boundary condition*
   - *Neumann B.C. fix $(\nabla_N u)_{|\partial K}$, i.e. the gradient in outer normal direction of ∂K. This fixes not the specific value of the size of interest, but its amount of change (that is the gradient)*

   At infinity we do the following: If there is no K, we assume that the fluid flows at constant speed (it does not hit any obstacle), i.e. $\vec{u}(x,t) = \vec{u}_\infty$ is constant.
4. *Impose initial conditions: Give $u(x,0) = \vec{u}_0(x)$, where $\vec{u}_0$ is a fixed velocity distribution.*

From PDE to physics

a) Which PDE are physically reasonable? This leads to *dimensional analysis.*

b) Usually one experiments on a small sized sample (small toy airplane) in order to get a describing PDE. Does this PDE also describe the life-size system (true airplane)? This leads to the *similarity principle.*

a) Dimensional Analysis

We cannot compare meters and seconds! All terms in a PDE must have the same dimension! We have the following basic dimensions:

L length

T time

M mass

Thus e.g. the dimension of the velocity is

$$[u] = \frac{L}{T}.$$

Consider the Navier Stokes equation:

$$-\nabla p + \eta \Delta u = \varrho_0 \partial_t u + \varrho_0 (u \cdot \nabla) u$$

For dimensional analysis we need to check the dimension of each of the occuring terms:

- $[u] = \frac{L}{T}$
- $[p] = \frac{[\text{force}]}{[\text{area}]}$ and $[\text{area}] = L^2$
- $[\text{force}] =?$? Newtons law tells us $F = ma$ so

  $$[F] = M \frac{L}{T^2}$$

  Thus $[p] = \frac{ML}{T^2} \frac{1}{L^2} = \frac{M}{T^2 L}$
- $[\nabla p] = [\frac{\partial}{\partial u_i} p] = \frac{[p]}{L} = \frac{M}{T^2 L^2}$
- $[\varrho_0 \partial_t u] =?$? We have

  $$[\partial_t u] = \frac{[u]}{T} = \frac{L}{T^2}$$

  and

  $$\varrho_0 = \frac{\text{mass}}{\text{volume}} \quad \Rightarrow \quad [\varrho_0] = \frac{M}{L^3}$$

  thus

  $$[\varrho_0 \partial_t u] = \frac{M}{L^3} \frac{L}{T^2} = \frac{M}{L^2 T^2}$$

- $[(u\nabla)u] = \frac{[u]^2}{L} = \frac{L^2}{T^2} \frac{1}{L} = \frac{L}{T^2}$. We can do the first step as u appears twice on the LHS, so its dimension enters quadratically
- $[\eta \Delta u] \stackrel{!}{=} \frac{M}{T^2 L^2}$ has to hold. We have

  $$[\eta] \underbrace{[\Delta u]}_{= \frac{u}{L^2}} = \frac{M}{L^2 T^2}$$

  and

  $$[\eta] \cdot \frac{L}{\cancel{T}} \frac{1}{\cancel{L^2}} = \frac{M}{\cancel{T^2} \cancel{L^2}}.$$

  We will see later that $[\eta] = \frac{M}{LT}$ really holds.

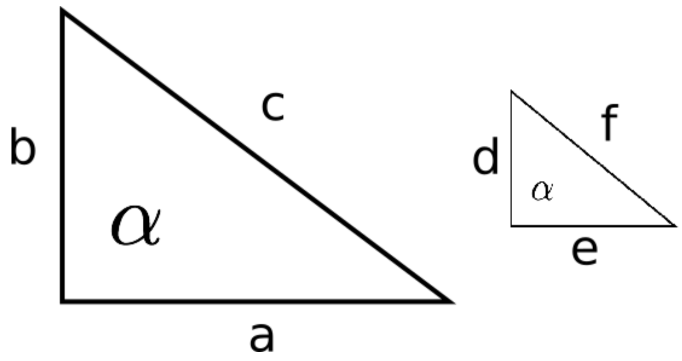

Figure 1.3: The triangles are similar, as $\sin\alpha = \frac{b}{a} = \frac{d}{e}$, so the adimensional parameters coincide

b) Similarity principle

Geometrically 2 triangles are similar if their *adimensional* parameter coincide. Analogeously to the case of triangles (see Fig. 1.3) two physical processes are similar if the corresponding adimensional patrameters of the processes coincide. This means we need first to identify the adimensional parameters and then write the PDE in a dimensionless form (this can be done for physical systems that are similar!)

Example.

Consider again the case of Navier-Stokes:

$$-\nabla p + \eta\Delta u = \varrho_0\partial_t u + \varrho_0(u\cdot\nabla)u$$

with the variables x, t. Define new variables

$$\begin{aligned} y &:= \frac{x}{x_0} \\ \tau &:= \frac{t}{t_0} \end{aligned}$$

with $[x_0] = L$, $[t_0] = T$. A natural choice for x_0 is $x_0 = \operatorname{diam} K$ s.t. near the obstacle we have $|y| \approx 1$ and $|y| >> 1$ far away from the obstacle. Unfortunately there is no natural choice for t_0. We have

$$\begin{aligned} \tilde{u}(\tau, y) &= u(t(\tau), x(y)) \\ \tilde{p}(\tau, y) &= p(t(\tau), x(y)) \end{aligned}$$

thus we get

$$\partial_t u(t,x) = \partial_t \tilde{u}(\tau(t), y(x)) = \partial_\tau \tilde{u}\cdot\frac{\partial\tau}{\partial t}$$

and

$$\frac{\partial}{\partial u_i} u = \sum_j \frac{\partial\tilde{u}}{\partial y_j}\frac{\partial y_j}{\partial u_i} = \left(\frac{\partial\tilde{u}}{\partial y_i}\right)\frac{1}{x_0}.$$

Then, $\tilde{u}, \tilde{p}$ satisfy

$$-\frac{1}{x_0}\nabla_y \tilde{p} + \eta \frac{1}{x_0^2}\Delta_y \tilde{u} = \varrho_0 \left[\frac{1}{t_0}\partial_\tau \tilde{u} + \frac{1}{x_0}\left(\vec{\tilde{u}} \cdot \vec{\nabla} y\right) \tilde{u}\right]$$

but $\tilde{p}, \tilde{u}$ still have a dimension. Define

$$\tilde{v}(\tau, y) := \frac{\tilde{u}(\tau, y)}{u_0}$$
$$q(\tau, y) := \frac{\tilde{p}(\tau, y)}{p_0}$$

using $u_0 > 0$ with $[u_0] = [velocity]$ and $p_0 > 0$ with $[p_0] = [pressure]$. How can we choose u_0 and p_0? A natural choice for u_0 would be $u_0 = |\vec{u}_\infty$ (where $\lim_{|x|\to\infty} u(x,t) = \vec{u}_\infty$ is a constant vector). Then

$$v = \frac{\tilde{u}}{v_0} \quad \Rightarrow \quad |v| \overset{|y|\to\infty}{\to} \frac{1}{.}$$

For p_0 there is no natural choice.
Replace in the PDE:

$$-\frac{p_0}{x_0}\underbrace{\vec{\nabla} q}_{adim.} + \frac{u_0 \eta}{x_0^2}\underbrace{\Delta v}_{adim.} = \frac{\varrho_0 u_0}{t_0}\underbrace{\partial_t v}_{adim.} + \frac{\varrho_0^2}{x_0}\underbrace{(\vec{v} \cdot \vec{\nabla})\vec{v}}_{adim.}$$

Divide now by $\frac{\varrho_0 v_0}{t_0}$:

$$\partial_t v + \underbrace{\frac{v_0 t_0}{x_0}}_{adim.}(v\nabla)v = \underbrace{-\frac{\varrho_0}{x_0}\frac{t_0}{\varrho_0 v_0}}_{adim.}\nabla q + \underbrace{\frac{\eta}{x_0^2}\frac{t_0}{\varrho_0}}_{adim.}\nabla v$$

Now we have

- *fixed v_0, x_0*
- *free t_0, p_0*
- *ϱ_0, η given by the physical system*

and we want to choose t_0 s.t. $\frac{v_0 t_0}{x_0} = L = v_0 = \frac{x_0}{t_0}$, so

$$\Rightarrow \frac{p_0 t_0}{x_0 \varrho_0 v_0} = \frac{p_0}{\varrho_0 v_0^2}.$$

Choose p_0 s.t. $\frac{p_0}{\varrho_0 v_0^2} = 1$ so $p_0 = \varrho_0 v_0^2$. Then

$$\frac{\eta t_0}{x_0^2 \varrho_0} = \frac{\eta}{\varrho_0 v_0 x_0} = \frac{1}{Re}$$

where Re is the so called Reynolds number. *In the end we get*

$$\begin{aligned} \partial_\tau v + (v \cdot \nabla) v = & \quad -\nabla q + \frac{1}{Re} \Delta v \\ \operatorname{div} v = & \quad 0 \\ v(\tau, y) \overset{\|y\| \to \infty}{\longrightarrow} & \quad \frac{\vec{u}_\infty}{u_0}. \end{aligned} \tag{1.1}$$

The reynolds number is the only term that contains information on the physical system!

1.2 A summary of point mechanics

A particle occupies a finite volume. However, often it's practical to describe it as a single point particle, located at the center of mass. This works also for big objects, as e.g. planets.

Our physical system

In a physical syste mwe have N point particles with masses $m_i > 0$, $i = 1, ..., N$. These particles are moving in $\mathbb{R}^d$ (typically $d = 3$).

a) **Kinematics** movement

$\vec{x}_i(t) \in \mathbb{R}^d$, $i = 1, ..., N$ and $t > 0$ is the position of the i-th particle at time t. Analogeously $\vec{v}_i(t) = \vec{x}_i'(t)$ is the velocity of the i-th particle at time t. If no force acts on the particles $\Rightarrow$ Trajectory of the i-th particle is a line:

$$\begin{aligned} \vec{v}_i(t) &= \vec{v}_i(0), \quad \forall t \forall i \\ \vec{x}_i(t) &= \vec{x}_i(0) + t\vec{v}_i(0), \quad \forall t \forall i. \end{aligned}$$

b) Forces modify the trajectory. We have two types of forces acting on particle i:

1. External forces $\vec{f}_i(t)$
2. Internal forces among the particles: $f_{i,j}(t)$ is the force applied on i due to interaction with the j-th particle

The effect of the forces on the trajectory is described by Newton's 2nd law:

$$\text{force} = \text{mass} \cdot \text{acceleration}.$$

Thus for particle i it holds that

$$m_i \vec{x}_i''(t) = \underbrace{F_i}_{\text{total force acting on } i} = \vec{f}_i + \sum_{j=1, j \neq i}^{N} \vec{f}_{i,j} \tag{*}$$

Eq. (*) is called the **equation of motion for the i-th particle**.

Constraints on the form of $\vec{f}_{i,j}$

We have a mutual interaction between two particles, so the force does not just act in one direction (from one particle to another). Newton's 3rd law states that

$$\text{force on } i \text{ due to } j = -\text{force acting on } j \text{ due to } i$$

so

$$\vec{f}_{i,j}(t) = -\vec{f}_{j,i}(t)$$

$\Rightarrow \vec{f}_{i,j}$ must be of the form

$$\vec{f}_{i,j} = \frac{\vec{x}_i - \vec{x}_j}{|x_i - x_j|} \cdot g_{i,j}(|x_i - x_j|)$$

for a scalar function $g_{i,j}$ with $g_{i,j} = g_{j,i}$.

In $d = 3$ we have some examples:

- **Gravitational force:**
  $$g_{i,j}(\tau) = -\frac{Gm_i m_j}{\tau^2}$$
  where $m_i > 0$ is the mass and G is the gravity constant
- **Electrical force:**
  $$g_{i,j}(\tau) = K\frac{Q_i Q_j}{\tau^2}$$
  where Q_i is the charge of the particle j

Here we $|\vec{x}|$ to denote the euclidean norm for some $\vec{x} \in \mathbb{R}^d$.

Till now we just considered the interaction between 2 particles of the system. There are more constraints to be considered, which appear if we consider the whole system of N particles $\Rightarrow$ **Conservation laws**

c) **Conservation laws**

c_1) **Conservation of momentum:**

$$m_i \vec{v}_i = m_i \vec{x}_i' = \vec{p}_i$$

is called the **momentum of the particle** i. The **equation of momentum for the i-th particle** can be written as

$$\vec{p}_i' = F_i$$

which is the total force acting on i.

Let

$$\begin{aligned}\vec{p}(t) &= \sum_{i=1}^{N} \vec{p}_i(t) = \text{total momentum}\\ \vec{f}(t) &= \sum_{i=1}^{N} \vec{f}_i(t) = \text{total external force.}\end{aligned}$$

Then

$$\vec{p}'(t) = \vec{f}(t) \tag{c1}$$

Note that in the equation of momentum for one particle we have external <u>and</u> internal forces, whereas in Eq. (c1) just external forces appear!

Proof (Proof of Eq. (c1)). We have

$$\begin{aligned}\vec{p}'(t) &= \sum_{i=1}^{N} p_i'(t)\\ &= \sum_{i=1}^{N} F_i(t)\\ &= \underbrace{\sum_{i=1}^{N} \vec{f}_i(t)}_{=:f} + \underbrace{\sum_{i=1}^{N} \sum_{j=1, j\neq i}^{N} f_{i,j}}_{=\frac{1}{2}\sum_{i\neq j}\underbrace{(f_{i,j}+f_{j,i})}_{=0}} .\end{aligned}$$

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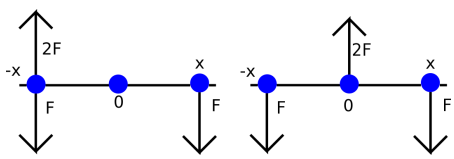

Figure 1.4: Two examples of force diagrams

c_2) **Conservation of angular momentum:**
In both cases of Fig. 1.4 we have total force equal to zero, but in the example on the left we have (clockwise) rotation.

Definition 1.1. For $d = 3$ the **cross product** (vector product) is defined as

$$\begin{aligned} x: \quad \mathbb{R}^3 \times \mathbb{R}^3 \quad & \to \mathbb{R}^3 \\ (a, b) \quad & \mapsto \vec{a} \times \vec{b} = |a|\,|b| \sin\Theta \end{aligned}$$

where $\Theta \in [0, \pi)$ is the angle between a and b. $\vec{n}$ is the unit vector $\perp$ to the plane spanned by a and b and its direction is given by the 'right hand rule':

$$\begin{aligned} (a \times b)_1 &= a_2 b_3 - a_3 b_2 \\ (a \times b)_2 &= a_3 b_1 - a_1 b_3 \\ (a \times b)_3 &= a_1 b_2 - a_2 b_1. \end{aligned}$$

It has the properties $a \times b = -b \times a$ and $a \times a = 0$.

We can represent the cross product by the *Levi-Civita* symbol $\varepsilon^{i,j,k}$:
Let $\pi(1,2,3) = \pi(1)\pi(2)\pi(3)$ and

$$\varepsilon^{\pi(1)\pi(2)\pi(3)} = \operatorname{sign} \pi$$

with $\varepsilon^{123} = 1 = \varepsilon^{312} = \varepsilon^{231}$. We have

$$\varepsilon : (1,2,3)^3 \to \{0, 1, -1\} \text{ with } (i,j,k) \mapsto \varepsilon^{ijk}.$$

It holds that $\varepsilon^{ijk} = 0$ if two f the indices coincide, otherwise we have $\varepsilon^{ijk} = \operatorname{sign} \pi$. Then

$$(a \times b)_i = \sum_{j,k=1}^{3} \varepsilon^{ijk} a_j b_k.$$

Definition 1.2. The **angular momentum of the external force on the i-th particle** (the torque) is defined as

$$\vec{M}_i := (\vec{x}_i - \vec{x}_0) \times \vec{f}_i,$$

where $\vec{x}_0$ is a fixed reference point in $\mathbb{R}^3$.

Definition 1.3. The **angular momentum of the i-th particle** is defined as

$$\vec{L}_i := (\vec{x}_i - \vec{x}_0) \times \vec{p}_i.$$

- c_2 **Conservation of angular momentum:**

Let

$$\begin{aligned} \vec{L} &= \sum_{j=1}^{N} \vec{L}_j \\ \vec{M} &= \sum_{j=1}^{N} \vec{M}_i \end{aligned}$$

be the **total angular momentum**, resp. the **total torque**. Then

$$\vec{L}'(t) = \vec{M}(t). \tag{c2}$$

PROOF. We have

$$\begin{aligned} L' &= \sum_{i=1}^{N} L_i' \\ &= \sum_{i=1}^{N} ((x_i - x_0) \times p_i)' \\ &= \sum_{i=1}^{N} \underbrace{x_i' \times p_i}_{m_i x_i' \times x_i' = 0} + \sum_{i=1}^{N} (x_i - x_0) \times p_i' \\ &= \sum_{i=1}^{N} (x_i - x_0) \times \underbrace{p_i'}_{\text{equal mot.}} \\ &= \sum_{i=1}^{N} (x_i - x_0) \times \underbrace{F_i}_{= \underbrace{f_i}_{\text{external}} + \underbrace{\sum_{j=1, j \neq i}^{N} f_{i,j}}_{\text{internal}}} \\ &= \underbrace{\sum_{i=1}^{N} (x_i - x_0) \times f_i}_{=M} + \underbrace{\sum_{i=1}^{N} \sum_{j=1, j \neq i}^{N} (x_i - x_0) \times f_{i,j}}_{:=A} \end{aligned}$$

where

$$A = \frac{1}{2} \sum_{i=1, i \neq j}^{N} (x_i - x_0) \times f_{i,j} + (x_j - x_0) \underbrace{f_{j,i}}_{=-f_{i,j}}$$

and from A terms cancel out using Newton's 3rd Law. ∎

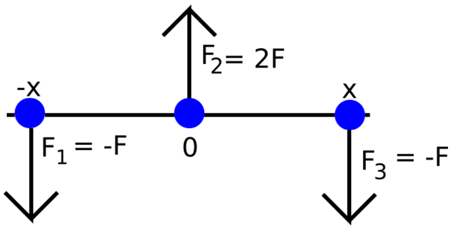

Figure 1.5: A force diagram

Example.
As seen in Fig. 1.5 the total force is $F_1+F_2+F_3=0 \Rightarrow P'=0$. *Using* $x_0=0$ *the total torque is*

$$\left.\begin{array}{ll} \vec{M}_1 = & (x_1-x_0)\times F_1 = \vec{x}\times\vec{F} \\ \vec{M}_2 = & (x_2-x_0)\times F_2 = -\vec{x}\times\vec{F} = -M_1 \\ \vec{M}_3 = & \underbrace{(x_0-x_0)}_{=0}\times F_3 = 0 \end{array}\right\} \Rightarrow M_1+M_2+M_3=0 \Rightarrow L'=0$$

thus the system is *<u>not rotating!</u>*

Another example:

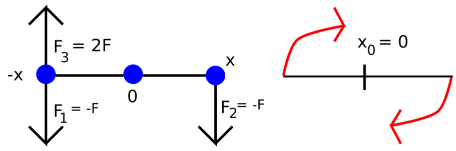

Figure 1.6: A force diagram and the resulting rotation of the system

Example.
For the situation in Fig. 1.6 we have that the total force $\tilde{F}_1+F_2=0$ *and* $P'=0$, *so there is no translation. However, the total torque is*

$$\left.\begin{array}{ll} M_1 = & (x_1-x_0)\times\tilde{F}_1 = -\vec{x}\times\vec{F} \\ M_2 = & (x_2-x_0)\times F+2 = -\vec{x}\times\vec{F} \end{array}\right\} \Rightarrow M_1+M_2 = -2\vec{x}\times\vec{F} \neq 0 \Rightarrow \underbrace{L'\neq 0}_{\textit{System rotates!}}$$

c_3) Energy conservation:

The energy of a particle system consists of kinetic energy (form movement) and internal energy (potential energy) from interactions between the particles. The kinetic energy (energy 'stored' in the movement) is given by

$$E_k=\sum_{i=1}^{N}\frac{|x_i'(t)|^2}{2}m_i=\sum_{i=1}^{N}\frac{|P_i|^2}{2m_i}.$$

For the potential energy, E_p, we need an

Assumption 1.4
E_p can be influenced only by internal forces!

To quentify we need the definition of 'work':

Definition 1.5. We define the **work** done per unit time on the particle i by the force F_i by

$$w_i := \vec{F}_i \cdot \vec{x}_i', \quad [w] = \text{force} \cdot \frac{\text{displacement}}{\text{time}}.$$

In our case we have

$$w_i = \underbrace{f_i \cdot x_i'}_{w_i^{=:\text{ext}}} + \underbrace{\sum_{j=1, j\neq i}^{N} f_{i,j} \cdot x_i'}_{=:w_i^{\text{int}}}.$$

E_p is controlled by internal forces only, i.e.

$$E_p'(t) = -w_{\text{int}}(t)$$

where

$$w_{\text{int}} := \sum_{i=1}^{N} w_i^{\text{int}}$$

Claim: $E_k' = w_{ext} + w_{int}$ with $w_{ext} = \sum_{j=1}^{N} w_j^{ext}$ and $w_{int} = \sum_{j=1}^{N} w_j^{int}$.
Proof. We know

$$\begin{aligned}
E_k' &= \frac{d}{dt}\left(\sum_{i=1}^{N} \frac{m_i}{2} x_i' \cdot x_i'\right) \\
&= \sum_{i=1}^{N} \underbrace{m_i x_i''}_{=F_i = f_i + \sum_{j=1, j\neq i}^{N} f_{i,j}} \cdot x_i' \\
&= \underbrace{\sum_{i=1}^{N} f_i \cdot x_i'}_{=w_{ext}} + \underbrace{\sum_{i=1}^{N} \sum_{j=1, j\neq i}^{N} f_{i,j} \cdot x_i'}_{=w_{int}}
\end{aligned}$$

∎

The claim and the assumption together give us the **conservation of total energy**: Let $E(t) = E_k + E_p$. Then

$$E' = w_{ext}. \tag{c3}$$

Form of the potential

Claim: Assume $E_p' = -w_{int}$. Then

$$E_p(t) = -\frac{1}{2}\sum_{j=1, j\neq i}^{N} G_{i,j}(|x_i - x_j|),$$

where if

$$\vec{f}_{i,j} = \frac{x_i \vec{-} x_j}{|x_i - x_j|} g_{i,j}(|x_i - x_j|)$$

then $G(\tau)$ is a primitive(?) of $g(\tau)$ (with $g_{i,j} = g_{j,i}$).
PROOF.

$$\begin{aligned}
E_p' &= -w_{int} \\
&= -\sum_{i=1}^{N}(\sum_{j=1, j\neq i}^{N} x_i' \cdot f_{i,j}) \\
&= -\frac{1}{2}\sum_{i\neq j}(\vec{x}_i' \cdot \vec{f}_{i,j} + \vec{x}_j' \cdot \vec{f}_{j,i}) \\
&= -\frac{1}{2}\sum_{i\neq j}\vec{f}_{i,j} \cdot (x_i' - x_j') \\
&= -\frac{1}{2}\sum_{i\neq j}\frac{(x_i \vec{-} x_j)}{|x_i - x_j|} \cdot (\vec{x}_i - \vec{x}_j)' \cdot \underbrace{g_{i,j}(|x_i - x_j|)}_{=G_{i,j}'(|x_i - x_j|)} \\
&= -\frac{1}{2}\sum_{i\neq j}\frac{d}{dt}G_{i,j}(|x_i(t) - x_j(t)|)
\end{aligned}$$

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1.3 Continuum Mechanics

From particle to continuum mechanics

Let $N >> 1$ and let $C_h(x)$ denote a cube of side length h centered at $x \in \mathbb{R}^d$. Then we have a fraction of particles inside $c_h(x)$. Moreover there is a fraction of mass inside $c_h(x)$ at time t given by

$$f_h(x,t) = \frac{1}{|c_h|}\sum_{i, x_i(t)\in c_h} m_i$$

where m_i is the corresponding mass / volume of particle i. Analogeously inside of c_h one has a fraction of p, that is

$$\vec{p}_h(x,t) = \frac{1}{|c_h|\sum_{i, x_i\in c_h}\vec{p}_i}$$

where $\vec{p}_i$ is the momentum / volume of particle i. One wants appropriate limits:

$$\begin{aligned} f_h(x,t) &\to f(x,t) \text{ mass density} && \text{for } h \to 0 \\ \vec{h}(x,t) &\to \vec{p}(x,t) \text{ momentum density} && \text{for } N \to \infty. \end{aligned}$$

The above constructions yield a velocity function

$$v_h := \frac{p_n}{f_n}\left(= \vec{v}_i - \frac{\vec{p}_i}{m_i}\right).$$

Dictionary

N particles $\Leftrightarrow$ Continuum

Initial position $\vec{x}_i(0) = \vec{x}_i \in \mathbb{R}^d \Leftrightarrow$ a piece of continuus material $\Omega \subset \mathbb{R}^d$

Notion $\vec{x}_i(t,x) \Leftrightarrow x : \mathbb{R} \times \Omega \to \mathbb{R}^d$ with $(t,x) \mapsto x(t,x)$

1.3.1 Definitions

Possible configurations for N particles: $(\vec{x}_1, \vec{x}_N) \in (\mathbb{R}^d)^N$ s.t. $\vec{x}_i \neq \vec{x}_j$ for $i \neq j$ (particles do not overlap).

For a continuous material, all possible deformations are either stationary, rotations, translations, ...

Definition 1.6 (Deformation). Let $\Omega \subset \mathbb{R}^d$ be a **domain** (i.e. open and connected), let $k \geq 1$. A **$\mathbf{C^k}$-deformation** (simply a **deformation**) is a map $\varphi : \Omega \to \mathbb{R}^d$ s.t.

i) $\varphi \in C^k(\Omega, \mathbb{R}^d)$

ii) φ has a continuous extension to $\overline{\Omega}$ and this extension is invertible (as a function of $\varphi(\overline{\Omega})$)

iii) φ preserves the orientation, i.e. $\det D\varphi(x) > 0$, $\forall x \in \Omega$

where $D\varphi(x) \in \mathbb{R}^{d \times d}$ is defined as

$$(D\varphi)_{i,j} = \frac{\partial \varphi_i}{\partial x_j}.$$

In this context, Ω is called the **reference configuration**.

ii) means that $x \neq y \Rightarrow \varphi(x) \neq \varphi(y)$ (so $\vec{c}_i \neq \vec{x}_j, \forall i \neq j$)

iii) means that φ is invertible $\Rightarrow \det D\varphi(x) \neq 0, \forall x \Rightarrow$ the determinant doesn't switch the sign so it's either always > 0 or < 0. If $\varphi(x) = x$ then

$$\det D\varphi = \det I = 1 > 0$$

and this excludes flipping. For $d = 2$ e.g. one has $\varphi(x_1, x_2) = (x_2, x_1)$ for $\varphi : \mathbb{R}^2 \to \mathbb{R}^2$. For this transformation we have

$$D\varphi = \begin{bmatrix} 0 & 1 \\ 1 & 0 \end{bmatrix} \Rightarrow \det D\varphi = -1 < 0.$$

We see that in $d = 2$ this is excluded. However, in $d = 3$ this is possible: It's a rotation along $x_1 = x_2$

A **special class of deformations** are translations and rotations.

Definition 1.7. A deformation $\varphi : \Omega \to \mathbb{R}^d$ is called **rigid** deformation, if

$$D\varphi(x) \in SO(d), \quad \forall x \in \Omega$$

Remark 1.8. Recall that

$$SO(d) := \left\{ A \in \mathbb{R}^{d\times d} : \; A^T A = I \wedge \det A = 1 \right\}$$

is the special orthogonal group.

Informally, rigid deformations locally look like a rotation + translation

Example.
Let $\varphi : \mathbb{R}^d \to \mathbb{R}^d$ be an affine map, i.e.

$$\exists A \in \mathbb{R}^{d\times d}, \, b \in \mathbb{R}^d$$

s.t.

$$\varphi(x) = A(x) + b, \quad \forall x.$$

φ is invertible iff A is invertible, i.e. $\det A \neq 0$*. φ is a deformation, iff* $\det A > 0$*!*

Is φ a rigid deformation?

This is true iff $D\varphi = A \in SO(d)$ and we know that a deformation is a rigid deformation, if it locally looks like $Ax + b$.

Surprise: *$\varphi \in SO(d) \Rightarrow$ motion is a rigid affine deformation!*

Theorem 1.9 (Liouville)
Let $\Omega \subset \mathbb{R}^d$ a domain and $\varphi : \Omega \to \mathbb{R}^d$ a deformation. The following are equivalent

i) *φ is a rigid deformation*

ii) *φ is a rigid affine deformation, i.e. $\exists b \in \mathbb{R}^d$ and $A \in \mathbb{R}^{d\times d}$ s.t. $\varphi(x) = Ax + b$, $\forall x \in \Omega$*

iii) *$\forall x, y \in \Omega$ it holds that φ is an isometry, i.e.*

$$\underbrace{|\varphi(x) - \varphi(y)|}_{\text{euclidean norm}} = |y - x|$$

iv) *(local version of ii)) φ is a local rigid deformation, i.e. $\forall x \in \Omega$ we can find $\kappa_x > 0, A_x \in SO(d), b_x \in \mathbb{R}^d$ s.t.*

$$\varphi(y) = A_x y + b_x, \quad \forall y \in B(x, \kappa)$$

v) *(local version if iii)) $\forall x \in \Omega \exists \kappa > 0 : |y - z| = |\varphi(y) - \varphi(z)|$, $\forall y, z \in B(x, \kappa)$*

Theorem 1.10
Let $\Omega \subset \mathbb{R}^d$ domain and φ a deformation. Then for all measurable sets $U \subseteq \Omega$ and for all integrable functions $g \in L^1(\varphi(U))$ we have

$$\int_{\varphi(U)} g(x)\, dx^d = \int_U g(\varphi(x)) \det D\varphi(x)\, dx^d$$

Proof. Change of coordinates. ■

1.3.2 Motion

Definition 1.11. Let $\Omega \subset \mathbb{R}^d$ a domain. A C^3-map $\chi : \mathbb{R} \times \Omega \to \mathbb{R}^d$ is a **motion**, if for each time $t \in \mathbb{R}$ the map $\chi_t : \Omega \to \mathbb{R}^d, \cdot \mapsto \chi(t, \cdot)$ is a deformation.

In general we study $f(t, \chi(t, x))$ (e.g. mass distribution, force,...), where t is the time and $\chi(t, x)$ is the position of the 'particle' x at time t. We can either use (t, x) independent variables (Lagrangian or material coordinates), or we use (t, u) as independent variables (Eulerian or spatial coordinates). The Lagrangian coordinates are better for use with particles and the Eulerian are more convenient when working with fluids ('moving coordinates', snapshot of the fluid at time t).

Definition 1.12. Let $x : \mathbb{R} \times \Omega \to \mathbb{R}^d$ be a motion.

1. $\Omega_t = \chi_t(\Omega) = \{(t, \chi(t,x) | \, x \in \Omega\}$ is the **region occupied by the body at time** t
2. $\mathcal{T} = \{(t,x) : \, t \in \mathbb{R}, x \in \Omega_t\}$ is the **trajectory in space-time of the body**
3. $\chi_t^{-1} : \Omega_t \to \Omega$ with $x \mapsto \chi_t^{-1}(x) = X$ s.t. $\chi(t,X) = x$ is the **reference map at time** t
4. $\chi^{-1} : \mathcal{T} \to \mathbb{R} \times \Omega$, $(t,x) \mapsto (t, \chi_t^{-1}(x))$ is the **reference map**

Definition 1.13 (Material and spatial fields). Let $\chi : \mathbb{R}\times\Omega \to \mathbb{R}^d$ be a motion.

1. A map $\Phi : \mathbb{R} \times \Omega \to \mathbb{R}^m$, $(t,x) \mapsto \Phi(t,x)$ with $m \geq 1$ is called a **material field**
2. A map $\varphi : \mathcal{T} \to \mathbb{R}^m$, $(t,\chi) \mapsto \varphi(t,\chi)$ is called a **spatial field**

Remark 1.14. In general, capital letters will be used for material fields and small letters for spatial fields.

Definition 1.15. We can relate material and spatial fields as follows:

1. Let $\varphi : \mathcal{T} \to \mathbb{R}^m$ a spatial field. The map $\varphi_m : \mathbb{R} \times \Omega \to \mathbb{R}^m$ defined by

$$\varphi_m(t,x) = \varphi(t, \chi(t,x)).$$

   is called the **material description of** φ

2. Let $\Phi : \mathbb{R} \times \Omega \to \mathbb{R}^m$ a material field. The map $\Phi_s : \mathcal{T} \to \mathbb{R}^m$ defined by

$$\Phi_s(t,\chi) = \Phi(t, \chi_t^{-1}(x))$$

   is called the **spatial description of** Φ

Example.
Let $\chi : \mathbb{R} \times \Omega \to \mathbb{R}^d$ a motion. This is a material field. The reference map $\chi^{-1} : \mathcal{T} \to \mathbb{R} \times \Omega$ is a spatial field.

The deformation gradient $(\frac{\partial \chi_i(t,x)}{\partial x_j})_{j=1}^d$ is a material field. Also the velocity $v(t,x) = \frac{\partial x}{\partial t}(t,x)$ is a material field.

***Define** the velocity in spatial coordinates: $\nu = V_s$, i.e.*

$$\nu(t,\chi) = V(t, X(t,\chi)) = V(t, \chi\hat{\ }{-1}_t(x)).$$

One usually computes first the time derivative in material coordinates!

Trajectory and streamlines

The trajectory is reconstructed from $\nu(t,x)$ for all t and the streamlines are reconstructed from $\nu(t_0,x)$ for some fixed t_0.

Lemma 1.16
Let $\nu(t,x)$ be a given spatial field $\nu:\mathcal{T}\to\mathbb{R}^d$. Let $x\in\Omega$ be a fixed point. Thenn the motion starting at x compatible with ν,

$$\chi_x: \quad \begin{aligned} &\mathbb{R}\to\mathcal{T}\\ &t\mapsto\chi(t,x)\end{aligned}$$

is a solution $y(t)$ of the (nonlinear) ODE

$$\vec{y}'(t)=\vec{\nu}(t,\vec{y}(t))$$

Proof.

$$\begin{aligned} y'(t)&=\partial_t\chi(t,x)\\ &=v(t,x)\\ &=\nu_m(t,x)\\ &=\nu(t,\underbrace{\chi(t,x)}_{=y(t)})\\ &=\nu(t,y(t)). \end{aligned}$$

Definition 1.17. Let ν be a given spatial field.

1. We call a **trajectory** a solution of the ODE
$$y'=\nu(t,y(t)).$$
We have different solutions $\forall x$
2. We call a **streamline** a solution of
$$z'(s)=\nu(t,z(s))$$

Example.
Let $d=2$, $\nu(t,\chi)=(\cos t,\sin t)$ (independent of spatial coordinate). The trajectory is given by
$$y(t)=(\alpha+\sin t,\beta-\cos t)$$
and a streamline is
$$z(s)=(\alpha+(\cos t)s,\beta+(\sin t)s).$$

Remark 1.18. If ν is time independent, then the streamlines coincide with the trajectory in the above example.