University of Groningen

# Dynamics of Engineering Systems: Course Reader

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*June 9, 2021*

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# Analogy of equivalent systems

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| Translational mechanical | $m\ddot{x} + c\dot{x} + kx = F$ |
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| Series RLC circuits | $L\ddot{q} + R\dot{q} + \dfrac{q}{c} = e$ |
| Parallel RLC circuits | $C\ddot{g} + G\dot{g} + \dfrac{g}{L} = \dot{z}$ |

# 1 Introduction

In front of you is the reader for the course Dynamics of Engineering Systems. The main aim of this course is to integrate the knowledge gained from preceding courses on mathematics, modelings and programming. In particular, this reader serves as reference work, next to the lectures and practicals.

The current version of the reader covers four main domains of dynamical systems treated in the course:

- Structural dynamics, such as harmonic oscillators, pendulum systems and electromechanical circuits;
- Fluid dynamics, such as hydraulics, ideal and real gas flows;
- Heat transfer and reaction kinetics, such as diffusion, viscoelasticity, and chemical reactions;
- Network dynamics, such as those relating to power networks or logistics systems.

In general, each chapter or main section of the reader first covers the theoretical background of the corresponding domain. Second, a step-by-step derivation of the appropriate mathematical model is provided. For most problems, the discretized numerical implementation in MATLAB is given in terms of pseudocode; a general description of the code, in simplified programming language. Note that a general introduction to discretization is provided in Appendix Appendix A.

Note that this course serves as the finalization of the mathematics learning path in the first year of the IEM bachelor programme and, as such, follows the two courses on Calculus for IEM (I and II) and Linear Algebra, while the course content thematically complements that of the courses on Programming, Modeling and Simulation and System Dynamics. Students are assumed to have prior knowledge from these preceding courses, especially on ordinary and partial differential equations, linear algebra and basic modeling and programming skills.

# 2 Modeling and Analysis of Structural Systems

The first main chapter of this reader is on the modeling and analysis of structural systems. In this chapter, you will learn how to derive mathematical models for common types of structural systems, and how to obtain the solution to the corresponding equations using numerical methods.

## 2.1 Single harmonic oscillators

In this chapter, we focus on the class of systems called harmonic oscillators. First, we will focus on a simple mass-spring system, which is then extended to the general mass-spring-damper. We show how to rewrite the corresponding 2nd order equations of motion into 1st order equations, which can be solved using conventional solver functions. We then demonstrate how the derived model can be extended to mass-spring-damper systems with multiple masses. Finally, we also touch briefly upon electromechanical systems and their similarity to other harmonic oscillators.

### 2.1.1 Simple mass-spring-damper systems

A general mass-spring-damper system is visualized as in Figure 2.1. For simplicity, any friction or gravitational force is often (and also in this chapter) neglected. We start the derivation of the mathematical model by neglecting the damper, and only considering the mass-spring system, which is not driven by any external force.

Starting from Newton's 2nd law of motion, we have

$$F = ma, \tag{2.1}$$

With $F$ the force exerted in N, $m$ the mass of the object in kg, and $a$ the acceleration in m/s$^2$. Given a simple harmonic oscillator with 1-dimensional position $z$, this yields the following expression:

$$F = ma = m\frac{d^2z}{dt^2} = m\ddot{z}. \tag{2.2}$$

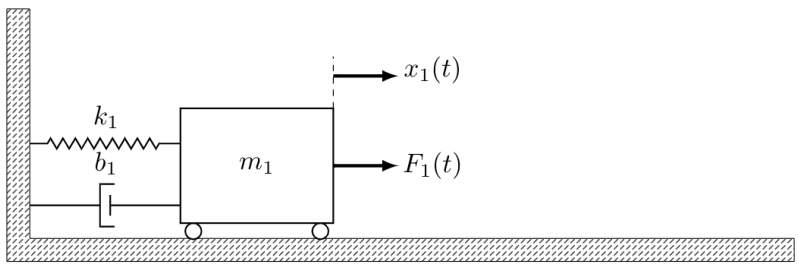



Figure 2.1: Mass-spring-damper system

On the other hand, the force exerted is exclusively described by the spring dynamics:

$$F = -kz, \tag{2.3}$$

where $k$ is the spring coefficient in $\mathrm{N\,m^{-1}}$. Combining Equation 2.2 and 2.3 yields:

$$m\ddot{z} + kz = 0. \tag{2.4}$$

The equality in Equation 2.4 is regarded as the equations of motion of the simply harmonic oscillator. Its general solution is described by

$$\begin{aligned} z(t) &= A\cos(\omega t + \phi), \\ \omega &= \sqrt{\frac{k}{m}}, \end{aligned} \tag{2.5}$$

which oscillates with period $T = \frac{2\pi}{\omega}$.

### 2.1.2 Damped harmonic oscillator

We now extend the model of the simple harmonic oscillator, by introducing a damper, which damps the oscillation over time. Because both the spring and the damper exert a force on the mass, we have to include both in the expression for the force:

$$F = F_{spring} + F_{damper} = -kz - c\frac{dz}{dt}, \tag{2.6}$$

where $c$ is the damping coefficient in $\mathrm{N\,s\,m^{-1}}$. Combining Equation 2.6 and 2.2 gives us the equations of motion for the damped harmonic oscillator:

$$m\ddot{z} + c\dot{z} + kz = \ddot{z} + J\dot{z} + \omega_0^2 z = 0, \tag{2.7}$$

where $J = \frac{c}{2\sqrt{mk}}$ and $\omega_0 = \sqrt{\frac{k}{m}}$. If the damping factor $J = 1$, the system is called *critically damped*, resulting in the quickest approach to zero (position and speed), without any overshoot. The system is *overdamped* if $J > 1$, resulting in a slower approach to zero, and the system is *underdamped* if $J < 1$, resulting in a oscillation which is slowly damped over time, but will initially always overshoot the equilibrium.

### 2.1.3 Driven, damped harmonic oscillator

A damped harmonic oscillator with damping coefficient $c > 0$ will always approach its equilibrium state over time, which is $z = 0$, $\dot{z} = 0$. However, if we add an external force, $F_{ext}$, the situation changes. The general equations of motion for a driven, damped harmonic oscillator are described by

$$m\ddot{z} + c\dot{z} + kz = F_{ext}(t). \tag{2.8}$$

The general solution of the system for an external force $F_{ext}(t) = m\omega_0^2$ for $t \geq 0$ is

$$\begin{aligned} z(t) &= 1 - \exp\Big\{ - J\omega_0 t \Big[\frac{\sin(\sqrt{1-J^2}\omega_0 t + \phi)}{\sin\phi}\Big]\Big\}, \text{ where} \\ \phi &= \cos^{-1} J \end{aligned} \tag{2.9}$$

As a second example, consider the sinusoidal external force $F_{ext}(t) = F_0 \sin(\omega t)$. Then, the steady-state solution is given by

$$\begin{aligned} z(t) &= \frac{F_0}{m z_m \omega} \sin(\omega t + \phi), \text{ where} \\ z_m &= \sqrt{(2\omega_0 J)^2 + \frac{1}{\omega^2}(\omega_0^2 - \omega^2)^2}, \text{ and} \\ \phi &= \tan^{-1}\big(\frac{2\omega\omega_0 J}{\omega^2 - \omega_0^2}\big) + n\pi \end{aligned} \tag{2.10}$$

Although the general solution to the system with sinusoidal external force consists of another term, called the *transient solution*, this term dies out fast enough to be ignored, leaving only the steady-state solution.

### 2.1.4 Numerical solution

In order to solve the equations of motion of the harmonic oscillator with a numerical solver, we need to rewrite the 2nd order ODE Equation 2.8 into a system of 1st order ODE's. To this end, we define the following two state variables:

$$\begin{aligned} z_1 &= z(t), \\ z_2 &= \dot{z}_1 = \dot{z}(t). \end{aligned} \tag{2.11}$$

Note that this gives $\dot{z}_2 = \ddot{z}(t)$. Rewriting the 2nd order ODE using the new state variables yields the following system of two 1st order ODE's:

$$\begin{bmatrix} \dot{z}_1 \\ \dot{z}_2 \end{bmatrix} = \begin{bmatrix} 0 & 1 \\ -\frac{k}{m} & -\frac{c}{m} \end{bmatrix} \begin{bmatrix} z_1 \\ z_2 \end{bmatrix} + \begin{bmatrix} 0 \\ \frac{F_{\text{ext}}(t)}{m} \end{bmatrix}. \tag{2.12}$$

### 2.1.5 Pseudocode

The pseudocode for solving the standard mass-spring-damper system is provided in Pseudocode 1. First, the workspace is cleared in step 1, and constants are defined in step 2. Then, the function handle is defined in step 3 (note that this is in fact Equation 2.12 in vector form), which is used as input for the solver in step 4. Although this specific example utilizes the built-in *ode45* solver, other ODE solvers can generally be used as well. Finally, the solution is plotted against time in step 5.

**Pseudocode 1:** Mass-spring-damper implementation

```
Clear all; clc;
Define constants:    m, k, c, and F_ext
f = @(t, z)[z(2);    -k/m * z(1) - c/m * z(2) + F_ext/m];
[t, s] = ode45(f, [t_start, t_end], [z_1(0), z_2(0)]);
plot(t,z);
```

## 2.2 Pendulum systems

### 2.2.1 Simple pendulum systems

In this chapter, we derive the equations of motion for the pendulum (Figure 2.2, and show how the equations can be solved using a numerical solver.

Starting from Newton's 2nd law for rotation, we have

$$\tau = I\alpha, \tag{2.13}$$

where $\tau$ is the torque in N m, $I$ the moment of inertia kg m m and $\alpha$ the angular acceleration in rad/s$^2$. From Figure 2.2, we observe that the gravitational force exerted on the mass is characterized by $F_g = mg$, with $g = 9.81\,\mathrm{m/s^2}$ the gravitational force. The vertical gravitational force is translated to the portion perpendicular to the pendulum rotation by

$$F = F_g \sin\theta. \tag{2.14}$$

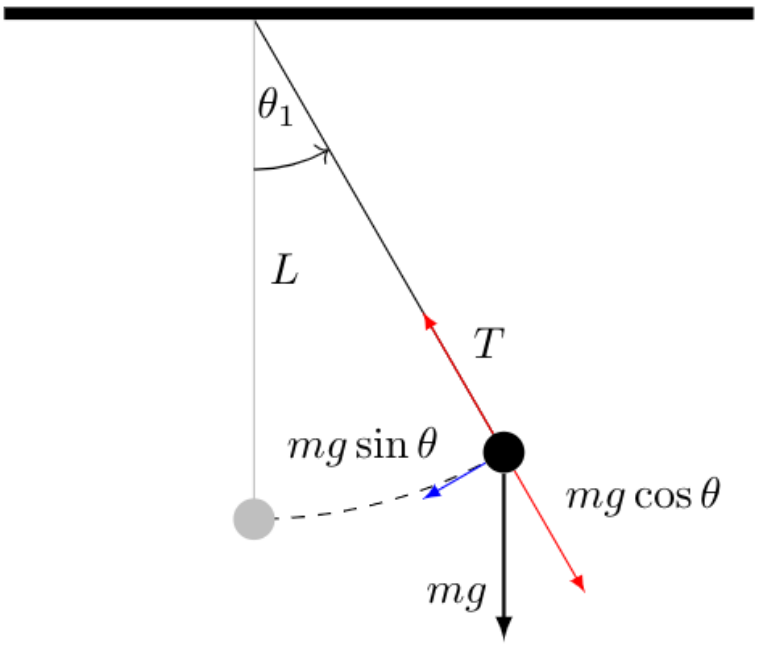



Figure 2.2: Simple pendulum

Rotational torque is defined as the force times the radius, yielding $\tau = -mgL\sin\theta$. Furthermore, the inertia of the mass is given by $I = mL^2$, and the angular acceleration $\alpha = \ddot{\theta}$, yielding the following equation of motion:

$$\ddot{\theta} + \frac{g}{L}\sin\theta = 0. \tag{2.15}$$

Although Equation 2.35 is similar to Equation 2.4, it contains a nonlinear sinusoidal term. To linearize this term, we make use of the so-called *small angle approximation*, which states that for angle $\theta$ small enough, we can estimate the sinusoidal term by

$$\sin\theta \approx \theta. \tag{2.16}$$

Using this approximation gives the linearized equation of motion:

$$\ddot{\theta} + \frac{g}{L}\theta = 0. \tag{2.17}$$

The general solution to Equation 2.17 is given by

$$\begin{aligned} \theta(t) &= A\cos(\omega t + \phi), \text{ where} \\ \omega &= \sqrt{\frac{g}{L}}, \end{aligned} \tag{2.18}$$

where $\omega$ is the natural frequency of the system (note again the equivalence between the pendulum and mass-spring-damper system).

### 2.2.2 Driven pendulum with damping

We extend upon the simple pendulum by adding a driving force and a damping term. To this end, we **do not** apply the *small angle approximation*, thus leaving us with the nonlinear equation of motion for the pendulum. Similar to the mass-spring-damper systems, the damping force is proportional to the angular velocity, $\dot{\theta}$, and the driving force is embedded as follows:

$$\ddot{\theta} + \alpha\dot{\theta} + \frac{g}{L}\sin\theta = \frac{M_{\text{ext}}}{mL^2}, \tag{2.19}$$

where $\alpha$ is the damping coefficient in $\mathrm{N\,rad\,s^{-1}}$. Note that the forcing term is different then for harmonic oscillators, because we now consider angular force.

**Dimensional analysis**

In order to gain understanding of the equation of motion, we take a step back, and perform a dimensional (unit) analysis to determine in what some of the analysis are written. We start by determining the unit of the forcing term::

$$\left[\frac{M_{\text{ext}}}{mL^2}\right] = \frac{\cancel{\text{N}}\,\cancel{\text{m}}}{\cancel{\text{kg}}\,\cancel{\text{m}^2}} \cdot \frac{\cancel{\text{kg}}\,\frac{\cancel{\text{m}}}{\cancel{\text{s}^2}}}{\cancel{\text{N}}} = \frac{1}{\text{s}^2} = \frac{\text{rad}}{\text{s}^2}, \tag{2.20}$$

which reveals that the forcing term is in radian per second squared! Next, we do the same for the units of the damping term, $\alpha$:

$$[\alpha\dot{\theta}] = [\ddot{\theta}] = [g/L][\sin\theta] = \left[\frac{M_{\text{ext}}}{mL^2}\right] = \frac{\text{radian}}{\text{s}^2}. \tag{2.21}$$

As we know that $[\dot{\theta}] = \frac{\text{rad}}{\text{s}}$ we conclude that the unit of the damping term is $[\alpha] = \frac{1}{\text{s}}$.

Next, what are the units of the $T$? We know that $[T\dot{\theta}] = [M_{\text{ext}}] = N \cdot m$, so that implies that

$$[T] = \frac{\text{N m}}{\dot{\theta}} = \frac{\text{N m}}{\text{rad s}^{-1}} = \frac{\text{N m s}}{\text{rad}} = \text{N m s}. \tag{2.22}$$

But, as we know that $\text{N} = \frac{\text{kg m}}{\text{s}^2}$, this means the units are further simplified to $[T] = \frac{\text{kgm}^2}{\text{second}}$

Finally, we put all units together, and check if the complete equation is consistent:

$$\begin{aligned} \alpha = \frac{T}{mL^2} \quad &\Rightarrow \quad \frac{[T]}{[m][L^2]} \\ &\Rightarrow \quad \frac{1}{\text{s}} = \frac{\cancel{\text{kg}}\,\frac{\cancel{\text{m}^2}}{\text{s}}}{\cancel{\text{kg}}\,\cancel{\text{m}^2}} = \frac{1}{\text{s}}, \end{aligned} \tag{2.23}$$

which is obviously correct!

### 2.2.3 Numerical solution

In order to solve the equations of motion for the pendulum numerically, we rewrite the 2nd order ODE as a system of 1st order ODEs. To this end, define

$$\begin{aligned} x_1 &= \theta(t), \\ x_2 &= \dot{x}_1 = \dot{\theta}(t). \end{aligned} \tag{2.24}$$

Note that this gives $\dot{x}_2 = \ddot{\theta}(t)$. Rewriting the 2nd order ODE using the new state variables yields the following system of two 1st order ODE's:

$$\begin{bmatrix} \dot{x}_1 \\ \dot{x}_2 \end{bmatrix} = \begin{bmatrix} 0 & 1 \\ -\frac{g}{L} & -\alpha \end{bmatrix} \begin{bmatrix} x_1 \\ x_2 \end{bmatrix} + \begin{bmatrix} 0 \\ F_{ext}(t) \end{bmatrix}. \tag{2.25}$$

### 2.2.4 Pseudocode

The system of first order differential equations can be solved in MATLAB by applying a suitable ODE solver, such as the ODE45 function. The pseudocode for solving the (driven) pendulum is provided in Pseudocode 2. First, the workspace is cleared in step 1, and constants are defined in step 2. Then, the function handle is defined in step 3 (note that this is in fact Equation 2.36 in vector form), which is used as input for the solver in step 4. Although this specific example utilizes the built-in *ode45* solver, other ODE solvers can generally be used as well. Finally, the solution is plotted against time in step 5. If desired, animation of the solution can be included as well.

### 2.2.5 Double (articulated) pendulum

The double (or articulated) pendulum is an extension of the simple pendulum discussed in the previous sections, and is shown in Figure 2.3. Although derivation of the equations of motion for the double pendulum is similar as for the simple pendulum, its behavior can be very different. The motion of the double pendulum is categorized as *chaotic*, as its trajectory depends extremely closely to its precise initial conditions.

Exact derivation of the equations of motion for the double pendulum is nicely done on the following Wolfram webpage: `http://scienceworld.wolfram.com/physics/DoublePendulum.html` (Weisstein, 2007). The resulting equation of motions are given by:

**Pseudocode 2:** Simple (driven) pendulum implementation

1: Clear all; clc;
2: Define constants: $g$, $L$, $\alpha$, $F_{\text{ext}}$ and $t_{\text{end}}$
3: $f = @(t, th)\big[th(2); (-g/L) * th(1) - \alpha * th(2) + F_{\text{ext}}\big]$
4: $[t,\ s] = \text{ode45}(f,\ [t_{start},\ t_{end}],\ \ [t(0),\ th(0)])$;
5: plot($t$,$z$);

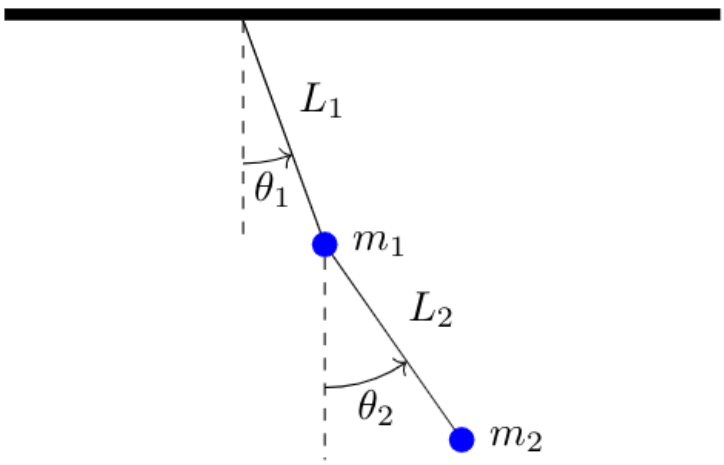



Figure 2.3: Double pendulum

$$
\begin{aligned}
(m_1 + m_2)l_1\ddot{\theta}_1 + m_2 l_2 \ddot{\theta}_2 \cos(\theta_1 - \theta_2) + m_2 l_2 \dot{\theta}_2^2 \sin(\theta_1 - \theta_2) + g(m_1 + m_2)\sin\theta_1 = 0 \\
m_2 l_2 \ddot{\theta}_2 + m_2 l_1 \ddot{\theta}_1 \cos(\theta_1 - \theta_2) - m_2 l_1 \dot{\theta}_1^2 \sin(\theta_1 - \theta_2) + m_2 g \sin\theta_2 = 0
\end{aligned}
\tag{2.26}
$$

If you look carefully into the derivation of Equation 2.26, you'll notice that the derivation is very similar compared to the simple pendulum. However, it also shows that the complexity of the system increases exponentially by doubling the amount of elements.

The exact derivation of the corresponding state-space system is nicely described in following reference: https://ir.canterbury.ac.nz/bitstream/handle/10092/12659/chen_2008_report.pdf (Chen, 2008).

Due to its chaotic behavior, solving the motion of the double pendulum can require a more sophisticated algorithm, or at least a smaller time-step, than for solving the simple pendulum. As any small integration or numerical error of the solver results in significantly larger deviations in output (the *butterfly effect*), solving the dynamics for the double pendulum is prone to errors. This is nicely visualized in the following YouTube movie by *Think Twice*: https://www.youtube.com/watch?v=d0Z8wLLPNE0 (Think Twice, 2017)

## 2.3 Hybrid systems

In this section, we will focus on the class of switching systems. We do this by introducing two examples. First, the model for dynamical contact of a bouncing ball is derived. This system can be in two states: the ball is either falling, or it is in contact with the ground. In this chapter, we will show how to deal with this switching between two states. Second, we will derive a similar model for a pendulum which is bouncing against a wall.

### 2.3.1 Dynamical contact for a bouncing ball

Consider the system of a bouncing ball, which is subject to the gravitational force, $g$. The ball is either falling, or it is in contact with the ground (i.e. the event of 'bouncing'). In order to capture such dynamics of the bouncing ball, we need to introduce a so-called *switching system*. Based on an IF-statement, we can determine if it is appropriate to activate the system in falling state, or to activate the system in contact with the ground.

In this section, we focus on the contact of the ball with the ground. In fact, the dynamical contact of the ball with the ground can be modeled similar to the mass-spring-damper in Equation 2.7. However in this case, the spring and damping coefficients are not constant. Instead, they are a function of the deformation of the ball, $w$.

The force applied to the ball is related to the deformation $w$ between the ball and the ground, and is defined by the Hertzian contact force, which is calculated as

$$
P(w) = \frac{4}{3} E^* R^{0.5} w^{1.5}, \tag{2.27}
$$

where $P(w)$ is the force in N as a function of the deformation ($w$), $E^*$ is the reduced elastic modulus in Pa (which is determined by the materials of the ball and ground), $R$ the radius of the ball in m, and $w$ the deformation of the ball.

The deformation of the ball should be calculated such that it only has a value in the case of contact, and is zero otherwise. This can be achieved by taking the difference between the radius $R$ and vertical position $z$, constrained by zero (as negative deformation does not make sense):

$$w = \max(0, R - z). \tag{2.28}$$

The calculated contact force is then substituted in the equations of motion, similar as for the mass-spring-damper systems, implying that the acceleration of the ball ($\ddot{z}$) is related to the force via the following expression:

$$\ddot{z} = \frac{P(w)}{m}. \tag{2.29}$$

As the value of $P$ is a function of the deformation $w$, which changes over time, the corresponding system is called a *time-variant system.*

### 2.3.2 Bouncing pendulum

We can now extend the model of the simple pendulum, and combine it with that of the bouncing ball, to derive a mathematical model for the bouncing pendulum. As for the bouncing ball, this requires the implementation of a switching system, which allows to make the system matrix time-variant.

Contact of the bouncing pendulum with the wall, occurs when the $x$-position is smaller than the radius $R$ of the ball, i.e. $x < R$. Assuming the wall to be rigid, this geometric violation results in deformation of the ball. As the model for the simple pendulum was written in terms of angular coordinates, we first translate this in $x$ (horizontal) and $z$ (vertical) coordinates:

$$x = L \sin\theta, z = L(1 - \cos theta). \tag{2.30}$$

Hence, contact is made if $x = L \in \theta < R$, and the resulting deformation of the ball is characterized by $d = |L \sin\theta - R|$.

Similar to the bouncing ball, we follow Hertzian mechanics theory to model the contact force:

$$P(w) = \frac{4}{3} E^* R^{0.5} w^{1.5}, \tag{2.31}$$

with $R$ the radius of the ball, $w$ the deformation of the ball, and $E^*$ the reduced elastic modulus, defined as

$$E^* = \left( \frac{1 - v_1^2}{E_1} + \frac{1 - v_2^2}{E_2} \right)^{-1}, \tag{2.32}$$

where $v_1$ and $v_2$ are the Poission's ratios associated with the bodies, and $E_1$ and $E_2$ the elastic moduli.

If the contact would take place between two spheres, we also need to take the effective radius into account:

$$R^* = \left(\frac{1}{R_1} + \frac{1}{R_2}\right)^{-1}, \tag{2.33}$$

where $R_1$ and $R_2$ are the radii of the two bodies. In this case, we consider sphere-on-flat contact, which means that we have $R_1 = R$ and $R_2 = \infty$, resulting in the effective radius being the same as the actual radius of the ball. So, the contact force is modelled by the following switching state:

$$P = \begin{cases} \frac{4}{3}E^* R^{0.5} w^{1.5} & \text{if } L\sin\theta < R \text{ (implying contact)}, \\ 0 & \text{otherwise.} \end{cases} \tag{2.34}$$

The next step is to combine the equation of motion (EoM) of the pendulum with the contact dynamics above. In this case, we do not apply the *small angle approximation*, yielding the non-linear equation of motion:

$$\ddot{\theta} + \alpha\dot{\theta} + \frac{g}{L}\sin\theta = \frac{M_{\text{ext}}}{mL^2} + \frac{P}{mL}, \tag{2.35}$$

as presented before, but with the contact force, $\frac{P}{mL}$ included as well. As the moment is $LP$ (and not just P), one $L$ in the denominator drops out for the contact force term. Note that the force $P$ is determined by the switching state in Equation 2.34.

Reformulating this 2nd order ODE into a system of two 1st order ODEs, and again adopting the small angle approximation yields:

$$\begin{bmatrix} \dot{x}_1 \\ \dot{x}_2 \end{bmatrix} = \begin{bmatrix} 0 & 1 \\ -\frac{g}{L} & -\alpha \end{bmatrix} \begin{bmatrix} x_1 \\ x_2 \end{bmatrix} + \begin{bmatrix} 0 \\ F_{ext}(t) + \frac{P}{mL} \end{bmatrix}, \tag{2.36}$$

where we defined state variables $x_1 = \theta$ and $x_2 = \dot{\theta}$.

In non-forced, non-contacting (bouncing) state, $M_{\text{ext}} = P = 0$, and the natural frequency of scillation is $\omega_0 = \frac{2\pi}{T_0} = \alpha = \sqrt{g/L}$.

If the case with damping, and $\alpha^2 - 4\omega_0^2 > 0 \Rightarrow \alpha > 2\omega_0$, the pendulum is overdamped. If $\alpha = 2\omega_0$, the pendulum is critically damped, and if $\alpha < 2\omega_0$, the pendulum is overdamped.

**Numerical solution**

We consider the classic Runge-Kutta 4th order method (RK4) to derive the numerical solution for the bouncing pendulum. In general, this method considers initial value problems of the form

$$\dot{y} = f(x, y), \quad y(x_0) = y_0. \tag{2.37}$$

As discussed in the Appendix on discretization, taking the Taylor series expansion gives

$$y(x+h) = y(x) + h\dot{y}(x) + \frac{h^2}{2!}\ddot{y}(x) + \cdots , \tag{2.38}$$

where $\dot{y} = f$, $\ddot{y} = \dot{f}$, etc. and $h$ is the time step. Euler's (explicit) method is one of the simplest methods derived from this Taylor series, and computes

$$y_{n+1} = y_n + hf(x_n, y_n). \tag{2.39}$$

The RK4 method finds its origin with Euler's method, but uses multiple function evaluations at each time, according to the following scheme:

$$y_n + 1 = y_n + \frac{1}{6}(k_1 + 2k_2 + 2k_3 + k_4), \quad \text{where} \tag{2.40a}$$

$$\begin{cases} k_1 = hf(x_n, y_n) \\ k_2 = hf(x_n + \frac{h}{2}, y_n + \frac{k_1}{2}) \\ k_3 = hf(x_n + \frac{h}{2}, y_n + \frac{k_2}{2}) \\ k_4 = hf(x_n + k, y_n + k_3) \end{cases} \tag{2.40b}$$

Finally, the bouncing pendulum is implemented in MATLAB using an *adaptive time step scheme*. This entails that time step $h$ is not constant, but is varied over time, depending on the error of the method for that iteration. Generally, the time step will be decreased in cases near contact, since that state is more prone to errors.

**Pseudocode**

The pseudocode for the bouncing pendulum implementation is provided below in Pseudocode 3. First, simulation (time) variables and the system parameters are defined, resulting in matrix $A$ (the internal, state-dependent system matrix). The main WHILE-loop iterates through time, and checks at each time step $t$ is contact with the wall is made. If so, the contact force is calculated; otherwise, $P = 0$. Similarly, it is checked if the external force (which is applied from $T_{\text{ext}}$ on) is apparent. The system of ODEs is then updated in lines 17-18, and solved using an appropriate method. If the resulting error in the solution exceeds the limit $\epsilon$, the step size $dt$ is reduced. At the end of each iteration, the results $\theta(t)$ and $\omega(t)$ are stored, and time proceeds according to $t = t + dt$. Finally, the results for the angle $\theta$ and angular velocity $\omega$ are plotted in time.

## 2.4 Multi degree of freedom (M-DOF) systems

In this section, we extend the model for harmonic oscillators, by adding multiple masses. Although derivation of the equations of motion is typically similar to the simple mass-spring-damper, the connection of different masses influences the respective dynamics.

Consider the system in Figure 2.4, consisting of two masses on wheels, connected via three springs to each other and two rigid walls. For simplicity, we assume that there is no friction between the wheels and the ground. The free body diagram (FBD) for cart 1 is shown in

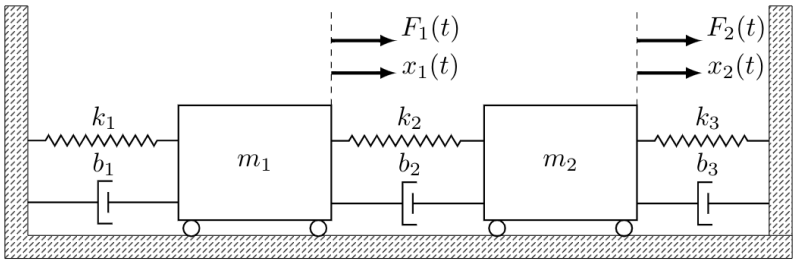



Figure 2.4: Mass-spring-damper system with two masses

Figure 2.5. Assume the first cart ($m_1$) moves $x_1$ to the right ($x_1 > 0$). This elongates the first spring ($k_1$) and compresses the second ($K_2$).

The second cart ($m_2$) moves $x_2$, but, depending on the stiffnesses of springs $k_2$ and $k_3$, $x_2$

**Pseudocode 3:** Bouncing pendulum implementation

```
Set simulation (time) variables
Set g, m, R, E*, L, α, M_ext
A = [0, 1; −g/L, −α];
while t ≤ t_end do
    w = L sin θ − R;
    if w > 0 then
        P = 0;
    else
        P = (4/3) E* R^0.5 w^1.5;
    end if
    if t > T_ext && mok= 0 then
        mok= 0;
        M = M_ext;
    else
        M = 0;
    end if
    f = [0; M/(mL^2) + P/(mL)];
    Update ODE ẋ = Ax + f
    Solve linear system (e.g. RK4, RK5)
    Calculate error (depending on method)
    if error > ϵ then
        Reduce step size dt;
    end if
    θ(t) = q(1);
    ω(t) = q(2);
    t = t + dt;
end while
plot(t,θ,ω);
```

may be positive or negative. If $x_1 > x_2$ for $x_2 > 0$, the second spring is compressed; if $x_2 < 0$, the second spring is compressed even more. Whether the third spring is compressed or tensioned will then depend on whether $x_2 > 0$ or $x_2 < 0$. Customarily, we assume positive displacements and let's also assume $x_1 > x_2$. Then, the free body diagram for cart 2 is as presented in ..

The corresponding equations of motion (EOM) are described as follows:

$$\begin{aligned} -k_1x_1 + k_2(x_2 - x_1) - b_1\dot{x_1} + b_2(\dot{x_2} - \dot{x_1}) &= m_1\ddot{x}_1, \\ k_2(x_1 - x_2) - k_3x_2 + b_2(\dot{x_1} - \dot{x_2}) - b_3\dot{x_2} &= m_2\ddot{x}_2, \end{aligned} \tag{2.41}$$

which, after rearranging yields:

$$\begin{aligned} m_1\ddot{x}_1 + (b_1 + b_2)\dot{x_1} - b_2\dot{x_2} + (k_1 + k_2)x_1 - k_2x_2 &= 0, \\ m_2\ddot{x}_2 - b_2\dot{x_2} + (b_2 + b_3)\dot{x_2} - k_2x_1 + (k_2 + k_3)x_2 &= 0. \end{aligned} \tag{2.42}$$

In matrix form, the EOM are described by

$$\begin{bmatrix} m_1 & 0 \\ 0 & m_2 \end{bmatrix} \begin{bmatrix} \ddot{x}_1 \\ \ddot{x}_2 \end{bmatrix} + \begin{bmatrix} b_1 + b_2 & -b_2 \\ -b_2 & b_2 + b_3 \end{bmatrix} \begin{bmatrix} \dot{x_1} \\ \dot{x_2} \end{bmatrix} + \begin{bmatrix} k_1 + k_2 & -k_2 \\ -k_2 & k_2 + k_3 \end{bmatrix} \begin{bmatrix} x_1 \\ x_2 \end{bmatrix} = \begin{bmatrix} 0 \\ 0 \end{bmatrix}. \tag{2.43}$$

Note that the EOM for a mass-spring system are identical to those of any linear system, i.e. $[M]\{\ddot{x}\} + [B]\{\dot{x}\} + [K]\{x\} = 0$.

## 2.5 Electromechanical systems (DC motor)

In this section, we briefly touch upon electromechanical systems, in order to highlight their resemblance to other harmonic oscillators. We consider the general DC motor electrical system (armature circuit) as shown in Figure 2.7.

From *Kirchhoff's Voltage law (KVL)*, we know that

$$\sum_{k=1}^{n} V_k = 0, \tag{2.44}$$

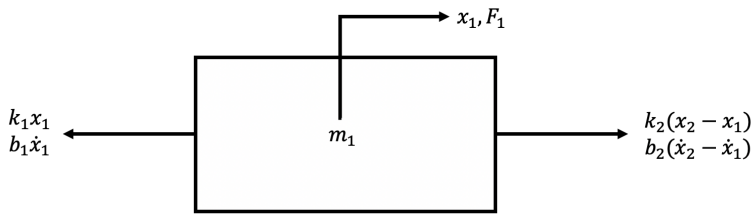



Figure 2.5: Free body diagram for cart 1 of the double MSD

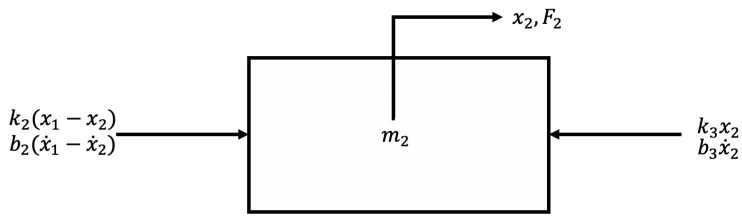



Figure 2.6: Free body diagram for cart 2 of the double MSD

where $n$ is the total number of voltages measured, i.e. the sum of voltages around a loop is equal to zero. The following sources of voltage are apparent in this circuit:

- Battery voltage, $V_B = V$ (input),
- Resistor voltage, $V_R = iR$ (Ohm's law),
- Inductor voltage, $V_L = L\frac{di}{dt}$,
- Electromotive voltage, $V_{\text{emf}} = kv\frac{d\theta}{dt}$.

Note that the electromotive voltage constant is determined by the flux density of the permanent magnet (back-emf constant). Writing Kirchhoff's Voltage law for the system yields the following balance:

$$\begin{aligned} V &= V_R + V_L + V_{\text{emf}} \\ V &= iR + L\frac{di}{dt} + k_v\frac{d\theta}{dt}, \end{aligned} \tag{2.45}$$

where term $R$ is the resistance, and $L$ is the inductance. Note that the current is the time derivative of the charge, i.e. $i = \frac{dq}{dt}$, so that the equation can also be written as $V = L\ddot{q} + R\dot{q} + k_v\dot{theta}$.

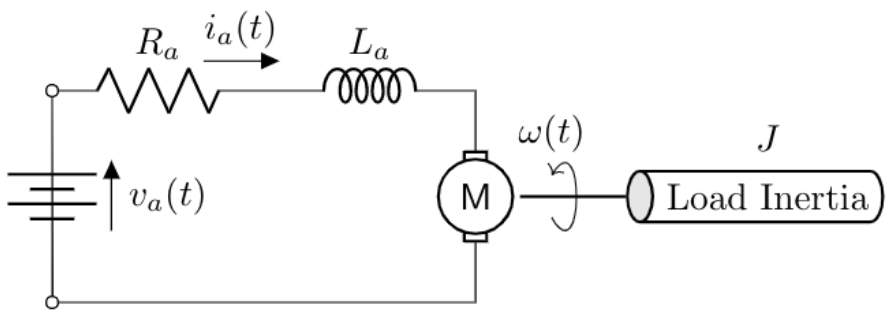



Figure 2.7: Electrical circuit of a DC motor, with resistor (R), inductor (L), and battery (v)

Then, Recall that Newton's second law for rotational systems is written as $\sum T = I\ddot{\theta}$ (Net external torque = I $\times$ angular acceleration). In the considered mechanical system, the output torque is $T = k_t i$, where $k_t$ is the torque constant, and the damping torque is $T_d = B\frac{d\theta}{dt}$, where $B$ is the damping coefficient. Note that the damping torque always opposes the motion, and is therefore reflected in the equation of motion with a negative sign:

$$k_t i - B\frac{d\theta}{dt} = I\frac{d^2\theta}{dt^2}. \tag{2.46}$$

The dynamics of the electromechanical system for the DC motor are written in matrix form as follows:

$$\frac{d}{dt}\begin{bmatrix}\dot{\theta}\\ i\end{bmatrix} = \begin{bmatrix}\frac{-B}{I} & \frac{k_t}{I}\\ \frac{-k_v}{L} & \frac{-R}{L}\end{bmatrix}\begin{bmatrix}\dot{\theta}\\ i\end{bmatrix} + \begin{bmatrix}0\\ \frac{1}{L}\end{bmatrix}V. \tag{2.47}$$

Finally, by defining the state vector $x = [\dot{\theta}\ \ i]^T$ and input $u = V$, the state-space representation of this system is written as

$$\dot{x} = Ax + Bu, \tag{2.48}$$

where

$$A = \begin{bmatrix}\frac{-B}{I} & \frac{k_t}{I}\\ \frac{-k_v}{L} & \frac{-R}{L}\end{bmatrix}, \qquad B = \begin{bmatrix}0\\ \frac{1}{L}\end{bmatrix} \tag{2.49}$$

## 2.6 The eigenvalue problem

In the absence of damping and applied loading, the previous EOM for an undamped free vibration can be assumed to have a harmonic solution of the form $\{x\} = \{V\}\sin\omega t$, where $\{V\}$ is a column vector (the eigenvector) called the *mode shapes*, and $\omega$ is the natural frequency.

Differentiating the assumed harmonic solution and plugging into the EOM yields the following:

$$-\omega^2[M]\{V\}\sin\omega t + [K]\{V\}\sin\omega t = 0. \tag{2.50}$$

After simplification, this becomes the following expression, which is called the eigenequation:

**Definition: The eigenequation for M-DOF harmonic oscillators**

$$\left([K] - \omega^2[M]\right)\{V\} = 0. \tag{2.51}$$

Note the similarity to the general eigenvalue problem, which is characterized by $[A - \zeta I]u = 0$.

The trivial solution is obtained when $\det\left[K] - \omega^2[M]\right) \neq 0$, with $\{V\} = 0$. Hence, solving $\det\left([K] - \omega^2[M]\right) = 0$ or $\det\left([K] - \zeta[M]\right) = 0$, where $\zeta = \omega^2$ in the solution of the eigenvalue problem.

In MATLAB, this can be solved by the code $[V, D] = \text{eig}(u\ K)$, where $V = [V]$ is a matrix containing the eigenvectors / mode shapes, $D = [D]$ is a diagonal marix containing the eigenvalues, and the operation $u > K$ is equivalent to $[K][M]^{-1}$.

So, for a 2-DOF system such as the one we examined, solving the eigenvalue problem will yield eigenvalues $\zeta = \omega^2$ so that $\zeta_1 = D(1,1) = \omega_1^2$ with mode shape $V(:,1)$, and $\zeta_2 = D(2,2) = \omega_2^2$ with mode shape $V(:,2)$.

**Example**

We conclude the analysis by illustrating an example. To this end, assume our system is characterized by the following parameters:

$$\begin{aligned} m_1 &= m_2 = 1\,\text{kg} \\ k_1 &= k_3 = 1\,\text{N}\,\text{m}^{-1} \\ k_2 &= 2\,\text{N}\,\text{m}^{-1}. \end{aligned} \tag{2.52}$$

Following the expressions above, this will yield (**check this yourself!**):

$$\begin{aligned} \omega_1 = 1\,\text{rad}\,\text{s}^{-1},\ \text{with}\ \{V\} &= \begin{bmatrix} --0.7071\,\text{m} \\ --0.7071\,\text{m} \end{bmatrix} \\ \omega_2 = 2.2361\,\text{rad}\,\text{s}^{-1},\ \text{with}\ \{V\} &= \begin{bmatrix} --0.7071\,\text{m} \\ -0.7071\,\text{m} \end{bmatrix} \end{aligned} \tag{2.53}$$

### 2.6.1 Physical meaning of the eigenvalue problem

According to wave theory, a mode is a standing wave state of excitation, in which all system components will be affected sinusoidally under a specified fixed frequency. The mode is characterized by a *modal frequency* and a *mode shape*.

### 2.6.2 Simplified 4-story building example (4-DOF)

In this example, we consider a so-called *shear-type building model*, and we model the walls as springs resisting the motion of each floor in the lateral direction $x$. We assume that all the mass of the building is lumped at the floor levels. Floor beams are rigid, and columns (walls) are axially rigid, i.e. they do not deform in the y-direction.

The EOM of the building model are given as follows:

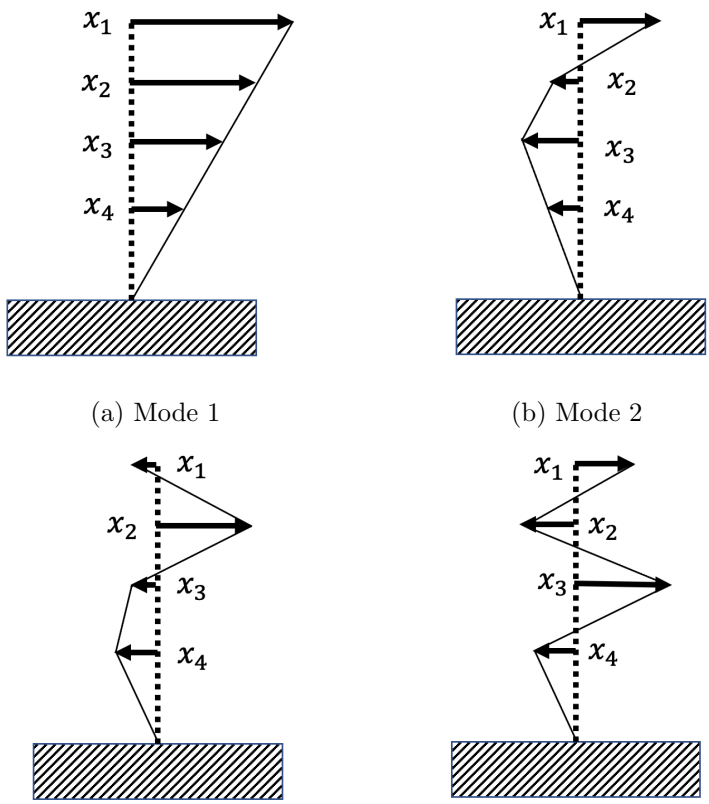
$$\begin{aligned} m_1\ddot{x}_1 &= 2k_1(x_2 - x_1) \\ m_2\ddot{x}_2 &= 2k_1(x_1 - x_2) + 2k_2(x_3 - x_2) \\ m_3\ddot{x}_3 &= 2k_2(x_2 - x_3) + 2k_3(x_4 - x_3) \\ m_4\ddot{x}_4 &= 2k_3(x_3 - x_4) - 2k_4x_4. \end{aligned} \tag{2.54}$$

In standard matrix form, $[M]\{\ddot{x}\} + [K]\{x\} = 0$, this yields

$$[M] = \begin{bmatrix} m_1 & 0 & 0 & 0 \\ 0 & m_2 & 0 & 0 \\ 0 & 0 & m_3 & 0 \\ 0 & 0 & 0 & m_4 \end{bmatrix}, \qquad [K] = \begin{bmatrix} 2k_1 & -2k_1 & 0 & 0 \\ -2k_1 & 2(k_1+k_2) & -k_2 & 0 \\ 0 & -2k_2 & 2(k_2+k_3) & -2k_3 \\ 0 & 0 & -2k_3 & 2(k_3+k_4) \end{bmatrix}. \tag{2.55}$$

**Example**

Consider the model of the 4-story building, and let $m_1 = 1500\,\mathrm{kg}$, $m_2 = 3000\,\mathrm{kg}$, $m_3 = 3000\,\mathrm{kg}$, $m_4 = 4500\,\mathrm{kg}$, and $k_1 = 400\,\mathrm{kN\,m^{-1}}$, $k_2 = 800\,\mathrm{kN\,m^{-1}}$, $k_3 = 1200\,\mathrm{kN\,m^{-1}}$, $k_4 = 1600\,\mathrm{kN\,m^{-1}}$.
You should be able to find the 4 modal shapes as presented in Figure 2.8. The corresponding natural frequencies are $\omega_1 = 10.9\,\mathrm{rad\,s^{-1}}$, $\omega_2 = 24.2\,\mathrm{rad\,s^{-1}}$, $\omega_3 = 33.6\,\mathrm{rad\,s^{-1}}$, and $\omega_4 = 45.6\,\mathrm{rad\,s^{-1}}$.




(a) Mode 1 (b) Mode 2

(c) Mode 3 (d) Mode 4

Figure 2.8: Modal shapes and natural frequencies and building example

# 3 Kuramoto Oscillators

## 3.1 Introduction

This is a (simple) mathematical model that can describe synchronization for (large) sets of coupled oscillators (aside: refer to the previous example of a Wilberforce pendulum).

### 3.1.1 Mechanical Analog

In order to study this system, a group of particles constrained to move along an unit circle, **without colliding**. Each of these has an angle $\theta$ and a frequency $\dot{\theta}$, as well as inertial and damping coefficients $M_i > 0$ and $D_i > 0$, respectively. Hence, external forces are: a viscous damping force opposing the velocity vector, equal to $D_i\dot{\theta}_i$; an external driving torque $\tau_i \in \mathbb{R}$; and an elastic restoring force $k_{ij}\sin(\theta_i - \theta_j)$ between pairs of particles (see Figure 3.1; note that $k_{ij} = k_{ji} > 0$).

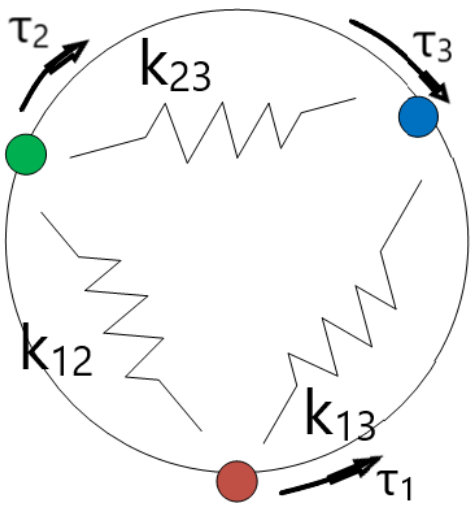



Figure 3.1: Mechanical analog

Based on this, we can write then the equation of motion as,

$$M_i\ddot{\theta}_i + D_i\dot{\theta}_i = \tau_i - \sum_{j=1}^{n} k_{ij}\sin(\theta_i - \theta_j), \text{ for } i \in [1, \ldots, n] \tag{3.1}$$

For small masses $M_i$ and uniformly-high viscous damping $D_i$, the relationship $\frac{M_i}{D_i} \approx 0$, and the EoM becomes,

$$\dot{\theta}_i = \omega_i - \sum_{j=1}^{n} a_{ij}\sin(\theta_i - \theta_j) \tag{3.2}$$

where $\omega_i = \frac{\tau_i}{D_i}$ are the natural rotational frequencies and $a_{ij} = \frac{k_{ij}}{D_i}$ are the coupling strengths. Thus, the following conclusions can be drawn,

- Weakly coupled and strongly heterogenous network (i.e., with strongly dissimilar natural frequencies) does not display any coherent behavior;
- Strongly coupled and sufficiently homogeneous network is amenable to synchronization when all frequencies $\dot{\theta}_i(t)$ become aligned.

The most popular form of the Kuramoto model is,

$$\dot{\theta}_i = \omega_i - \frac{K}{n}\sum_{j=1}^{n} \sin\left(\theta_i - \theta_j\right), \text{ for } i \in [1, \ldots, n]. \tag{3.3}$$

This model considers uniform weights $a_{ij} = \frac{K}{n}$. Kuramoto (1975) showed that the synchronization takes place if $K$ exceeds a certain threshold value $K_{critical}$, which is a function of the distribution of the rotational frequencies $\omega_i$.

### 3.1.2 Pseudocode

The theory described up to now can be easily programmed to find the behavior of such systems.

**Pseudocode 4:** Kuramoto Model

1: Set $n$, $K$, and the number of iterations;
2: Pre-allocate memory for $\theta = zeros(n, iterations)$ and $\omega =$ rand(n,1);
3: Populate the first column of $\theta$ (first iteration) with the random initial positions $\theta(:,1) = 2 \cdot \pi \cdot rand(n,1)$;
4: Run the loop over a number of iterations, use RK-4 to integrate the ODE numerically $f = \omega + \frac{K}{n}\sum_{j=1}^{n} \sin\left(\theta_j - \theta_i\right)$ for the Kuramoto function $[\theta(i,j), K, n, \omega]$.

The question is how can we perform the *sum* operation element-wise? Let's look at the function definition:

1. We pass $\theta(:,j)$ that is a column vector of size $(n,1)$;
2. $K$ and $n$ are scalar constants, while $\omega$ is also of size $(n,1)$;
3. Look into Matlab's *sum* function (Matlab SUM help); what we need is the sum of the sine of each pair of angles $\theta_i$ and $\theta_j$. This can be done by assembling a matrix $\theta(:,1) \cdot ones(1,n)$ of size $(n,n)$ and subtracting from this a matrix $ones(n,1) \cdot \theta(:,1)^T$ of equal size;
4. Therefore, if $\omega$ is a column vector, the operation can be completed to yield a $(n,1)$ vector of $\theta$ values;
5. Calculate the Cartesian positions $x = \sin\theta$ and $y = \cos\theta$ and plot the kinematics.

### 3.1.3 Examples

Several phenomena and applications can be explained using the Kuramoto coupled oscillator model:

- Biological synchronization and rhythmic phenomena;

- Physical systems (e.g. coupled metronomes (Synchronization of metronomes), chemical oscillators);
- Networks (e.g. opinion dynamics, decision making in animal groups);
- Power systems, and the list goes on...

## 3.2 Electrical Power Networks

Synchronization refers to the process of matching the speed and frequency of a generator (or other source) to a running AC power network. An AC generator cannot deliver power to the electrical grid unless it runs in the same frequency as the network.

**Definition: Synchronous speed**

In an AC network with a supply frequency $f$ $[Hz]$, the speed of rotation $[rpm]$ of the magnetic field in a generator with a number of poles $p$ is (attention, the speed of rotation of the shaft may be different!),

$$n_s = \frac{120f}{p} \tag{3.4}$$

The forces and moments acting on the system are: the electromagnetic torque ($T_e$); the electromagnetic power ($P_e = T_e\omega_m$; the mechanical torque ($T_m$); the mechanical power ($P_m = T_m\omega_m$. The terms $\omega_m$ and $\omega_s$ are the rotor and the synchronous (see **Definition**) angular velocities, respectively.

### 3.2.1 Networks with Synchronous Generators

The swing dynamics for the electromagnetic system are,

$$M_i\ddot{\theta}_i + D_i\dot{\theta}_i = P_{m,i} - \sum_{j=1}^{n} k_{ij}\sin(\theta_i - \theta_j) \tag{3.5}$$

where $P_{m,i} > 0$ is the mechanical power input. Another form of the swing equation (for synchronous machines) can be derived from the electromagnetic system (refer to earlier section on DC motors for comparison).

$$I\frac{d^2\theta_m}{dt^2} = T_a = T_m - T_e \tag{3.6}$$

where $I$ is the rotor's moment of inertia, $T_a$ is the net accelerating torque and $\theta_m$ is the angular position of the rotor with respect to the stationary axis.
Relative to a synchronously frame (with frequency $\omega_s$), the angular position is $\omega_m = \omega_s t + \delta_m$, where $\delta_m$ is the angular position with respect to the synchronously rotating frame. Taking the time derivatives of this last expression yields

$$\frac{d\omega_m}{dt} = \omega_s + \frac{d\delta_m}{dt}. \tag{3.7}$$

In other words, synchronization will only take place when $\frac{d\delta_m}{dt} = 0$. This term represents the deviation of the rotor speed from the synchronization (leading later to the concept of $slip = \frac{\omega_s - \omega_m}{\omega_s}$). If now we take the second derivative and introduce this in the EoM, we get

$$\frac{d^2\omega_m}{dt^2} = \frac{d^2\delta_m}{dt^2} \tag{3.8}$$

$$I\frac{d^2\delta_m}{dt^2} = T_a = T_m - T_e. \tag{3.9}$$

Let us define $\omega_m = \frac{d\theta_m}{dt}$ as the angular velocity of the rotor, and multiply this with both sides of the equation,

$$I\omega_m\frac{d^2\delta_m}{dt^2} = T_a\omega_m = (T_m - T_e)\omega_m. \tag{3.10}$$

The torque terms on the right-hand side of the equation represent the accelerating, mechanical and electric power, respectively. At the synchronous speed we can define the parameter $H$, the inertia constant of the machine as,

$$H = \frac{\text{Stored kinetic energy at synchronous speed}}{\text{Machine rating}}\frac{[MJ]}{[MVA]} = \frac{I\omega_s^2}{2S_{rated}}[s] \tag{3.11}$$

where $S_{rated}$ is the three-phase rating of the machine, while the relationship between the electrical and mechanical power angles is $\delta = \frac{p}{2}\delta_m$, and $\omega = \frac{p}{2}\omega_m$ is the relationship between electrical and mechanical speeds ($p$ being the number of poles).
In steady-state conditions $\omega_m = \omega_s$, such that,

$$\frac{2H}{\omega_s}\frac{d^2\delta}{dt^2} = P_a = P_m - P_e \quad [per - unit]^{1}. \tag{3.12}$$

Let us now take a look at the simplest form of the swing equation and grouping in $M$, a constant of the machine,

$$M\frac{d^2\delta}{dt^2} = P_a = P_m - P_e \longrightarrow \frac{d^2\delta}{dt^2} = \frac{P_a}{M}. \tag{3.13}$$

We can use this to determine the transient stability, i.e. whether or not synchronism is maintained after the machine has been subjected to severe disturbance (e.g. a sudden application of load, loss of generation, loss of a large load, or a fault in the system).
Adding damping to the system yields (compare it with Eq. 3.5),

$$M\frac{d^2\delta}{dt^2} + D\frac{d\delta}{dt} = P_m - P_e. \tag{3.14}$$

[1] The electrical power angle $\delta$ is the angle of the generator's internal electromagnetic field, also called the load angle.

If we have synchronous machines, their EoM's will then be,

$$M_1 \frac{d^2\delta_1}{dt^2} + D_1 \frac{d\delta_1}{dt} = P_{m,1} - P_{e,1} = P_{m,1} - a_{1,2} \sin(\delta_1 - \delta_2) \tag{3.15a}$$

$$M_2 \frac{d^2\delta_2}{dt^2} + D_2 \frac{d\delta_2}{dt} = P_{m,2} - P_{e,2} = P_{m,2} - a_{2,1} \sin(\delta_2 - \delta_1). \tag{3.15b}$$

Equivalently,

$$M_i \ddot{\delta}_i + D_i \dot{\delta}_i = P_{m,i} - \sum_{j=1}^{n} a_{ij} \sin(\delta_i - \delta_j) \quad \text{and } a_{i,j} = a_{j,i} \tag{3.16}$$

In the case of our example with two machines,

$$\sum_{j=1}^{2} a_{ij} \sin(\delta_i - \delta_j) = a_{11} \cancel{\sin(\delta_1 - \delta_1)} + a_{12} \sin(\delta_1 - \delta_2) \quad \text{for } i = 1 \tag{3.17}$$

If the system runs at steady-state conditions $\theta_i = \delta_i$ ($\omega_s = \omega_m$).

**Definition: State variable representation**

Let $\frac{d\delta_i}{dt} = \dot{\delta}_i = \Delta\omega_i$ so that $\frac{d^2\delta_i}{dt^2} = \frac{d}{dt}(\Delta\omega_i)$. Hence,

$$M_i \frac{d}{dt}(\Delta\omega_i) + D_i \Delta\omega_i = P_{m,i} - \sum_{j=1}^{n} a_{ij} \sin(\delta_i - \delta_j) \tag{3.18a}$$

$$\frac{d}{dt}(\Delta\omega_i) = -\frac{D_i}{M_i}\Delta\omega_i + \frac{P_{m,i}}{M_i} - \frac{1}{M_i}\sum_{j=1}^{n} a_{ij} \sin(\delta_i - \delta_j) \tag{3.18b}$$

For two synchronous machines,[a]

$$\frac{d}{dt}\begin{bmatrix} \delta_1 \\ \Delta\omega_1 \\ \delta_2 \\ \Delta\omega_2 \end{bmatrix} = \begin{bmatrix} 0 & 1 & 0 & 0 \\ 0 & -\frac{D_1}{M_1} & 0 & 0 \\ 0 & 0 & 0 & 1 \\ 0 & 0 & 0 & -\frac{D_2}{M_2} \end{bmatrix} \cdot \begin{bmatrix} \delta_1 \\ \Delta\omega_1 \\ \delta_2 \\ \Delta\omega_2 \end{bmatrix} + \begin{bmatrix} 0 \\ \frac{P_{m,1}}{M_1} - \frac{a_{1,2}}{M_1}\sin(\delta_1 - \delta_2) \\ 0 \\ \frac{P_{m,2}}{M_2} - \frac{a_{2,1}}{M_2}\sin(\delta_2 - \delta_1) \end{bmatrix} \tag{3.19}$$

[a] $a_{i,j} = a_{j,i}$

# 4 Systems and Control Volumes

Systems and Control Volumes

Discrete view ⟷ Continuum view (simplified view)

Let us take a look at how everything connects

Black box (for now) | Material (or body or...) | Response (output) → How does a mtl (physical object or) react to/with its environment?

Boundary

MECHANICS

A) Applying force(s) and pressure(s) / traction(s)
B) Applying deformation(s) / displacement(s)
C) Applying heating/cooling
D) Allow for chemical reactions
⋮

Constraints. BCs, ICs

Changes in energy over time

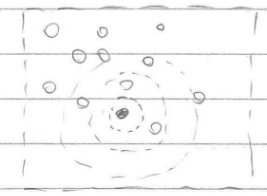
Object/system → Component → Material → Molecules → Atoms → ⋮

Macroscale → Microscale → Nanoscale

If we could track the movement of every particle* in our system, we could predict the behavior across all these scales and up to the macroscale. (Or could we?) Do we even need this information?

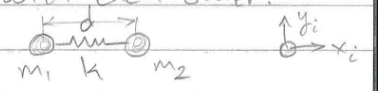
* Particle can be an atom or molecule or clusters of molecules, etc.

I. Start small: molecular dynamics (and statics)



Particles interact with each other.

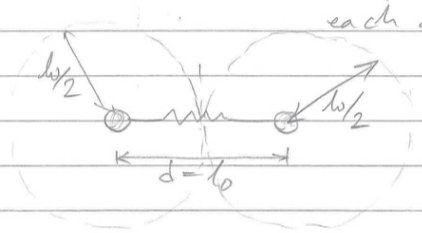
Simplest case:




Spring wants to stay relaxed so that distance d is always equal to the spring's original length $l_0$

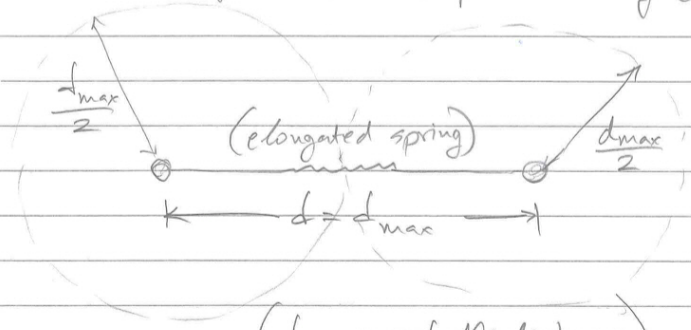
But, even small changes to $d$ away from $l_0$ will cause the system to start oscillating.
In the simplest case when $k = \text{const.}$ the spring will have an internal force $F_S = k\delta = k(l_0 - d)$ : if $d > l_0$ the spring elongates and the force wants to bring the two particles together; if $d < l_0$ the spring compresses and the force wants to separate the particles more. The stiffness $k$ would correspond to the strength of these interactions.

Complication #1: In systems with more than two particles, all particles should somehow interact with each other (think of Kuramoto, f.e.)




Any particle that comes within a distance of $l_0$ from another would repel each other; but this is only half the story...

Starting from $d = l_0$, how large should $d$ become for the two particles to stop interacting (= attracting) each other?




($d_{max}$ = cut-off distance)

Assumption:
If the distance between the particles becomes larger than $d_{max}$ then they stop interacting with each other.

[On the other hand, there is also a limiting close distance beyond which you cannot compress the spring further ($d_{min}$)]

Note: to better approximate reality, the force in the spring should smoothly go to zero (or become negligible) at $d_{max}$ $\therefore$ $F_S$ is not really linear, nor would $k$ be constant...

How would this look for a multi-particle system?

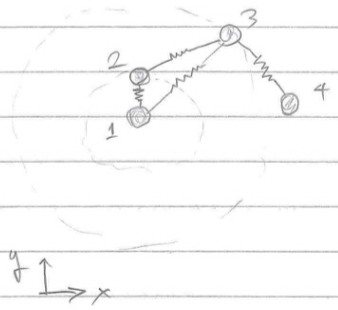
> If $d_{ij}$ between particles $i$ and $j$ becomes smaller than $d_{max}$, then they should start interacting with each other under a nonlinear spring force that wants to bring them together.

> At some point, $d_{ij}$ will become equal to $l_0$ (the desired spacing between them) but, because the masses have inertia, $d_{ij} < l_0$ and the spring will compress.

> So, pairs of particles (in the absence of damping) will oscillate around their equilibrium positions depending on the spring stiffness.

> If the repulsion (or contact?) between particles is strong enough, they may go out of interaction ($d_{ij} > d_{max}$) if the stiffness of the spring is low enough.

So, this is a M-DOF multi-body system with nonlinear springs engaging between any pair of particles that comes close enough.




Focus on particle 1.

> Particle 2 is close enough to 1 so that they repel each other, but is also close enough to 3 so that 2 and 3 attract each other.

> Particle 4 is far enough from 1 and 2 so that it is only attracted by 3, etc.

How do we solve the dynamics of such a system?
Solve Newton's equations of motion (2nd law)!

$$\boxed{\sum F_i = m_i a_i \quad \text{for the } i^{th} \text{ particle}}$$

We need to solve $N \times M$ equations simultaneously for $N$ particles each having $M$ DOF.

Peak into MD: we actually use potential energies instead of forces (that change as a function of the distance between particle pairs).

(Refer to tool shared in prep. assignment)

$$F_i = -\nabla_i V \Rightarrow \boxed{-\frac{dV}{dr_i} = m_i \frac{d^2 r_i}{dt^2}}$$

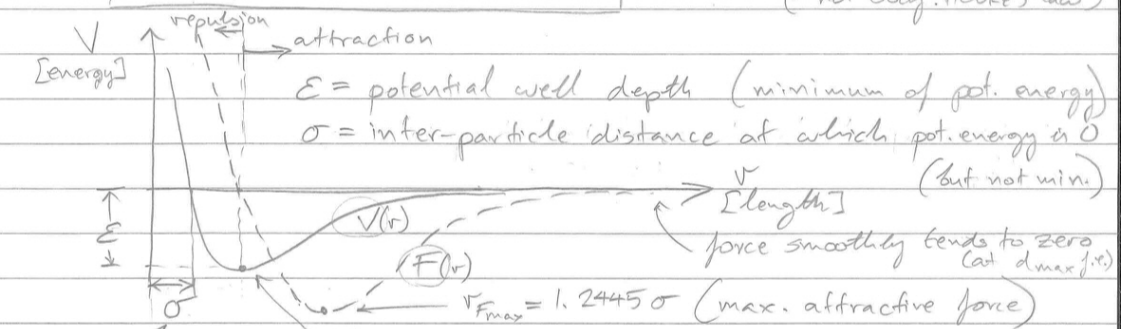
potential energy — distance — mass — acceleration

Aside:

A good approximation for the interactions between particles is the Lennard-Jones (LJ) potential

$$\boxed{V_{LJ}(r) = 4\varepsilon \left(\frac{\sigma}{r}\right)^{12} - \left(\frac{\sigma}{r}\right)^{6}}$$

(Obviously, this does not obey Hooke's law)




$\varepsilon$ = potential well depth (minimum of pot. energy)

$\sigma$ = inter-particle distance at which pot. energy is 0 (but not min.)

force smoothly tends to zero (at $d_{max}$ i.e.)

$r_{F_{max}} = 1.2445\sigma$ (max. attractive force)

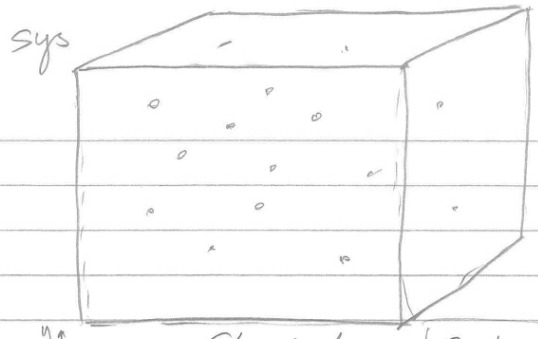
This is the original spring length, i.e. where the particles want to sit relative to each other ($r_{equil} = 2^{1/6}\sigma$)

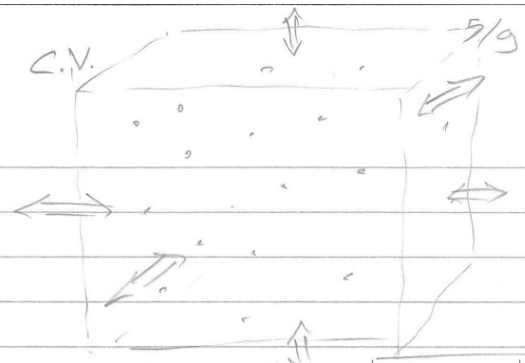
referred to as particle size (or $d_{min}$)

Note: more advanced many-atom (particle) potentials are also widely used in MD to account for more than pair-wise interactions

Question: if particles are always oscillating around their equilibrium positions, what happens to the energy they generate?

Answer: this is heat! A lot of movement corresponds to high temperature and vice versa. In fact, if we set the temperature to absolute zero (MD uses thermostats!) then the particles freeze in their positions $\Rightarrow$ molecular statics




Closed box ⇒ System
Fixed number of particles

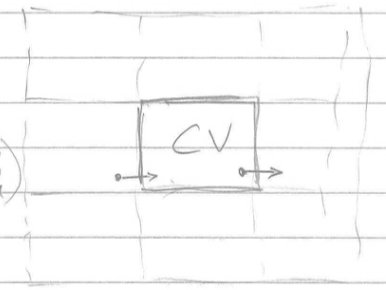
Open box ⇒ Control Volume
Fixed in space

⇓

Apply conditions such that particles cannot cross the walls (boundaries) and bounce inside the closed box

Apply periodic boundary conditions (PBCs) to allow the "flow" of particles through the CV

⇓




A particle exits from the bottom right and reappears from the left

## II. Discrete Element Method (DEM)

- Same concept but at the microscale.
- Not using LJ potential but focusing on particle collisions but also accounting for rotations, deformations, etc (with FEM)
  (MD actually also models rotations, which become important for aggregates of particles, e.g. polymer molecules)

- Suitable to model particulates (sand, powders, etc.) but can also be used together with computational fluid dynamics (coupled CFD-DEM programs) to simultaneously solve the fluid (dynamics) flow; so, it is widely used f.e. in soil mechanics

BUT: many of these problems can also be solved by looking at matter as a continuum rather than discrete particles

Before we switch to continuum...

sys or CV of particles

gases → relatively few particles with little chance to interact; heat → more mobility

compressible fluids!

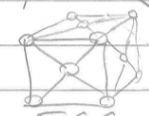
liquids → (nearly) incompressible fluids that can flow and take the shape of their container; volume (nearly) constant

solids → tightly packed particles → structural rigidity exhibiting strong resistance to force

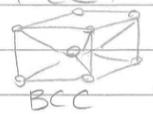
→ crystalline solids bound in regular geometric lattices (e.g. metals)

→ amorphous solids bound irregularly (e.g. glass)

Strength of interactions depend on chemistry and various types of bonds between atoms



FCC



BCC

etc.

Note:

Choosing the appropriate potential in MD can let us model any of the states of matter (including chemical interactions) as functions of the conditions of the system (or CV): number of particles, temperature, pressure, ...

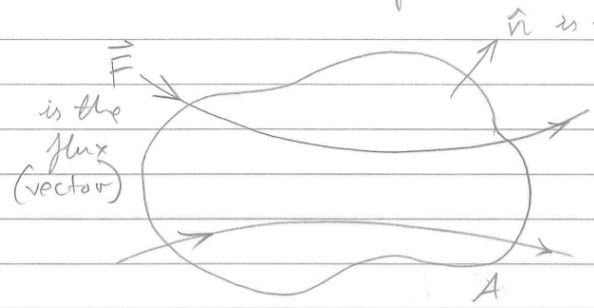
---

III. Continuum mechanics: looking at the mechanical behavior of materials modeled as a continuous mass rather than as discrete particles

- Ignore that matter is made of atoms (i.e. not continuous): this is valid on length scales much greater than those of inter-atomic distances
- Assume that the substance of an object completely fills (i.e. is well distributed) in the space it occupies
- Fundamental laws: Conservation of mass, Conservation of momentum, Conservation of energy } formulate diff. equations to describe behavior
- Material constitutive behavior

$\boxed{\text{We will keep coming back to this ...}}$

Mathematical representation of CV




Here, we want to track the conservation of quantity $q$ (assumed as scalar) within the enclosed domain of volume $V$. $\vec{F}$ represents the flux of quantity $q$ entering and leaving this domain via a small patch of area $A$, defined by its normal unit vector $\hat{n}$. The accumulation is the balance of what enters, what leaves and what may be produced ($P_V$, also a scalar) in the domain.

Integral form of general conservation equation

$$\underbrace{\frac{d}{dt}\left[\int_V q\, dV\right]}_{\text{accumulation}} = \underbrace{-\oint_A \hat{n}\cdot\vec{F}\, dA}_{\substack{\text{in-out} \\ \text{(net input rate)}}} + \underbrace{\int_V P_V\, dV}_{\text{production}}$$

$[q] = \text{unit}/m^3$ depending on quantity of interest (e.g. mass, energy)

$[\vec{F}] = \text{unit}/m^2 s$ and $[P_V] = \text{unit}/m^3 s$

Recall the divergence theorem such that $\oint_A \hat{n}\cdot\vec{F}\, dA = \int_V \nabla\cdot\vec{F}\, dV$

where $\nabla\cdot\vec{F} = \frac{\partial F_x}{\partial x} + \frac{\partial F_y}{\partial y} + \frac{\partial F_z}{\partial z}$

(Recall Calc. I / high school)

Itself, this is a 3D generalization of the Fundamental theorem of calc.

$F(x_1) - F(x_2) = \int_{x_1}^{x_2} \frac{dF}{dx}\, dx$. ($\hat{n}$ ← $x_1$ ——— $x_2$ → $\hat{n}$ → $x$)

Provided that the fixed volume doesn't move over time, the divergence theorem let's us transform the integral representation into differential form: $\int_V \left(\frac{\partial q}{\partial t} + \nabla\cdot\vec{F} - P_V\right) dV = 0$

If we use the mean value theorem (i.e. shrink down the volume to being infinitely small and sum over the volume elements), we can simplify further: $\boxed{\frac{\partial q}{\partial t} + \nabla\cdot\vec{F} = P_V}$

viscosity → $\tau = -\nu \frac{\partial \rho u}{\partial x}$

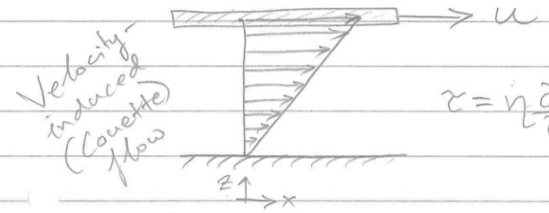
heat conduction → $\frac{q}{A} = -k \frac{dT}{dx}$

diffusion → $J = -D \frac{\partial C}{\partial x}$

A) Gases: harder to model beyond idealizations (e.g. ideal gas law $PV = nRT$) because real gases are compressible and their dynamics are complicated

B) Liquids: stress depends on the strain rate

$(\sigma \propto \dot{\varepsilon})$ $\left(\sigma = F/A,\ \varepsilon = \frac{\text{deformation}}{\text{original size}}\right)$



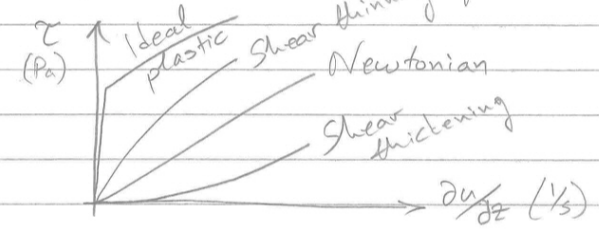

$\tau = \eta \frac{\partial u}{\partial z}$

$\tau$ = shear stress

$\eta$ = dynamic viscosity

$\frac{\partial u}{\partial z}$ = velocity gradient

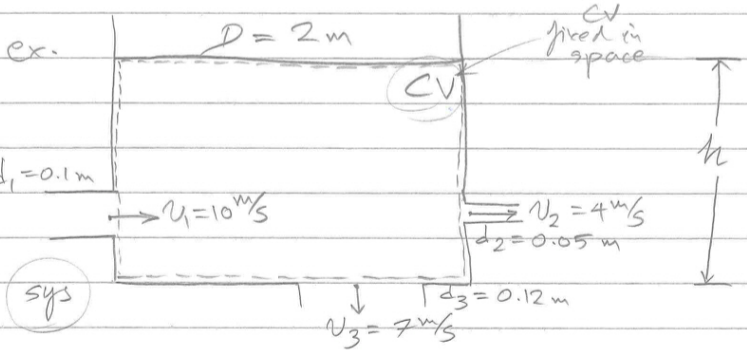
Note: show animations of Couette and Poisseuille flows from MD




Non-Newtonian behavior

↳ VISCOELASTICITY

ex.




$A_{tank} = \frac{\pi D^2}{4} = \pi\ m^2$

$V_{tank} = A_{tank} h = \pi h\ [m^3]$

In CVs we deal with FLUXES

$M_{sys}(t) = M_{CV}(t)$

$\Delta t$ = change in time

$\Delta M$ = change in mass

After $\Delta t$ passes, $M_{sys}(t+\Delta t) = M_{CV}(t+\Delta t) + \Delta M_{out} - \Delta M_{in}$

So, $\frac{dM_{sys}}{dt} = \frac{dM_{CV}}{dt} + \dot{m}_{out} - \dot{m}_{in}$ for infinitessimally small $\Delta t$ ↓ $dt$

But, there is no change in the number of particles in the system, i.e. $\frac{dM_{sys}}{dt} = 0$

$$\therefore \boxed{\frac{dM_{cv}}{dt} = \dot{m}_{in} - \dot{m}_{out}} \text{ for the CV}$$

For more than one input and output, $\frac{dM_{cv}}{dt} = \sum \dot{m}_{in} - \sum \dot{m}_{out}$

In our example, $M_{CV} = \rho V_{tank} = \pi \rho h D^2 [kg]$ where $\rho$ = density

usual assumption

$\frac{dM_{cv}}{dt} = \frac{d}{dt}\left(\rho \overset{A}{\pi D^2} h\right)$ but $A$ = const. and $\rho$ = const. so $\frac{dM_{cv}}{dt} = \rho A \frac{dh}{dt}$

cross-sectional area

and $\boxed{\frac{dh}{dt} = \frac{dM_{cv}}{dt}\frac{1}{\rho A}}$ Also, in general, $\boxed{\dot{m} = \rho \bar{v} A}$

avg velocity

So, $\frac{dM_{cv}}{dt} = \underbrace{\pi\rho\left(\frac{d_1}{2}\right)^2 v_1}_{\text{inflow}} - \underbrace{\pi\rho\left[\left(\frac{d_2}{2}\right)^2 v_2 + \left(\frac{d_3}{2}\right)^2 v_3\right]}_{\text{outflows}}$

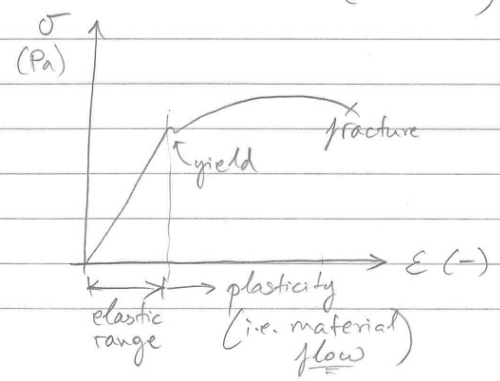
$$\Rightarrow \frac{dM_{cv}}{dt} = \frac{\pi\rho}{4}\left(v_1 d_1^2 - v_2 d_2^2 - v_3 d_3^2\right)$$

Plugging this into the eq'n for $\frac{dh}{dt}$ yields the following:

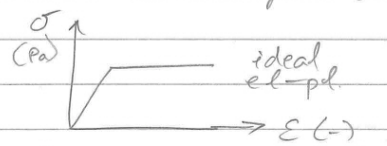
$$\boxed{\frac{dh}{dt} = \frac{1}{4}\left(v_1 d_1^2 - v_2 d_2^2 - v_3 d_3^2\right)}$$

and $\frac{dh}{dt} = -0.0027$ m/s (level in the tank falls by 27 mm every second)

C) Solids: stress depends on strain ($\sigma \propto \varepsilon$)




Interesting case: elastic-plastic constitutive behavior used to model soil (instead of DEM)




(Drucker-Prager model)

# 5 Linear Viscoelasticity

Introduction to viscoelasticity: let's start from elasticity...
(Source: Wikipedia)

- Continuum* mechanics
  - Solid mechanics
    - Elasticity
    - Plasticity
  - Fluid mechanics
    - Non-Newtonian fluids
    - Newtonian fluids

Rheology

*Reminder: A continuum is a body that can be continually sub-divided into infinitessimal elements with properties being those of the bulk material

Aside: $\frac{\partial q}{\partial t} + \nabla \cdot \vec{F} = P_v$ is the conservation law we defined previously.

In solid mechanics, this law has to do with the conservation of momentum (Cauchy momentum equation):

$$\boxed{\frac{\partial \vec{j}}{\partial t} + \nabla \cdot \vec{F} = \vec{s}}$$

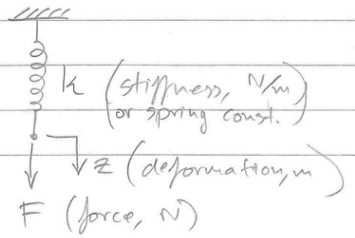
$\vec{j} = \rho \vec{u}$ is the momentum density, where $\vec{u}$ is the flow velocity (vector)

$\vec{F} = \rho \vec{u} \otimes \vec{u} - \vec{\sigma}$ is the flux (tensor) associated to the momentum density, where $\vec{\sigma}$ is the stress tensor

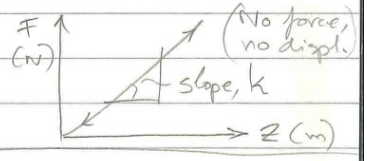
($\vec{u} \otimes \vec{u}$ is the dyad of the flow velocity)

$\vec{s} = \rho \vec{f}$ contains all the body forces per unit volume

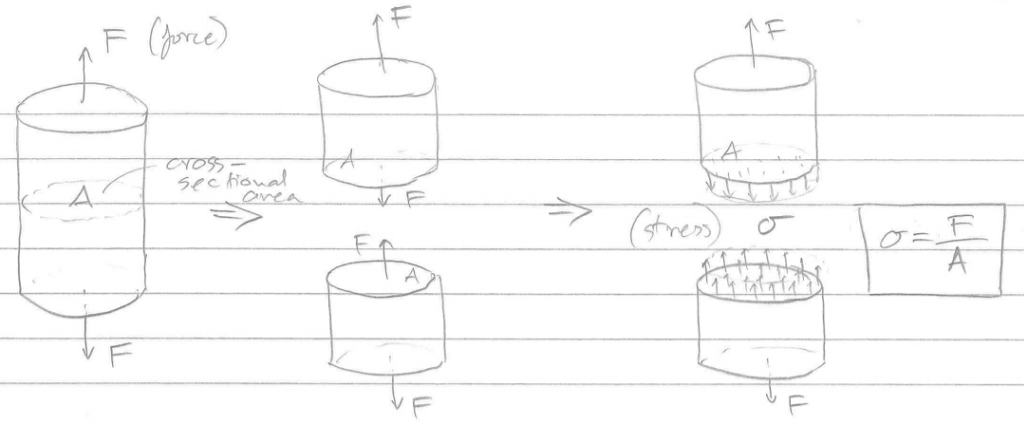
In this course, we limit our scope to linear elasticity. For most elastic materials, stress and strain are linearly related for small deformations. The starting point is Hooke's law, i.e. let's go back to our springs...




$F = kz$
(Hooke's law)

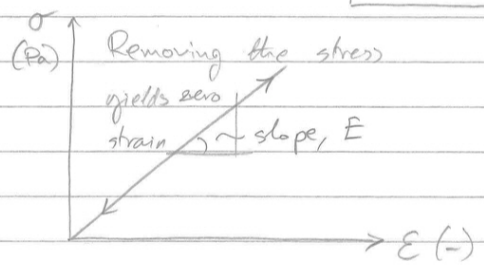


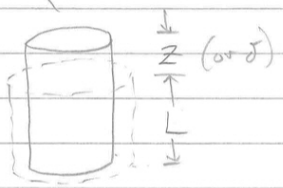

For small deformations, we can represent elastic materials as springs...




Stress distribution in a straight rod of uniform material and cross-section (uniaxial normal stress)

Young's modulus, $\boxed{E = \frac{\sigma}{\varepsilon}}$ $\left(\text{Poisson ratio, } \nu = -\frac{\varepsilon_{transverse}}{\varepsilon_{axial}}\right)$




Strain (axial) $\boxed{\varepsilon = \frac{z}{L}}$

stiffness (from Hooke's law)

$$\therefore \quad E = \frac{\sigma}{\varepsilon} = \frac{F/A}{z/L} = \frac{F}{z}\frac{L}{A} = k\frac{L}{A} \Rightarrow \boxed{k = \frac{EA}{L}}$$

So, applying force F (tensile, axial) to an elastic rod will deform it by amount z (or δ) as a fcn of $k = EA/L$.

OR (in other words...)

Elasticity can be modelled using a Hookean spring.

---

Aside: (Wikipedia) Stress is a physical quantity that expresses the internal forces that neighboring particles of a continuous material exert on each other.

Strain is a measure of deformation representing the displacement between particles in the body relative to a reference length.

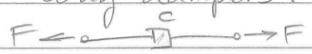
$E$ = Young's modulus $\qquad$ $\eta$ = dynamic viscosity



3/8

Viscoelasticity combines elastic behavior (springs) and viscous behavior (dampers) to model the time-dependent behavior of non-Newtonian fluids.

Why dampers? Because viscoelastic materials exhibit energy loss due to dissipation (friction inside material transformed into heat)




$F = cv = c\dot{z}$

→ In terms of $\sigma - \dot{\varepsilon}$, viscoelasticity uses $\eta$ in place of $c$

Note: We will look at the fluid dynamics of a viscous damper in the next lecture (ie. what is $c$?)

Stress v. strain relations do not give a complete picture of viscoelastic material response: we must include time, i.e. the same material will behave differently if we take less or more time to apply our changes (e.g. force or displacement)

Aside: (Rayleance 2001) 1st and 2nd Laws of Thermodynamics: an increment in mechanical work done on a system $F\,dx$ can produce an increment in the internal energy $dU$ or a decrease in entropy, with the relative importance of the entropic contribution increasing with temperature:

$$\boxed{F\,dx = dU - T\,dS}$$

(Entropy, $S \approx$ degree of disorder (randomness))

Such changes are complex and time-dependent

Arrhenius-type eq'n — apparent activation energy

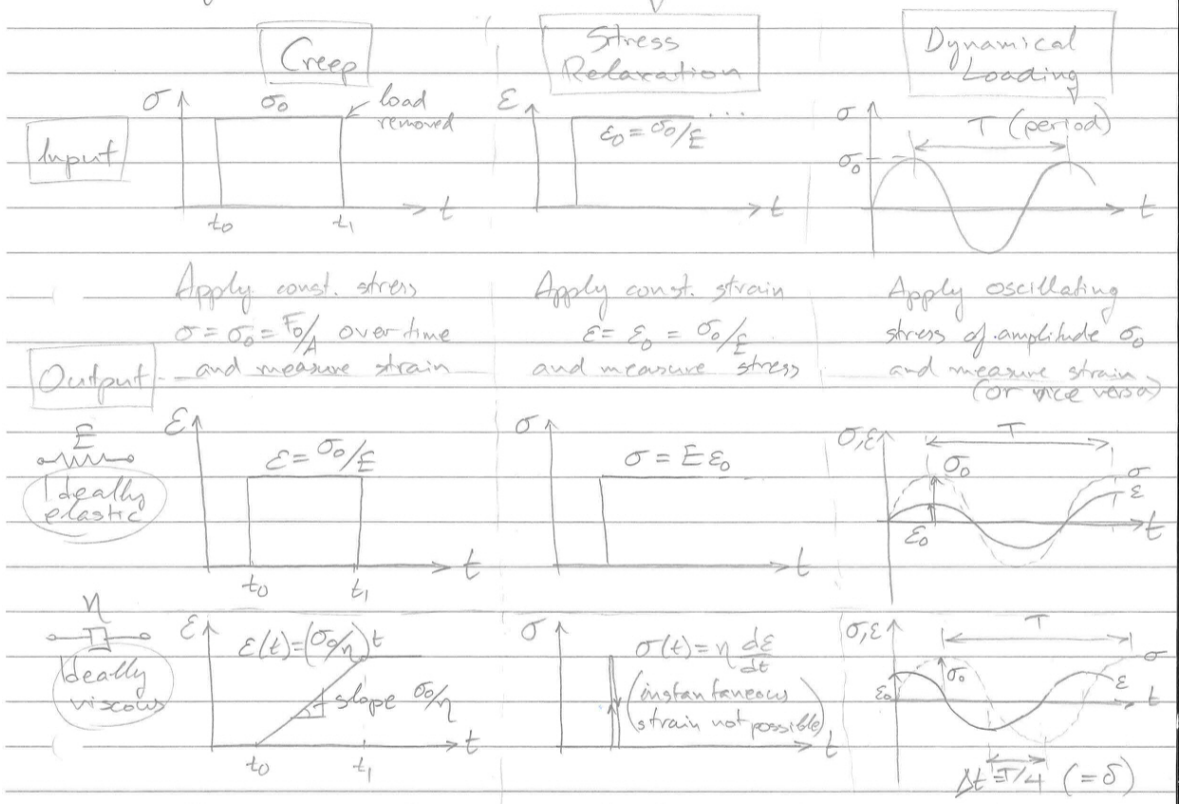
$$\gamma \propto \exp\left(\frac{-\Delta H}{RT}\right)$$

E.g. If you hold a rubber band elongated for increasing temperature, the retractive force will increase as "the increased thermal agitation will make the internal structure more vigorous in its natural attemps to restore randomness. But, if you do the same with steel, "which shows little entropic elasticity", you will observe that the retractive force "will decrease with temperature, as thermal expansion will act to relieve the internal stress."

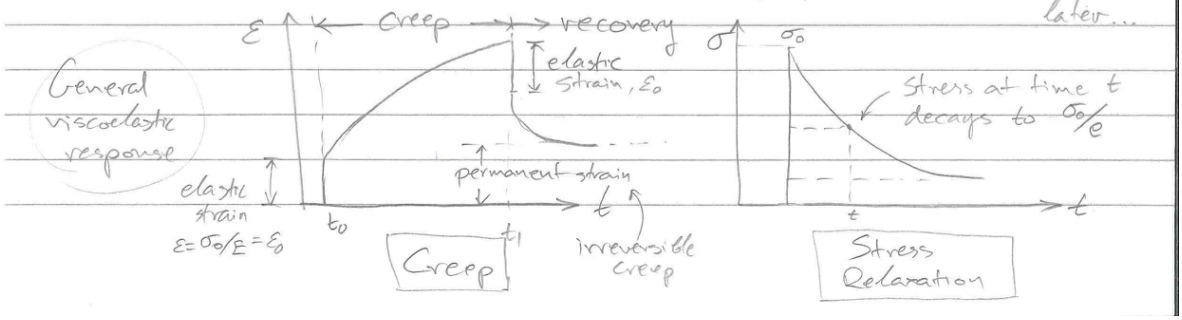
4/8 (Sources: Roylance, MIT, 2001
We et al., Nat. Meth., 2018
Koeder, Char. Biomater., 2013)

Phenomenology of viscoelastic material behavior
> Creep
> Stress relaxation
> Dynamic (sinusoidal) loading

(observed via "viscoelastic tensile tests")




The response to dynamical loading for viscoelastic materials will resemble both that for ideally elastic and that for ideally viscous materials, i.e. the phase shift between the stress and strain curves will be $0 < \Delta t < T/4$ (so, 90° out-of-phase). More on this later...

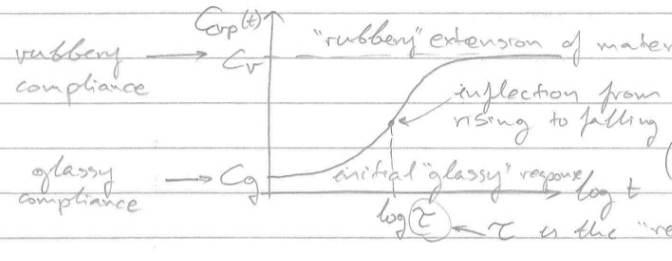


(For linear viscoelastic materials...)

Creep: for various constant stress values, we can calculate the ratio of strain to stress as the compliance, $C_{crp}$:

$$C_{crp}(t) = \frac{\varepsilon(t)}{\sigma_0}$$

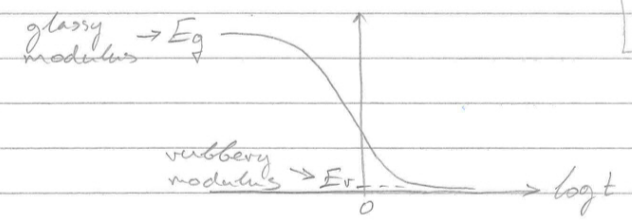
If we plot this against the logarithm of time, we get (typically) a curve of the following form.




(Note: why log t? Because creep occurs over long time)

Stress relaxation: for various constant strain values, we can calculate the ratio of stress to strain as the relaxation modulus, $E_{rel}$:

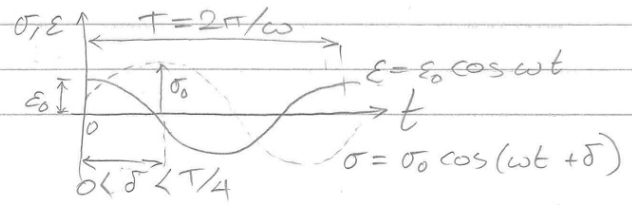
$$E_{rel}(t) = \frac{\sigma(t)}{\varepsilon_0}$$




"Creep and relaxation are both manifestations of the same molecular mechanisms"

Molecular mechanisms: conformational extension ("rubbery" response) v. bond distortion ("glassy" response).

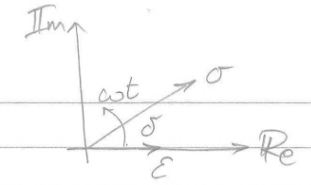
Creep and relaxation tests capture well the viscoelastic response over long times (minutes to days) but are less accurate at shorter times. This is where dynamic tests come into play.




We can represent stress and strain in the complex plane...

complex quantity $\qquad i=\sqrt{-1}$

$$\sigma^* = \underbrace{\sigma_0' \cos\omega t}_{\substack{\text{real part}\\ \text{in-phase with}\\ \text{strain}}} + \underbrace{i\,\sigma_0'' \sin\omega t}_{\substack{\text{imaginary part}\\ 90^\circ \text{ out-of-phase}\\ \text{with strain}}}$$




$$\tan\delta = \sigma_0''/\sigma_0' \qquad |\sigma^*| = \sigma_0 = \sqrt{(\sigma_0')^2 + (\sigma_0'')^2}$$

$$\sigma_0' = \sigma_0 \cos\delta$$

$$\sigma_0'' = \sigma_0 \sin\delta$$

"Real" or "storage" modulus is $\boxed{E' = \sigma_0'/\varepsilon_0}$ (in-phase)

"Imaginary" or "loss" modulus is $\boxed{E'' = \sigma_0''/\varepsilon_0}$ (out-of-phase)

---

Aside: Mechanical work per loading cycle

$$W = \oint \sigma\, d\varepsilon = \oint \sigma \frac{d\varepsilon}{dt}\, dt = \oint \sigma \dot{\varepsilon}\, dt$$

$$\Rightarrow W = \int_0^{T=2\pi/\omega} (\sigma_0' \cos\omega t)(-\varepsilon_0 \omega \sin\omega t)\, dt + \int_0^{2\pi/\omega} (\sigma_0'' \sin\omega t)(-\varepsilon_0 \omega \sin\omega t)\, dt$$

$$\Rightarrow W = \underset{\substack{\uparrow\\ \text{in-phase}\\ \text{components produce}\\ \text{no net work}\\ \text{(over cycle)}}}{0} - \underbrace{\pi \sigma_0'' \varepsilon_0}_{\text{net dissipation per cycle}}$$

$\therefore$

$$W_{dis} = \pi \sigma_0'' \varepsilon_0$$

$$\Rightarrow \boxed{W_{dis} = \pi \sigma_0 \varepsilon_0 \sin\delta}$$ per cycle

Max. stored energy occurs at $T/4 = \pi/2\omega$:

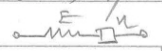
$$W_{st} = \int_0^{\pi/2\omega} (\sigma_0' \cos\omega t)(-\varepsilon_0 \omega \sin\omega t)\, dt = -\tfrac{1}{2}\sigma_0' \varepsilon_0$$

$$\Rightarrow \boxed{W_{st} = -\tfrac{1}{2}\sigma_0 \varepsilon_0 \cos\delta}$$ at the quarter-cycle point (when $\varepsilon$ is max.)

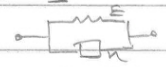
---

Mathematical models for linear viscoelasticity

> Maxwell



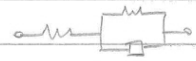

> Kelvin-Voigt



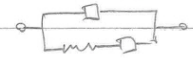

> Standard Linear Solid (SLS)


(Stand. Solid II or Maxwell type)

There can be other 3-element models: (and generalized Maxwell or Kelvin ones)



Stand. Solid I

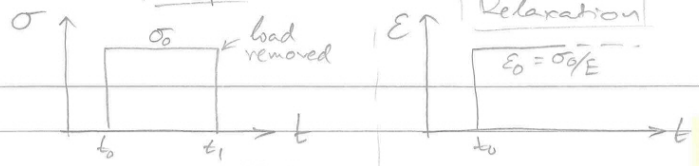


Stand. Fluid I

Stand. Fluid II

**Creep** | **Stress Relaxation**

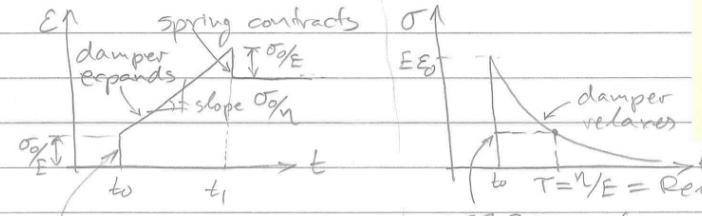
**Input**




What is $0.37E\varepsilon_0$?
This is $\frac{1}{e}E\varepsilon_0$
(Refer to example)

**Output**

Maxwell

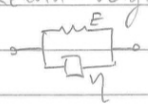

spring expands ("isotonic" response)

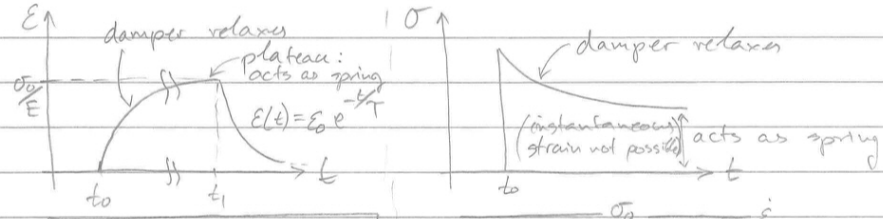
$0.37E\varepsilon_0$ (plug $t = T$ in the eq'n) ("Isometric" response)

$$\boxed{\varepsilon(t) = \frac{\sigma_0}{E} + \left(\frac{\sigma_0}{\eta}\right)t} \qquad \boxed{\sigma(t) = E\varepsilon_0 e^{-t/T}}$$

Standard form of constitutive equation: $\boxed{\sigma + \frac{\eta}{E}\dot{\sigma} = \eta\dot{\varepsilon}}$

Kelvin-Voigt

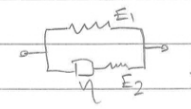


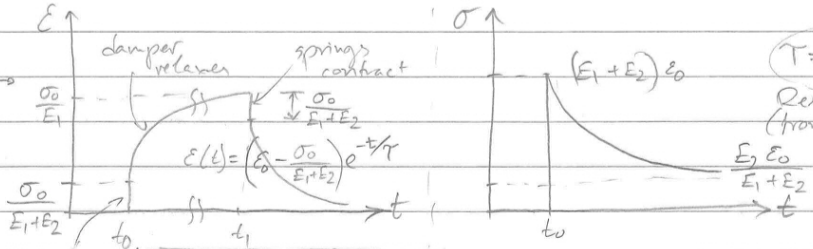




$$\boxed{\varepsilon(t) = \frac{\sigma_0}{E}\left(1 - e^{-t/T}\right)} \qquad \boxed{\sigma(t) = \overset{\sigma_0}{E\varepsilon_0} + \eta\overset{\dot{\varepsilon}}{\frac{d\varepsilon}{dt}}}$$

Standard form of constitutive equation: $\boxed{\sigma = E\varepsilon + \eta\dot{\varepsilon}}$

SLS




$T = \frac{\eta}{E_2}$ Relaxation time (from stress rel. test)

$$\boxed{\varepsilon(t) = \frac{\sigma_0}{E_1}\left(1 - \frac{E_2}{E_1+E_2}e^{-t/T}\right)} \qquad \boxed{\sigma(t) = \varepsilon_0\left(E_1 + E_2 e^{-t/T}\right)}$$

$T = \frac{\eta}{E_1} + \frac{\eta}{E_2}$ Relaxation time (from creep test)

Standard form of constitutive equation:

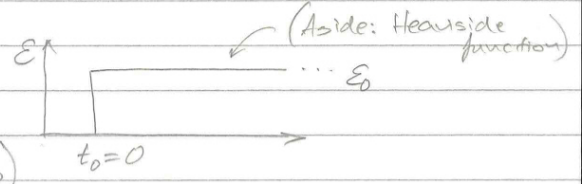
$$\boxed{\sigma + \frac{\eta}{E_2}\dot{\sigma} = E_1\varepsilon + \frac{\eta(E_1+E_2)}{E_2}\dot{\varepsilon}}$$

Example. Derive an expression for the stress as a function of time for the stress relaxation behavior of a Maxwell material.

Stress relaxation:

$\therefore\ \dot{\varepsilon} = 0$

(since $\varepsilon$=const. for $t > t_0$)




$$\boxed{\sigma + \frac{\eta}{E}\dot{\sigma} = \eta\dot{\varepsilon}}$$ for


Plug in $\dot{\varepsilon}=0$ into the equation: $\sigma + \frac{\eta}{E}\dot{\sigma} = 0$

Separate variables and integrate.

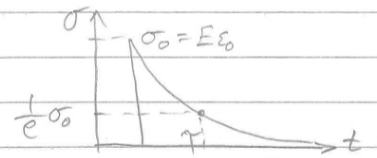
$$\frac{\eta}{E}\underbrace{\frac{d\sigma}{dt}}_{\dot{\sigma}} = -\sigma \Rightarrow \frac{1}{\sigma}\frac{d\sigma}{dt} = -\frac{E}{\eta} \Rightarrow \frac{d\sigma}{\sigma} = -\frac{E}{\eta}dt$$

value for $t > t_0$ $\rightarrow \sigma$

value at $t_0 = 0$ $\rightarrow \sigma_0$

$$\int_{\sigma_0}^{\sigma}\frac{d\sigma}{\sigma} = -\frac{E}{\eta}\int_{t_0=0}^{t} dt \Rightarrow \ln\sigma - \ln\sigma_0 = -\frac{E}{\eta}t$$

$$\Rightarrow \ln\left(\frac{\sigma}{\sigma_0}\right) = -\frac{E}{\eta}t \Rightarrow \frac{\sigma}{\sigma_0} = e^{-\frac{E}{\eta}t}$$




$$\Rightarrow \boxed{\sigma = \sigma_0 e^{-t/\tau}} \quad \text{with } \tau = \eta/E$$

relaxation time

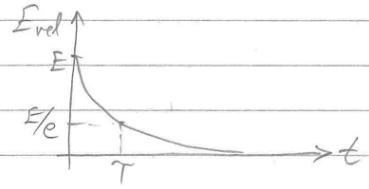
What is $\tau$? Physically, this is the time needed for the stress to fall to $1/e$ $(=0.368)$ of its initial value $(\sigma_0 = E\varepsilon_0)$. This is also the inflection point in the plot with $\log t$.

glass transition temperature

(Above $T_g$, $\tau$ very short
Below $T_g$, $\tau$ very long)

Aside: Revisiting the relaxation modulus: $E_{rel}(t) = \frac{\sigma(t)}{\varepsilon_0}$

In our example, $E_{rel}(t) = \frac{\sigma_0}{\varepsilon_0}e^{-t/\tau} = Ee^{-t/\tau}$




Initially, you can set $E = E_g$ and vary $\tau$ when trying to match $E_{rel}(t)$ to experimental data

# 6 Fluid Dynamics

(Source: COMSOL documentation)

Fluid dynamics: a flow field is characterized by balance in mass, momentum and (total) energy.

Continuity equation: (conservation of mass) $\boxed{\frac{\partial \rho}{\partial t} + \nabla\cdot(\rho\vec{u}) = 0}$ Remember, $\vec{F} = \rho\vec{u}$ (flux; velocity field)

Aside:

Navier-Stokes equations: (conservation of momentum) $\boxed{\frac{\partial \rho\vec{u}}{\partial t} + \nabla\cdot(\rho\vec{u}\vec{u}) = -\nabla p + \nabla\cdot\tau + \vec{F}}$ ($\tau$: Reynolds stress tensor)

Total energy equation: (conservation of energy) $\boxed{\frac{\partial}{\partial t}\left[\rho\left(e+\frac{1}{2}u^2\right)\right] + \nabla\cdot\left[\rho\vec{u}\left(e+\frac{1}{2}u^2\right)\right] = \nabla\cdot(k\nabla T) + \nabla\cdot(-p\vec{u} + \tau\cdot\vec{u}) + \vec{u}\cdot\vec{F} + Q}$ ($e$: extension)

Incompressible fluid flow: density variations are very small (for liquids and gases under moderate pressure / temp. variations)

$$\boxed{\begin{aligned} &\nabla\cdot\vec{u} = 0 \\ &\rho\frac{\partial\vec{u}}{\partial t} + \rho\vec{u}\cdot\nabla\vec{u} = -\nabla p + \nabla\cdot\left[\mu\left(\nabla\vec{u} + \nabla\vec{u}^T\right)\right] + \vec{F} \end{aligned}}$$

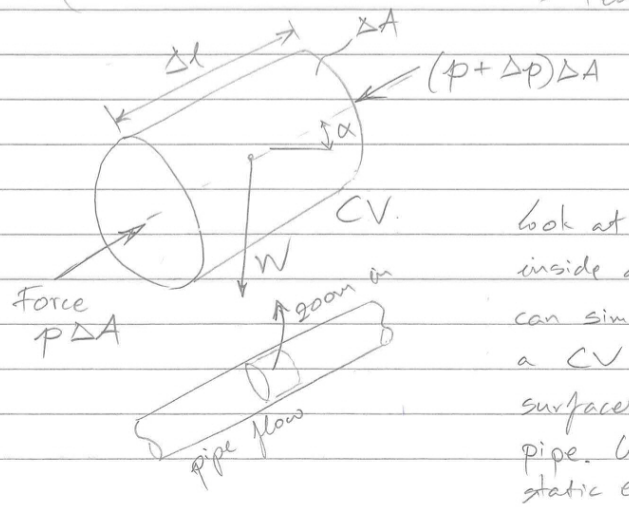
($\mu$: dynamic viscosity) Common form of Navier-Stokes eq'ns $\Rightarrow$ pressure and velocity fields

(Temp. eq'n is completely uncoupled from first two, unless the viscosity depends on temp.)

Note: dynamic viscosity $\mu$ is the same quantity as $\eta$ used in rheology.

Let's take a pause and start from a static description.

(Aside: Fluid mechanics $\longrightarrow$ Fluid statics; $\longrightarrow$ Fluid dynamics)




Take a control volume (CV) at static equilibrium. The more general case would look at a CV of random shape inside a body of fluid; however, we can simplify the case by looking at a CV in which the cylindrical surfaces coincide with the walls of a pipe. What does it mean to be in static equilibrium? $\boxed{\Sigma F = 0}$ (i.e. acceleration of fluid is zero)

What is the weight of this volume of fluid, W?

$W = mg = \rho V g = \rho g V$ and in fluid mechanics, $\boxed{\rho g = \gamma}$ is the specific weight

not the same as the angle

(Aside: What are the units of $\gamma$? $[\gamma] = [\rho][g] = \frac{kg}{m^3} \cdot \frac{m}{s^2} = kg/m^2 s^2$)

The volume of fluid is $V = \Delta A \Delta l$, so that $\boxed{W = \gamma \Delta A \Delta l}$

Now, let's go to trigonometry:


$\sin\alpha = \Delta z / \Delta l$

We should now calculate $\Delta p$ due to inclination

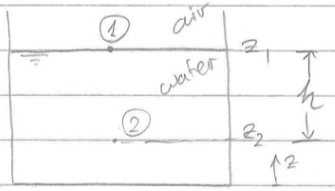
So, $\Sigma F = 0 \Rightarrow p\Delta A - (p + \Delta p)\Delta A - \gamma \Delta A \cdot \Delta l \sin\alpha = 0$

$\Rightarrow \cancel{p\Delta A} - \cancel{p\Delta A} - \Delta p \cancel{\Delta A} - \gamma \cancel{\Delta A} \Delta l \sin\alpha = 0$

$\Rightarrow -\Delta p - \gamma \underbrace{\Delta l \sin\alpha}_{\Delta z} \Rightarrow \boxed{\Delta p = -\gamma \Delta z}$

The pressure is higher at the bottom, which is compressed by the weight of the fluid above it. $\Delta p = -\gamma \Delta z$ means that pressure decreases linearly with increasing elevation.

Ex.




What is the pressure at point 2?

$\Delta p = -\gamma \Delta z$ and we know that $p_2 > p_1$

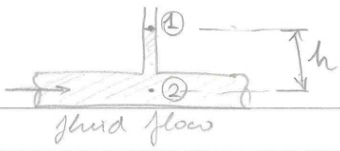
$\therefore \underbrace{p_1 - p_2}_{-ve} = -\gamma \underbrace{(z_1 - z_2)}_{+ve}$ with $z_1 > z_2$

Note: Gage (or gauge) pressure is zero-referenced against ambient air pressure ($p_{atm}$): $p_g = p_{abs} - p_{atm}$

We usually (and will) use gage pressure from here on. Therefore, $p_1 = 0$, i.e. $p_{g,1} = 0$ and $p_{abs,1} = p_{atm}$

So, $-p_2 = -\gamma(z_1 - z_2) = -\gamma \Delta h \Rightarrow \boxed{p_2 = \gamma h = \rho g h}$

Piezometer



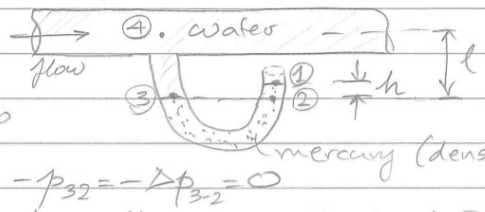

$\Delta p = -\gamma \Delta z$ $\quad \because p_1 = 0$, $p_1 = p_{atm}$ (gage)

$\therefore \boxed{p_2 = \gamma h = \rho g h}$

Measuring $h$ gives you $p_2$.

---

Differential manometer




$p_1 = 0$ (gage pressure)

$\Delta p_{2-1} = p_{21} = p_2 - \cancel{p_1}^{\,0}$

$\Delta p_{2-3} = p_{23} = p_2 - p_3 = -p_{32} = -\Delta p_{3-2} = 0$

Why? Because we have the same fluid at 2 and 3 and it is at rest.

$\Delta p_{3-4} = p_{34} = p_3 - p_4 = \gamma_{water}\, l$

$\Delta p_{1-4} = p_{14} = \cancel{p_1}^{\,0} - p_4$

Why positive? We know that $p_4 > p_3$, so

$\underbrace{p_3 - p_4}_{-ve} = -\gamma_{water} \underbrace{(z_3 - z_4)}_{-ve\ (-l)}$

$\therefore p_3 - p_4 = \gamma_{water}\, l$

From algebra, $\cancel{p_1}^{\,0} - p_4 = \cancel{(p_1 - p_2)} + \cancel{(p_2 - p_3)} + \cancel{(p_3 - p_4)}$ ✓ BUT $p_{14} = p_{12} + p_{23} + p_{34}$

In our example, $p_{23} = 0$ such that $p_{14} = p_{12} + p_{34} = -p_{21} + p_{34}$

$\Rightarrow -p_4 = -p_2 + \gamma_{water}\, l$

$\Rightarrow p_4 = p_2 - \gamma_{water}\, l$

So, what is $p_2$?

$\Delta p_{21} = \underbrace{p_2 - \cancel{p_1}^{\,0}}_{+ve} = -\gamma_{Hg}\, h \Rightarrow p_2 = -\gamma_{Hg}\, h$

Put it all together: $\boxed{p_4 = -(\gamma_{Hg}\, h + \gamma_{water}\, l)}$

Measuring $h$ and $l$ and knowing $\gamma_{Hg}$ and $\gamma_{water}$ gives you $p_4$.

$\boxed{\text{Ref. to OG part of assignment 3.}}$

---

More concepts...

I. Laminar flow: no mass exchange perpendicular to the flow
Why? Because strong viscous effects prevent the particles from moving elsewhere in the flow.

V. Turbulent flow: we have transport of momentum perpendicular to the flow due to strong inertial effects

So, the relative importance of viscous versus inertial effects (and forces) determines the type of flow we have.

$$Re = \frac{\text{Inertial forces}}{\text{Viscous forces}} = \frac{\rho \mathcal{V} L}{\mu}$$

$\mathcal{V}$ ← avg. velocity in direction of flow; $L$ ← significant length; $\mu$ ← dynamic viscosity

E.g. for pipe flow, $L = D$ and the flow is laminar for $Re < 2{,}300$.

(Source: Wiki)

II. Streamlines: family of curves that are instantaneously tangent to the velocity vector of the flow; they show the direction in which a massless fluid element will travel at any point in time

Pathlines: the trajectories that individual fluid particles follow; they can be thought as "recording" the path of a fluid element in the flow over some amount of time. (Direction depends on streamlines.)

III Bernoulli's equation (and principle) for incompressible fluids. Derived by integrating Newton's 2nd law (conservation of momentum) or by applying conservation of energy between two sections along a streamline, ignoring viscosity (i.e. for frictionless flow), compressibility and thermal effects; also, the flow is assumed to be steady.

$$\boxed{p + \gamma z + \frac{\rho \mathcal{V}^2}{2} = \text{constant}}$$

(in terms of pressure)

OR $\frac{p}{\rho} + gz + \frac{\mathcal{V}^2}{2} = \text{constant}$ (in terms of energy)

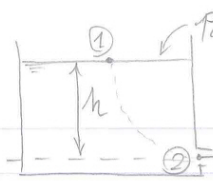
OR $\frac{p}{\gamma} + z + \frac{\mathcal{V}^2}{2g} = \text{constant}$ (in terms of head)

> Principle: within a flow of constant energy, fluid that flows through a region of lower pressure accelerates, and vice versa.

Aside: for compressible flows with small elevations ($z \ll$ size of earth) and sufficiently small fluid flow scales (adiabatic eqn of state), the Bernoulli eqn for an ideal gas is $\left(\frac{\gamma}{\gamma-1}\right)\frac{p}{\rho} + gz + \frac{\mathcal{V}^2}{2} = \text{constant}$, where $\gamma$ is the ratio of specific heats

$$\left(\gamma = \frac{C_p}{C_v} = \frac{\text{heat capacity at constant pressure}}{\text{heat capacity at constant volume}}\right)$$

Ex.




Hole discharges at $p_{atm}$ ($p_g$ @ pt. 2 = $p_2$ = 0)

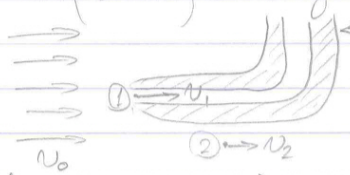
$$\cancel{p_1}^{0} + \gamma z_1 + \cancel{\frac{\rho v_1^2}{2}}^{\approx 0} = \cancel{p_2}^{0} + \gamma z_2 + \frac{\rho v^2}{2}$$

$$\Rightarrow \frac{\rho}{2} v^2 = \gamma \underbrace{(z_1 - z_2)}_{h}$$

$$\Rightarrow \boxed{v = \sqrt{2gh}}$$

Velocity at pt. 1 assumed negligible ($v_1 = 0$) due to large area of container compared to outlet.

Ex. Pitot (-static) or stagnation tube




(at static pressure, $p_s$)

← connect to manometer (i.e. read pressure based on change of head of fluid in manometer)

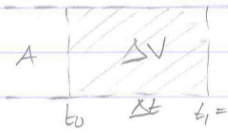
Pt. 1 is the stagnation point at stagnation pressure, $p_t$, where $\boxed{v_1 = 0}$

We could show that $h = \frac{p}{\gamma} + z$ for the manometer, so that $\Delta h = \left(\frac{p_1}{\gamma} + z_1\right) - \left(\frac{p_2}{\gamma} + z_2\right)$

From Bernoulli's principle, $\frac{p_1}{\gamma} + z_1 + \frac{v_1^2}{2g}^{\approx 0} = \frac{p_2}{\gamma} + z_2 + \frac{v_2^2}{2g}$

$$\Rightarrow v_2 = \sqrt{2g\left[\left(\frac{p_1}{\gamma} + z_1\right) - \left(\frac{p_2}{\gamma} + z_2\right)\right]} \Rightarrow v_2 = \boxed{v = \sqrt{2g\Delta h} = \sqrt{\frac{2}{\rho}(p_t - p_s)}}$$

## IV. Conservation of mass




$$\frac{\Delta V}{\Delta t} = \frac{\overbrace{(\bar{v}\Delta t)}^{\text{distance covered in } \Delta t} A}{\Delta t} \Rightarrow \boxed{Q = A\bar{v}}$$

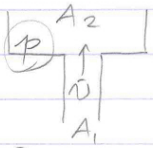
cross-sectional area; avg. velocity; volumetric flow-rate ($\Delta V / \Delta t$)

The mass flow-rate is $\boxed{\dot{m} = \rho Q = \rho A \bar{v}}$

$$\left.\begin{aligned} Q &= \int_A \bar{v}\, dA \\ \dot{m} &= \int_A \rho \bar{v}\, dA \end{aligned}\right\} \text{for variable cross-sections}$$

Mass conservation dictates that $\boxed{Q = A_1\bar{v}_1 = A_2\bar{v}_2}$

## V. Capacitance:



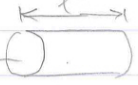

starting from mass conservation, the change in (hydraulic) head over time is $\frac{dh}{dt} = \dot{h} = \frac{Q}{A}$ (since $\dot{h}$ = velocity). Since $p = \gamma h$, $\dot{p} = \gamma \dot{h}$ such that $\boxed{\dot{p} = \gamma \frac{Q}{A}}$

$Q = A_1\bar{v}$ and the head rises in $A_2$ so that $\dot{p} = \gamma \frac{A_1}{A_2}\bar{v}$

VI. Inertance: a measure of the pressure difference in a fluid required to cause a unit change in the rate of change of volumetric flow-rate with time

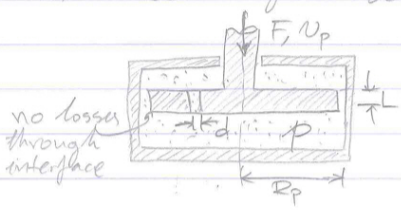
$$\boxed{\Delta p = I\dot{Q}} = I\frac{dQ}{dt}$$

inertance




e.g. for a tube, $I = \rho l/A$

Ex. Viscous fluid damping: a piston moves inside a cylinder containing a viscous fluid (usually liquid) that is forced to pass through an orifice of size d as it is pressurized by the piston; the casing does not move.




Damping coefficient, $C = \dfrac{\text{damping force}}{\text{squeeze velocity}} = \dfrac{F}{v_h}$ ← through hole

$Q_p = v_p A_p$, $Q_h = v_h A_h$ } The flow of the fluid displaced by the piston must be accommodated via the hole, $Q_p = Q_h$

Also, the force on the piston is $F = A_p \Delta p$ (pressure difference across the piston)

Hagen-Poisseuille equation for laminar flow in a tube:

$$\boxed{\Delta p = \frac{128 Q L}{\pi d^4}\mu} \therefore F = (\pi R_p^2)\frac{128 Q L}{\pi d^4}\mu \Rightarrow F = 128\pi\mu L\left(\frac{R_p}{d}\right)^2 v_h$$

So, the damping coefficient is $\boxed{C = 128\pi\mu L\left(\frac{R_p}{d}\right)^2}$.

Aside: Hagen-Poisseuille eq'n (laminar, incompressible, Newtonian flow for $L/d > 48$; no fluid acceleration in tube). If the flow is turbulent, use Darcy-Weisbach eq'n insted.

Navier-Stokes in 3D: $\frac{1}{r}\frac{\partial}{\partial r}\left(r\frac{\partial u}{\partial r}\right) = \frac{1}{\mu}\frac{dp}{dx}$ (cylindrical coords where $u_x = u$)

$$\begin{cases} \text{steady flow} \\ u_r = u_\theta = 0 \\ \frac{\partial(\ldots)}{\partial\theta} = 0 \text{ axisymm. flow} \\ \frac{\partial u_x}{\partial x} = 0 \text{ fully-developed} \end{cases}$$

Soln: $u = \frac{G}{4\mu}(R^2 - r^2)$ parabolic velocity profile

Hence, $u_{max} = u(r=0) = \frac{GR^2}{4\mu}$ and $u_{avg} = \frac{1}{\pi R^2}\int_0^R 2\pi r u\, dr = \frac{1}{2}u_{max}$

If $Q = (\pi R^2)u_{avg}$ and $G = \frac{\Delta p}{L}$, $\Delta p = \frac{8\mu Q L}{\pi R^4}$ ✓

# 7 Heat Transfer and Reaction Kinetics

1/7 (Sources: Wikipedia, Lund Uni. YouTube)

Heat transfer: Conduction (Fourier's law) } + mass transfer
Convection (Newton's law)
Radiation (Stefan-Boltzmann law)

I. Conduction: heat conduction (or heat diffusion) is the direct microscopic exchange of kinetic energy of particles through the boundary between two systems

(for solids or stationary fluids)

> 2nd Law of Thermodynamics:
> Heat transfer always occurs spontaneously from a region of high temperature to another region of lower temperature.

So, heat flows through a body so that it reaches the same temperature as its surroundings (thermal equilibrium)

Fourier's law: $\boxed{\vec{q} = -k \nabla T}$ (differential form)
(isotropic medium)

$\vec{q}$: heat flux (rate of flow of heat energy per unit area)
$k$: thermal conductivity
$\nabla T$: temperature gradient (across medium)

Note: $\tilde{q}_x = -k \frac{\partial T}{\partial x}$, $\tilde{q}_y = -k \frac{\partial T}{\partial y}$, $\tilde{q}_z = -k \frac{\partial T}{\partial x}$ } fluxes

$\vec{q} = -k\left(\frac{\partial T}{\partial x}\hat{i} + \frac{\partial T}{\partial y}\hat{j} + \frac{\partial T}{\partial z}\hat{k}\right) = -k\vec{\nabla T}$

$\vec{q}$: vector quantity; $\hat{i}$: unit vector in x-direction; $\hat{j}$: y-dir.; $\hat{k}$: z-dir.; $\vec{\nabla T}$: vector quant

For a medium of uniform cross-sectional area $A$ and material with (isotropic) thermal conductivity $k$, let us define the heat transfer rate (scalar) relative to $\vec{q}$ so that $\boxed{\dot{Q}_{cond} = -kA\frac{\partial T}{\partial x}}$ along length $x$, i.e. $\vec{q} = \frac{d\dot{Q}}{dA}$

What is $k$? Thermal conductivity is the ability of a material to transport (conduct) heat.

$[k] = \frac{W}{m \cdot K}$ ← Kelvin (abs. temp.)

$\left( W = \frac{J}{s} \quad Pa = \frac{N}{m^2} \right)$

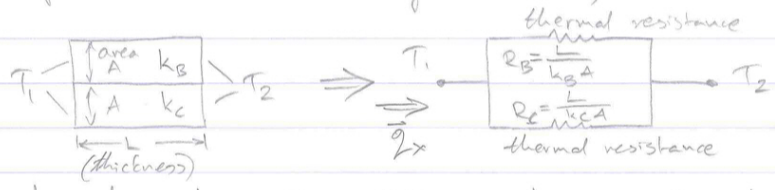
Aside: Analogical models (Wikipedia: thermal resistance)

| Type | Mechanical analogy | Hydraulic analogy | Thermal analogy | Electrical analogy |
|---|---|---|---|---|
| Quantity | momentum, $P$ [Ns] | volume, $V$ [$m^3$] | heat, $Q$ [J] | charge, $q$ [C] |
| Potential | velocity, $v$ [$\frac{m}{s}$] | pressure, $p$ [Pa] | temp., $T$ [K] | potential, $V$ [V] |
| Flux | force, $F$ [N] | flow-rate, $Q$ [$\frac{m^3}{s}$] | heat transfer rate, $\dot{Q}$ [W] | current, $I$ [A] |
| Flux density | stress, $\sigma$ [Pa] | velocity, $v$ [$\frac{m}{s}$] | heat flux, $\dot{q}$ [$\frac{W}{m^2}$] | current density, $j$ [$\frac{A}{m^2}$] |

Further analogies: thermal resistance, $R$ [$\frac{K}{W}$] v. electrical resistance, $R$ [$\Omega$]
thermal conductance, $G$ [$\frac{W}{K}$] ($G = 1/R$)
mechanical stiffness, $k$ [$\frac{N}{m}$] v. thermal conductivity, $k$ [$\frac{W}{mK}$]

Ex. from previous courses (PAIS)

Composite wall under steady conditions; what is the heat flow?




$$\frac{1}{R_{tot}} = \frac{1}{R_B} + \frac{1}{R_C} \Rightarrow R_{tot} = \frac{R_B R_C}{R_B + R_C} = \frac{L}{(k_B + k_C)A}$$ where $k_B$ and $k_C$ are thermal conductivities

From Fourier's law: $\Delta T = \dot{Q} R_{tot} \Rightarrow \dot{Q} = \frac{\Delta T}{R_{tot}} = \frac{T_2 - T_1}{R_{tot}}$

heat transfer rate (or heat flow)

Back to thermal conductivity: other quantities can be derived...

Thermal conductance, $G = kA/L$

Thermal resistance, $R = 1/G = L/kA$ } reciprocal

Thermal insulance is the reciprocal of the thermal admittance, also referred to as the heat transfer coefficient, $h = k/L$ (simplified)

Let us revisit our general conservation equation:

$$\frac{\partial q}{\partial t} + \nabla \cdot \vec{F} = P_v \quad \text{with} \quad [q] = \text{unit}/m^3, \; [\vec{F}] = \text{unit}/m^2 s \text{ and } [P_v] = \text{unit}/m^3 s$$

Take $q$ to be enthalpy per unit volume. But what is enthalpy?

Enthalpy: we need to go into the thermodynamics of chemical reactions...

Enthalpy is the sum of the system's internal energy and the product of its pressure and volume: $\boxed{H = U + pV}$

enthalpy, internal energy

While enthalpy is not something we can measure experimentally, the change in enthalpy corresponds to the heat of reaction

Heat of reaction, $\boxed{\Delta H = H_f - H_i}$ ← initial enthalpy (reactants), final enthalpy (products)
(change in enthalpy)

$\boxed{\Delta H = q}$ where $q$ is the heat transferred $[q] = \frac{J}{mol}$

If $\Delta H < 0$, the reaction is exothermic (heat released to surroundings)
If $\Delta H > 0$, the reaction is endothermic (requires heat to occur)

So, $\boxed{\Delta H = \Delta U + p\Delta V}$ at constant pressure and usually $p\Delta V \ll \Delta U$ so that $\Delta H \approx \Delta U$

E.g. for $2CO(g) + O_2(g) \rightarrow 2CO_2(g)$, $\Delta H = -566.0$ kJ and
(combustion of CO) $\Delta U = -563.5$ kJ

But what is internal energy? It is the sum of the kinetic and potential energies of the particles that form the system.

(change in internal energy)
$\boxed{\Delta U = U_f - U_i}$ (e.g. for an ideal gas, $U = \frac{3}{2}RT$)

1st Law of Thermodynamics: ($\Delta U_{universe} = 0$)
Energy can be transferred from the system to its surroundings and vice versa, but it cannot be created or destroyed.

If $\Delta U > 0$, the system gains heat from its surroundings
If $\Delta U < 0$, the system loses heat to its surroundings

From 1st law: $\boxed{\Delta U = q + w}$
heat, work

For constant pressure, the internal energy of the system decreases when the system does work on its surroundings, i.e. $\boxed{w = -p\Delta V}$ for $p = \text{const}$.

So, $\Delta U = q + w = q - p\Delta V$ and $\Delta H = \Delta U + pV$.

Therefore, $\boxed{\Delta H = q}$ at constant pressure ✓

---

We need one more property before we return to our general conservation equation: heat (or thermal) capacity.

Heat capacity is the amount of heat to be supplied to a given mass of material to produce a unit change in its temperature: $\boxed{q = C\,\Delta T}$ $\quad [C] = \frac{J}{K}$

Specific heat capacity is the heat capacity per mass: $\boxed{C_p = \frac{C}{m}}$ for constant pressure.

Therefore, $q = \Delta H = m C_p \Delta T$ and $\boxed{dH = m C_p dT}$ for infinitessimally small changes.

---

Now, back to our general conservation equation where we introduce $H_V = H/V$ as the enthalpy per unit volume (and $dH_V = dH/V$), heat flux $\vec{q} = -k\nabla T$ as our flux ($\vec{F}$) and $q_V$ as the rate at which energy is generated per unit volume:

$$\frac{\partial H_V}{\partial t} + \nabla\cdot(-k\nabla T) = q_V$$

Then, $dH_V = \frac{dH}{V} = \frac{m}{V} C_p\, dT = \rho C_p\, dT$ and $\frac{\partial H_V}{\partial t} = \rho C_p \frac{\partial T}{\partial t}$

$\therefore$

$$\boxed{\rho C_p \frac{\partial T}{\partial t} = k\nabla^2 T + q_V}$$ Fourier-Biot equation (for heat conduction)

If there is no heat generation ($q_V = 0$), then we get the heat (diffusion) equation:

"Heat equation"

$$\rho c_p \frac{\partial T}{\partial t} = k \nabla^2 T \Rightarrow \boxed{\frac{\partial T}{\partial t} = \alpha \nabla^2 T}$$ where $\alpha = k / \rho c_p$ is the thermal diffusivity $[\alpha] = \frac{m^2}{s}$

At steady-state with heat generation, we get:

$$\boxed{k \nabla^2 T + q_v = 0}$$ Poisson equation

And at steady-state without heat generation, we get:

$$\boxed{\nabla^2 T = 0}$$ Laplace equation

---

II. Convection: heat convection occurs when bulk flow from a fluid (liquid or gas) carries heat along with the flow of matter.

Note: all convective processes also move heat partly by diffusion.

heat transfer coefficient

$$\boxed{\dot{Q}_{conv} = h A (T - T_f)^b}$$

scaling exponent

fluid temperature

heat transfer rate

surface temperature

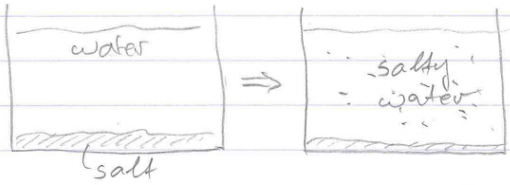
What is the heat transfer coefficient? $h = \frac{\vec{q}}{\Delta T}$ (heat flux; temp. diff.)

$[h] = \frac{W}{m^2 K}$

Convection occurs on the macroscale: an entire "package" (bulk) of fluid moves together transferring heat to and from its surroundings.

V.

At the molecular level, particles always move (Brownian motion) and collide with each other: if you separate two sets of particles with a barrier and then remove the barrier, the particles will spontaneously mix. This is diffusion.




After mixing

$V = V_A = V_B$ (why? fluids move to occupy space)

$\boxed{m = m_A + m_B}$

$\rho = \rho_A + \rho_B$

Concentration $\boxed{C = C_A + C_B}$

Mass transfer (diffusion) described by Fick's laws
(Also derived from our general conservation equation)
Fick's 1st law:

$$\boxed{J = -D \nabla C}$$

concentration (also denoted $c$) (= amount of substance per unit volume)
diffusivity (= rate of collision of molecules)
diffusion flux (= amount of substance per unit area per unit time)

According to Fick's first law, a solute will move from a region of high concentration to a region of low concentration across a concentration gradient. (minus sign)

Fick's 2nd law: this describes how diffusion causes the concentration to change with respect to time.

$$\boxed{\frac{\partial C}{\partial t} = D \nabla^2 C}$$

---

Aside: Reaction-diffusion systems can be used to describe the spreading of biological populations, Rayleigh-Bénard convection (resulting convection patterns in a planar horizontal fluid heated from below; example of a self-organizing nonlinear system), combustion (Zeldovich equation, etc.)

(in 1D) if $R(u)$ vanishes, this becomes Fick's 2nd law

E.g. $\boxed{\partial_t u = D^2 \partial_x^2 u + R(u)}$ (Kolmogorov-Petrovsky-Piskunov)

---

III. Radiation: heat radiation occurs through vacuum or any transparent medium. It is the transfer of energy by means of photons in electromagnetic waves.

$$\boxed{\dot{Q}_{rad} = \varepsilon \sigma T^4}$$

Stefan-Boltzman constant ($\sigma = 5.67\cdots \times 10^{-8} \frac{W}{m^2 K^4}$)
Stefan-Boltzman equation
heat transfer rate
emissivity ($\varepsilon < 1$ since $\varepsilon = 1$ for an ideal black body)

---

Let us look at an example of how to solve a heat transfer problem numerically, before moving on to reaction kinetics...

Ex. Find the temperature distribution in a square plate for conduction only, i.e. using $\frac{\partial T}{\partial t} = \alpha \nabla^2 T$, in 2D.

In 2D, $\frac{\partial^2 T}{\partial x^2} + \frac{\partial^2 T}{\partial y^2} = \frac{1}{\alpha}\frac{\partial T}{\partial t}$ (since $\nabla^2 T = \frac{1}{\alpha}\frac{\partial T}{\partial t}$)

FDM

$$\frac{\partial^2 T}{\partial x^2} \approx \frac{T_{i-1,j}^{k} - 2T_{i,j}^{k} + T_{i+1,j}^{k}}{\Delta x^2}$$

$$\frac{\partial^2 T}{\partial y^2} \approx \frac{T_{i,j-1}^{k} - 2T_{i,j}^{k} + T_{i,j+1}^{k}}{\Delta y^2}$$

$$\frac{\partial T}{\partial t} \approx \frac{T_{i,j}^{k+1} - T_{i,j}^{k}}{\Delta t}$$

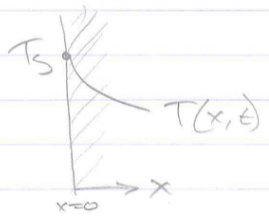
Refer to course reader §5.2-3. Solve for $T_{ij}^{k+1}$ and set stability criterion for $\Delta t$.

But, we also need BCs...

Boundary conditions (BCs) for heat transfer.

1. Constant surface temperature

$$\boxed{T(0,t) = T_s}$$




2. Constant surface heat flux

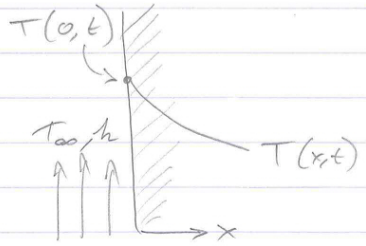
$$\boxed{-k\left.\frac{\partial T}{\partial x}\right|_{x=0} = \dot{q}_s}$$ for finite heat flux

$$\boxed{\left.\frac{\partial T}{\partial x}\right|_{x=0} = 0}$$ for an adiabatic or insulated surface

Note: adiabatic refers to a process occurring without transferring heat or mass between the system and its surroundings

3. Convection surface condition

$$\boxed{-k\left.\frac{\partial T}{\partial x}\right|_{x=0} = h\left[T_\infty - T(0,t)\right]}$$



## 7.1 Boundary and Initial Conditions

The Boundary and Initial Conditions are a set of additional qualitative and quantitative constraints which are also solution of the Partial Differential Equations (PDE's) and help defining the conditions under which the system works. In heat transfer we can find three different type of boundary conditions: Dirichlet, Neumann and Robin.

1. **Dirichlet** or First Type: the value of the variable is defined in the boundary. In other words, there is a constant surface temperature at the boundary which is given by $T(0,t) = T_s$.
2. **Neumann** or Second Type: the value of the derivative if defined in the boundary. This essentially implies there is a constant surface heat flux. If there is a finite heat flux, then it is given by $-k\frac{\partial T}{\partial x}|_{x=0}$. When there is a adiabatic or insulated surface, then it is given by $\frac{\partial T}{\partial x}|_{x=0} = 0$
3. **Robin** or Third Type: usually used in convection, the heat transfer by convection is defined in the boundary which is simply the convection surface condition and is given by $-k\frac{\partial T}{\partial x}|_{x=0} = h[T_\infty - T(0,t)]$.

## 7.2 Heat Diffusion Equation - Solutions

We have defined the differential equations and the BC's and IC's, so the "only" thing we need to do is to solve them. Generally speaking, we can find two types of solutions...

- Analytical: the PDE is completely solved, finding a function of one or several variables. This type of solution is restricted to very few, specific cases;
- Numerical: we do not solve the PDE, but we find the solution of something that "looks like" the PDE. Therefore, the solution is approximate... But how do we approximate the solution?

There are many different approaches nowadays with computers, but in almost all the numerical techniques (the exception are the meshfree methods) our domain in study is discretized in a mesh with a finite number of points in which the PDE is solved... how does this look???

The most commonly used numerical techniques in heat transfer are...

- Finite Difference Methods (FDM): we transform every derivative into approximate relationships between the variables in study (see Appendix A for more information on FDM). The approximation is in the derivative;
- Finite Element Methods (FEM) or Finite Volume Methods (FVM): in this case we do not approximate every derivative but we approximate the solution of the PDE. The approximation is in the solution of the PDE;
- Boundary Element Methods (BEM): based on finding the solution of boundary integral equations, solutions of the PDE, using only the values at the boundaries. Once the solution of this equation is found, the values in the whole domain are obtained straightforwardly.

The easiest and most commonly numerical technique used/taught is the FDM. If we apply

this concept to a generic point inside the domain $(m, n)$ we get,

$$\left.\frac{\partial^2 T}{\partial x^2}\right|_{m,n} \approx \frac{\frac{\partial T}{\partial x}\Big|_{m+\frac{1}{2},n} - \frac{\partial T}{\partial x}\Big|_{m-\frac{1}{2},n}}{\Delta x} = \frac{T_{m-1,n} - 2T_{m,n} + T_{m+1,n}}{\Delta x^2} \tag{7.1}$$

$$\left.\frac{\partial^2 T}{\partial y^2}\right|_{m,n} \approx \frac{\frac{\partial T}{\partial y}\Big|_{m,n+\frac{1}{2}} - \frac{\partial T}{\partial x}\Big|_{m,n-\frac{1}{2}}}{\Delta y} = \frac{T_{m,n-1} - 2T_{m,n} + T_{m,n+1}}{\Delta y^2} \tag{7.2}$$

Inserting this into the Laplace equation,

$$T_{m+1,n} + T_{m,n+1} + T_{m-1,n} + T_{m,n-1} - 4T_{m,n} = 0 \tag{7.3}$$

And into Poisson,

$$T_{m+1,n} + T_{m,n+1} + T_{m-1,n} + T_{m,n-1} + \frac{\dot{E}_{trans,m,n}\Delta x^2}{k} - 4T_{m,n} = 0 \tag{7.4}$$

### 7.2.1 Transient Problems

The addition of the time derivatives in transient problems usually complicates everything (*golden rule in numerical simulation!*), since the solution of the PDE becomes dependant on this derivative. In this case, the time derivative is approached using,

$$\left.\frac{\partial T}{\partial t}\right|_{m,n} \approx \frac{T_{m,n}^{k+\Delta t} - T_{m,n}^{k}}{\Delta t} \tag{7.5}$$

and then...

$$\frac{1}{\alpha}\frac{T_{m,n}^{k+\Delta t} - T_{m,n}^{k}}{\Delta t} = \frac{T_{m-1,n} - 2T_{m,n} + T_{m+1,n}}{\Delta x^2} + \frac{T_{m,n-1} - 2T_{m,n} + T_{m,n+1}}{\Delta y^2} + \frac{\dot{E}_{trans,m,n}}{k} \tag{7.6}$$

But now there is problem... the spatial derivatives and the heat addition must also be approximated to a specific time-step. This gives us three options...

- Explicit (*Euler Explicit*): the values used are those from the previous time-step ($k$)... Easier to solve but is not unconditionally stable. Thus, oscillations may appear in the solution, which are not physically possible. These may grow boundlessly, making the whole simulation to crash.
- Implicit (*Euler Implicit*): the values used are those from the time-step being calculated ($k + \Delta t$). Harder to solve, but these are usually unconditionally stable (i.e., no oscillations!).
- A linear combination of the previous ones (*Crank-Nicolson*).

**Explicit**

$$\frac{1}{\alpha}\frac{T_{m,n}^{k+\Delta t} - T_{m,n}^{k}}{\Delta t} = \left(\frac{T_{m-1,n} - 2T_{m,n} + T_{m+1,n}}{\Delta x^2} + \frac{T_{m,n-1} - 2T_{m,n} + T_{m,n+1}}{\Delta y^2} + \frac{\dot{E}_{trans,m,n}}{k}\right)^k \tag{7.7}$$

$$\frac{1}{Fo}\left(T_{m,n}^{k+\Delta t} - T_{m,n}^{k}\right) = \left(T_{m-1,n} + T_{m+1,n} + T_{m,n-1} + T_{m,n+1} + 4T_{m,n} + \frac{\dot{E}_{trans,m,n}\Delta x^2}{k}\right)^k \tag{7.8}$$

With the $Fo$ Fourier number being defined by,

$$Fo = \frac{\alpha \Delta t}{\Delta x^2} \tag{7.9}$$

**Implicit**

$$\frac{1}{Fo}\left(T_{m,n}^{k+\Delta t} - T_{m,n}^{k}\right) = \left(T_{m-1,n} + T_{m+1,n} + T_{m,n-1} + T_{m,n+1} + 4T_{m,n} + \frac{\dot{E}_{trans,m,n}\Delta x^2}{k}\right)^{k+\Delta t} \tag{7.10}$$

**Crank-Nicolson**

$$\begin{aligned}\frac{1}{\alpha}\frac{T_{m,n}^{k+\Delta t} - T_{m,n}^{k}}{\Delta t} = \\ \frac{1}{2}\left(\frac{T_{m-1,n} - 2T_{m,n} + T_{m+1,n}}{\Delta x^2} + \frac{T_{m,n-1} - 2T_{m,n} + T_{m,n+1}}{\Delta y^2} + \frac{\dot{E}_{trans,m,n}}{k}\right)^k + \\ \frac{1}{2}\left(\frac{T_{m-1,n} - 2T_{m,n} + T_{m+1,n}}{\Delta x^2} + \frac{T_{m,n-1} - 2T_{m,n} + T_{m,n+1}}{\Delta y^2} + \frac{\dot{E}_{trans,m,n}}{k}\right)^{k+\Delta t}\end{aligned} \tag{7.11}$$

### 7.2.2 Solving the Heat Equation for a Rod

We consider a square plate with lengths $x$ by $y$, and assume that we can neglect the thickness $z = 0$. The square plate is connected to a heat source at one of its bases. We are interested in the temperature distribution of the rod in both dimensions as function of time. The change of heat in the body is determined by the inflow and outflow of heat. In other words, we have

$$\begin{aligned}\frac{\partial T}{\partial t} &= \text{In} - \text{Out} \\ &= Q_x + Q_y - Q_{x+dx} - Q_{y+dy},\end{aligned} \tag{7.12}$$

where

$$\begin{aligned}Q_{x+dx} &= Q_x + \frac{\partial Q}{\partial x}dx \\ Q_{y+dy} &= Q_y + \frac{\partial Q}{\partial y}dy,\end{aligned} \tag{7.13}$$

which yields the following equation:

$$-\frac{\partial Q}{\partial x}dx - \frac{\partial Q}{\partial y}dy = \frac{\partial T}{\partial t}. \tag{7.14}$$

The thermal conductivity $k$ is given in the units of $\mathrm{W\,m^{-1}\,K^{-1}}$. To express the heat transfer in Watt for this specific plate, we need to multiply with the corresponding factors:

$$\begin{aligned} Q_x &= -kA_x\frac{\partial T}{\partial x} \\ Q_y &= -kA_y\frac{\partial T}{\partial y}, \end{aligned} \tag{7.15}$$

where the areas are given by $A_x = xdy$ and $A_z = ydx$. Combining the equations yields:

$$-\frac{\partial}{\partial x}\big(-kA_x\frac{\partial T}{\partial x}\big)dx - \frac{\partial}{\partial y}\big(-kA_y\frac{\partial T}{\partial y}\big)dy = \rho r C_p\frac{\partial T}{\partial t} \tag{7.16}$$

$$\frac{\partial^2 T}{\partial x^2} + \frac{\partial^2 T}{\partial y^2} = \frac{1}{\alpha}\frac{\partial T}{\partial t} \tag{7.17}$$

**Numerical solution**

In order to calculate the numerical solution to the heat equation for the rod, we discretize Equation 7.17 using indices $i$, $j$, and $k$, where $i$ and $j$ are spatial dimensions for $x$ and $y$, respectively, and $k$ represents time:

$$\frac{\partial^2 T}{\partial x^2} \approx \frac{T^k_{i-1,j} - 2T^k_{i,j} + T^k_{i+1,j}}{\Delta x^2} \tag{7.18a}$$

$$\frac{\partial^2 T}{\partial y^2} \approx \frac{T^k_{i,j-1} - 2T^k_{i,j} + T^k_{i,j+1}}{\Delta y^2} \tag{7.18b}$$

$$\frac{\partial T}{\partial t} \approx \frac{T^{k+1}_{i,j} - T^k_{i,j}}{\Delta t} \tag{7.18c}$$

Putting together all equations to solve for $T(i,j)$ at $k+1$, we obtain:

$$T^{k+1}_{i,j} = T^k_{i,j} + \alpha\Delta t\left(\frac{T^k_{i-1,j} - 2T^k_{i,j} + T^k_{i+1,j}}{\Delta x^2} + \frac{T^k_{i,j-1} - 2T^k_{i,j} + T^k_{i,j+1}}{\Delta y^2}\right), \tag{7.19}$$

where Equation 7.18c is rewritten such that $T^{k+1}_{i,j}$ becomes the left hand side of Equation 7.17, and the other approximations in Equation 7.18 are used to approximate the other partial derivatives.

Finally, for stability of this explicit scheme, we set

$$\Delta t \leq \frac{\min(x^2, y^2)}{4\alpha}. \tag{7.20}$$

Hence, we require that the maximum $\Delta t$ depends on the square of dimension $x$ if $x < y$, and on the square of dimension $y$ otherwise.

### 7.2.3 Pseudocode

**Pseudocode 5:** Heat Transfer

```
Set Δt, Δx ∧ Δy, k, c_p, ρ, q̇(x, y), min_error and max_time;
Initial Condition T^0_{x,y};
Boundary Condition T^{∀t}_{x,y} = T ∨ (∂T/∂n)^{∀t} = Q   ∀(x, y) ∈ boundary;
α = k/(ρ c_p);
Fo = α Δt/Δx^2;
t = Δt;
while t ≤ max_time do
    Assembly Temperature vector C⃗ = (T_1^{t−Δt}, T_2^{t−Δt}, ··· , T_n^{t−Δt});
    Assembly Conductivity/Temperature matrix A⃜;
    if Solver = Direct then
        Find A⃜^{−1};
        T^t = A⃜^{−1} · C⃗;
    else
        while error ≥ min_error do
            Solve linear system (e.g., Gauss-Seidel, Jacobi, SOR);
            Calculate error ‖ΔT⃗‖;
        end while
    end if
    plot(T,x, y);
    t = t + Δt;
end while
```

## Reaction kinetics

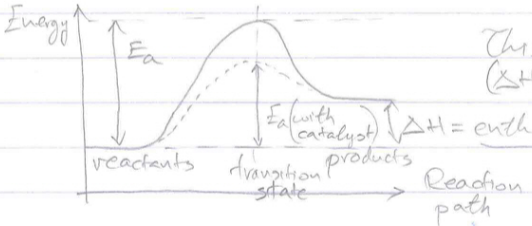
Let's start from collision theory (Wikipedia page link on Nestor) and refer to "Rates of Reaction" videos by FuseSchool (on Nestor)

Reaction rate, $v = \frac{\text{change in amount of reactants or products}}{\text{time}}$

To increase the reaction rate, you need more frequent and more successful collisions

- give particles more energy, or lower the activation energy
- increase particle speed, or increase number of particles (i.e. increase concentration)

What is activation energy? It is the minimum amount of energy that must be provided to reactants to result in a chemical reaction. $[E_a] = \frac{J}{mol}$




This is an endothermic reaction. Why? ($\Delta H > 0$)

$\Delta H$ = enthalpy of formation $\neq$ enthalpy of reaction (not exactly the same)

for compounds, this is the enthalpy change between the elements in their standard state (reactants) and the compound (product).

Arrhenius equation:

Temperature-dependence in reaction rate constant

$$\boxed{k = A e^{-E_a/RT}}$$

- $k$: rate constant
- $A$: pre-exponential factor
- $E_a$: activation energy
- $R$: universal gas constant ($R = 8{,}314.3 \frac{J}{kg\,K}$)
- $T$: absolute temp.

In general, the reaction rate obeys the following rate law:

$$\boxed{v = k\,[A]^m [B]^n \ldots}$$

$v$ = reaction rate $[v] = mol/L/s$

$[A], [B]$ = molar concentration of A or B $\frac{mol}{m^3}$

$m, n$ = partial orders of reaction

So, for a reaction $aA + bB \rightarrow cC$, $v = k\,[A]^m [B]^n$, i.e. the partial orders of reaction are not equal to the stoichiometric coefficients $(a, b, c)$ but depend on the reaction mechanism and can be determined experimentally.

However, we can relate the reaction rate to the stoichiometric coefficients for the reaction $aA + bB \rightarrow cC$ as follows:

$$\boxed{v = -\frac{1}{a}\frac{d[A]}{dt} = -\frac{1}{b}\frac{d[B]}{dt} = \frac{1}{c}\frac{d[C]}{dt}}$$

If we know the order of the reaction (see videos on Nestor), we can also write the rate law.

E.g. for a first order reaction, $\boxed{v = k[A]^1[B]^1 = k[A][B]}$

Combining the two yields: $\boxed{-\frac{1}{a}\frac{d[A]}{dt} = k[A][B]} = -\frac{1}{b}\frac{d[B]}{dt} = \frac{1}{c}\frac{d[C]}{dt}$

Note: rate law for $n^{th}$ order (elementary) reaction is $-\frac{1}{a}\frac{d[A]}{dt} = k[A]^n$

---

Ex. Let's assume that the following are first order reactions:

$$\left.\begin{array}{l} A + B \xrightarrow{k_1} AB \\ AB \xrightarrow{k_2} A + B \end{array}\right\}$$ Another way to write this system would be as $A + B \underset{k_2}{\overset{k_1}{\rightleftharpoons}} AB$

(Reversible reaction ($\rightleftharpoons$): both reactions occur simultaneously)

The reaction rates for each step are $v_1 = k_1[A][B]$ and $v_2 = k_2[AB]$, where concentrations are fcns of time.

First, we need to assemble the stoichiometric matrix where reactant stoichiometric coefficients are negative and products' are positive

$$\vec{\alpha} = \begin{array}{c} \begin{array}{ccc} A & B & AB \end{array} \\ \begin{bmatrix} -1 & -1 & 1 \\ 1 & 1 & -1 \end{bmatrix} \end{array} \begin{array}{l} \leftarrow \text{step 1} \\ \leftarrow \text{step 2} \end{array}$$

Note: $aA + bB \underset{k_2}{\overset{k_1}{\rightleftharpoons}} cAB$ in our example has $a = b = c = 1$

The rate vector is $\vec{v} = \begin{Bmatrix} v_1 \\ v_2 \end{Bmatrix} = \begin{Bmatrix} k_1[A][B] \\ k_2[AB] \end{Bmatrix}$

Then, the rate of change in the concentration of every component taking part in the reaction is:

$$\boxed{\frac{d}{dt}\vec{C}(t) = \vec{\alpha}^T \vec{v}(t)} \Rightarrow \frac{d}{dt}\underset{3\times1}{\begin{Bmatrix} [A] \\ [B] \\ [AB] \end{Bmatrix}} = \underset{3\times2}{\begin{bmatrix} -1 & 1 \\ -1 & 1 \\ 1 & -1 \end{bmatrix}} \underset{2\times1}{\begin{Bmatrix} k_1[A][B] \\ k_2[AB] \end{Bmatrix}}$$

$$\frac{d[A]}{dt} = -k_1[A][B] + k_2[AB]$$

$$\frac{d[B]}{dt} = -k_1[A][B] + k_2[AB]$$

$$\frac{d[AB]}{dt} = k_1[A][B] - k_2[AB]$$

**Example**

Do the same analysis with the following reactions...

$$2\,\mathrm{A} \underset{k_2}{\overset{k_1}{\rightleftharpoons}} 2\,\mathrm{B} + \mathrm{C}$$
$$\mathrm{A} + \mathrm{B} \underset{k_4}{\overset{k_3}{\rightleftharpoons}} 2\,\mathrm{D}$$
$$\mathrm{B} + \mathrm{D} \underset{k_6}{\overset{k_5}{\rightleftharpoons}} \mathrm{E}$$

In the solution procedure of these systems, an important concept of matrix plays an important role: the stoichoimetric matrix *rank*.

**Definition: Rank of a matrix**

The rank of a matrix is defined as the maximum number of linearly independent column vectors in the matrix, or the maximum number of linearly independent row vectors in the matrix.

Using this concept, we can reduce the number of equations to be solved in the system, rendering an easier system to model the reaction kinetics. Let's consider a different system,

$$\mathrm{A} + \mathrm{B} \underset{k_2}{\overset{k_1}{\rightleftharpoons}} \mathrm{C}$$
$$\mathrm{C} + \mathrm{C} \underset{k_4}{\overset{k_3}{\rightleftharpoons}} \mathrm{D}$$

Thus, we assembly the stoichoimetric matrix and the rate vector,

$$\frac{d}{dt}\vec{C}(t) = \begin{pmatrix} -1 & -1 & 1 & 0 \\ 1 & 1 & -1 & 0 \\ 0 & 0 & -2 & 1 \\ 0 & 0 & 2 & -1 \end{pmatrix}^T \cdot \begin{pmatrix} k_1[C]_a[C]_b \\ k_2[C]_c \\ k_3[C]_c^2 \\ k_4[C]_d \end{pmatrix} \tag{7.21}$$

If you analyze the stoichiometrix matrix in the previous equation, you will see it is not a *full rank* matrix, but one of rank 2. This means that the system can be solved using only two rows of the matrix. We will continue the analysis considering the components $C$ and $D$.

$$\frac{d[C]_c}{dt} = k_1[C]_a[C]_b - k_2[C]_c - 2k_3[C]_c^2 + 2k_4[C]_d \tag{7.22a}$$
$$\frac{d[C]_d}{dt} = k_3[C]_c^2 - k_4[C]_d \tag{7.22b}$$

Since the system has four unknowns and only two linearly independent equations, we need two more relationships to determine the system. In this case, it is necessary to find an expression to calculate the concentrations of $A$ and $B$ as a function of the components $C$ and $D$. In this case we can also use the mass balance in the equations, assuming the whole process is confined in a closed system. Then, the total mass at the beginning of the reaction will be

equal to the sum of the masses in every time step, which can be also expressed as function of concentration and molar masses. Thus,

$$\sum_i m_0^i = \sum_i m^i \tag{7.23}$$

$$\sum_i C_0^i M_{mol}^i = \sum_i C^i M_{mol}^i \tag{7.24}$$

and therefore,

$$\underline{\underline{\alpha}} \cdot \vec{M_{mol}} = \vec{0} \tag{7.25}$$

Then, applying this to the example we get,

$$\underline{\underline{\alpha}} \cdot \vec{M_{mol}} = \vec{0} \longrightarrow \begin{cases} -M_{mol,a} - M_{mol,b} + M_{mol,c} = 0 \\ -2M_{mol,c} + M_{mol,d} = 0 \end{cases} \tag{7.26}$$

Furthermore, the initial mass is equal to,

$$\sum_i m_0^i = [C]_{0,a} M_{mol,a} + [C]_{0,b} M_{mol,b} \tag{7.27}$$

and the mass after a certain period of the reaction,

$$\sum_i m^i = [C]_a M_{mol,a} + [C]_b M_{mol,b} + [C]_c M_{mol,c} + [C]_d M_{mol,d} \tag{7.28}$$

Finally, we can find a relationship between the concentration of $A$ and $B$ as a function of initial masses and the concentrations of products $C$ and $D$.

$$[C]_a = [C]_{0,a} - [C]_c - 2[C]_d \tag{7.29a}$$

$$[C]_b = [C]_{0,b} - [C]_c - 2[C]_d \tag{7.29b}$$

As it was mentioned before, these type of ODE systems have either an analytical or numerical solution. However, in chemical kinetics it is always possible to find an analytical solution if a reaction model is a linear system of first-order ODE's. A sequence of elementary first-order reaction steps is an example of such system. In order to analyze this, we will use the following example,

$$\mathrm{B} \xleftarrow{k_1} \mathrm{A} \xrightarrow{k_2} \mathrm{C} \underset{k_4}{\overset{k_3}{\rightleftharpoons}} \mathrm{D}$$

With this model, we can set up the set of differential equations corresponding to the reaction steps,

$$\frac{d}{dt}\begin{pmatrix} [C]_a(t) \\ [C]_b(t) \\ [C]_c(t) \\ [C]_d(t) \end{pmatrix} = \begin{pmatrix} -1 & 1 & 0 & 0 \\ -1 & 0 & 1 & 0 \\ 0 & 0 & -1 & 1 \\ 0 & 0 & 1 & -1 \end{pmatrix}^T \cdot \begin{pmatrix} k_1[C]_a(t) \\ k_2[C]_a(t) \\ k_3[C]_c(t) \\ k_4[C]_d(t) \end{pmatrix} \tag{7.30}$$

The first step in this technique consists in rearrange the stoichoimetric matrix and rate vector in order to leave only the concentrations in the vector. Thus,

$$\frac{d}{dt}\begin{pmatrix}[C]_a(t)\\ [C]_b(t)\\ [C]_c(t)\\ [C]_d(t)\end{pmatrix} = \begin{pmatrix}-(k_1+k_2) & 0 & 0 & 0\\ k_1 & 0 & 0 & 0\\ k_2 & 0 & -k_3 & k_4\\ 0 & 0 & k_3 & -k_4\end{pmatrix} \cdot \begin{pmatrix}[C]_a(t)\\ [C]_b(t)\\ [C]_c(t)\\ [C]_d(t)\end{pmatrix} \tag{7.31}$$

$$\frac{d}{dt}[\vec{C}](t) = \underline{\underline{k}}^v \cdot [\vec{C}](t) \tag{7.32}$$

The solution to this system of ODE's has the following form,

$$[\vec{C}](t) = e^{\left(\underline{\underline{k}}^v t\right)}[\vec{C}]_0 \tag{7.33}$$

The solution presented though it looks simple, has a major problem: how to calculate the exponent of the reaction matrix? We use for this purpose two familiar concepts: *eigenvalues* and *eigenvectors*. According to the properties of these,

$$\underline{\underline{k}}^v \cdot \vec{X}^n = \lambda^n \cdot \vec{X}^v \tag{7.34}$$

where $\lambda^n$ is the *nth* elements of the eigenvalues vector and $\vec{X}^n$ is the *nth* column of the matrix of eigenvectors. Moreover, we can replace the matrix $\underline{\underline{k}}^v$ by a system of matrices, which is known as *diagonalization* of the matrix,

**Definition: Diagonalization of a matrix**

$$A \in \mathbf{F}^{n\times n} \text{ is diagonalizable } \iff \exists P, P^{-1} \in \mathbf{F}^{n\times n} : P^{-1}AP \text{ is diagonal}$$

Applying this definition to the system we obtain,

$$e^{\left(\underline{\underline{k}}^v t\right)} = \underline{\underline{X}} \cdot e^{\left(\underline{\underline{\Lambda}} t\right)} \cdot \underline{\underline{X}}^{-1} \tag{7.35}$$

The matrix related to the reaction rates was replaced then by a system of matrices in which $\underline{\underline{X}}$ is the matrix form by the *eigenvectors* of the the original matrix and $\underline{\underline{\Lambda}}$ is a diagonal matrix whose elements are the *eigenvalues* of the original matrix. Thus,

$$e^{\left(\underline{\underline{\Lambda}} t\right)} = \begin{pmatrix} e^{\lambda_1 t} & 0 & \cdots & 0\\ 0 & e^{\lambda_2 t} & \cdots & 0\\ \vdots & \vdots & \ddots & \vdots\\ 0 & 0 & \cdots & e^{\lambda_n t}\end{pmatrix} \tag{7.36}$$

This allows transforming our system of ODE's into the following equation,

$$[\vec{C}](t) = \underline{\underline{X}} \cdot e^{\left(\underline{\underline{\Lambda}} t\right)} \cdot \underline{\underline{X}}^{-1} \cdot [\vec{C}]_0 \tag{7.37}$$

Thus, our original system of ODE's was reduced to find the *eigenvalues* and *eigenvectors*. The diagonal matrix with the *eigenvalues* is equal to,

$$\underline{\underline{\Lambda}} = \begin{pmatrix} -(k_1+k_2) & 0 & 0 & 0\\ 0 & 0 & 0 & 0\\ 0 & 0 & 0 & 0\\ 0 & 0 & 0 & -(k_3+k_4)\end{pmatrix} \tag{7.38}$$

And subsequently, the matrix of *eigenvectors* associated to these *eigenvalues* is presented hereafter. It is noteworthy that in this case special attention should be paid in order to get the *nth eigenvalue* aligned with the *nth* column of the matrix of *eigenvectors*.

$$\underline{\underline{X}} = \begin{pmatrix} (k_1+k_2)\frac{k_1+k_2-k_3-k_4}{k_2k_3} & 0 & 0 & 0 \\ -k_1\frac{k_1+k_2-k_3-k_4}{k_2k_3} & 0 & 1 & 0 \\ -\frac{k_1+k_2-k_4}{k_3} & \frac{k_4}{k_3} & 0 & -1 \\ 1 & 1 & 0 & 1 \end{pmatrix} \tag{7.39}$$

$$\underline{\underline{X}}^{-1} = \begin{pmatrix} \frac{k_2k_3}{(k_1+k_2)(k_1+k_2-k_3-k_4)} & 0 & 0 & 0 \\ \frac{k_2k_3}{(k_1+k_2)(k_3+k_4)} & 0 & \frac{k_3}{k_3+k_4} & \frac{k_3}{k_3+k_4} \\ \frac{k_1}{k_1+k_2} & 1 & 0 & 0 \\ -\frac{k_2k_3}{(k_3+k_4)(k_3+k_4)} & 0 & -\frac{k_3}{k_3+k_4} & \frac{k_4}{k_3+k_4} \end{pmatrix} \tag{7.40}$$

Therefore, the final system and analytical solution of the concentration in this multi-step reaction is as follows,

$$\begin{pmatrix} [C]_a(t) \\ [C]_b(t) \\ [C]_c(t) \\ [C]_d(t) \end{pmatrix} = \begin{pmatrix} (k_1+k_2)\frac{k_1+k_2-k_3-k_4}{k_2k_3} & 0 & 0 & 0 \\ -k_1\frac{k_1+k_2-k_3-k_4}{k_2k_3} & 0 & 1 & 0 \\ -\frac{k_1+k_2-k_4}{k_3} & \frac{k_4}{k_3} & 0 & -1 \\ 1 & 1 & 0 & 1 \end{pmatrix} \cdot \begin{pmatrix} e^{[-(k_1+k_2)]t} & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & e^{[-(k_3+k_4)]t} \end{pmatrix} \cdot$$

$$\cdot \begin{pmatrix} \frac{k_2k_3}{(k_1+k_2)(k_1+k_2-k_3-k_4)} & 0 & 0 & 0 \\ \frac{k_2k_3}{(k_1+k_2)(k_3+k_4)} & 0 & \frac{k_3}{k_3+k_4} & \frac{k_3}{k_3+k_4} \\ \frac{k_1}{k_1+k_2} & 1 & 0 & 0 \\ -\frac{k_2k_3}{(k_3+k_4)(k_3+k_4)} & 0 & -\frac{k_3}{k_3+k_4} & \frac{k_4}{k_3+k_4} \end{pmatrix} \cdot \begin{pmatrix} [C]_{0,a} \\ 0 \\ 0 \\ 0 \end{pmatrix} \tag{7.41}$$

$$[C]_a(t) = e^{-(k_1+k_2)t}[C]_{0,a} \tag{7.42a}$$

$$[C]_b(t) = \left[-k_1\frac{e^{-(k_1+k_2)t}}{k_1+k_2} + \frac{k_1}{k_1+k_2}\right][C]_{0,a} \tag{7.42b}$$

$$\begin{aligned} [C]_c(t) = \Bigg[(k_4-k_1-k_2)\frac{e^{-(k_1+k_2)t}}{(k_1+k_2)(k_1+k_2-k_3-k_4)}k_2 + \frac{k_2k_4}{(k_1+k_2)(k_3+k_4)} + ... \\ e^{-(k_3+k_4)t}\frac{k_2k_3}{(k_3+k_4)(k_1+k_2-k_3-k_4)}\Bigg][C]_{0,a} \end{aligned} \tag{7.42c}$$

$$\begin{aligned} [C]_d(t) = \Bigg[e^{-(k_1+k_2)t}\frac{k_2k_3}{(k_1+k_2)(k_1+k_2-k_3-k_4)} + \frac{k_2k_3}{(k_1+k_2)(k_3+k_4)} - ... \\ e^{-(k_3+k_4)t}\frac{k_2k_3}{(k_3+k_4)(k_1+k_2-k_3-k_4)}\Bigg][C]_{0,a} \end{aligned} \tag{7.42d}$$

**Example**

Plot the behavior of the analyzed multi-step reaction using the following values (until you observe a steady-state system): $k_1 = 0.5[s^{-1}], k_2 = 0.25[s^{-1}], k_3 = 1[s^{-1}], k_4 = 2[s^{-1}]$ and $[C]_{0,a} = 1[mol/m^3]$

(Source: Wiki)

Aside: how does this all come together?

Diffusion-controlled reactions

"The process of chemical reaction can be considered as involving the diffusion of reactants until they encounter each other in the right stoichiometry and form an activated complex which can form the product species. The observed rate of chemical reactions is, generally speaking, the rate of the slowest or "rate determining" step. In diffusion-controlled reactions, the formation of products from the activated complex (ref. intermediate state) is much faster than the diffusion of reactants and thus the rate is controlled by collision frequency (the rate of collisions between two atomic or molecular species in a given volume, per unit time).

Diffusion control is more likely in solution: examples include catalysis and enzymatic reactions.

Is the rate of a reaction affected by stirring or agitation? Then, the reaction is almost certainly diffusion-controlled.

E.g. for the reaction $A + B \longrightarrow C$, via Fick's law:

$$k = \frac{4\pi D_{AB} \beta k_r}{k_r + 4\pi D_{AB} \beta \exp\left(\frac{U(AB)}{k_B T}\right)}$$

$k_r$ = inherent reaction const.
$D_{AB}$ = diffusion coefficient
$U(AB)$ = chemical potential
$k_B$ = Boltzmann constant
$T$ = absolute temperature
$\beta^{-1} = \int_{R_{AB}}^{\infty} \frac{1}{r^2} \exp\left(\frac{U(r)}{k_B T}\right) dr$
$R_{AB}$ = distance between molecules A and B
$r$ = distance

# 8 Bibliography

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# Appendices

# A Discretization

In this Appendix, we give an introduction to some discretization methods. We start by highlighting why discretization is relevant for many engineering problems, and discuss some basic properties. Then, the concept of the *mesh* is introduced, and we discuss how it is applied to discretize different types of problems, including different formulations of the *finite difference method*.

## A.1 Why discretization?

As you will have seen by now, many problems in engineering cannot be solved analytically. Especially problems involving Navier-Stokes, diffusion and waves are difficult to solve in multiple dimensions or with coupled physics as these are typically PDEs. Analytical solutions are often only obtainable if one reduces the problem using restrictive assumptions, thereby often rendering the problem devoid of practical interest.

When we are interested in the behavior of a physical system of which the behavior is dependent on space and time and need to solve it numerically, we employ discretization. In essence we are decomposing a continuous set of equations describing this system into discrete elements which can be evaluated using a numerical scheme. By calculating these elements in time and space we can then evaluate system behavior, whether that be steady state or its dynamics.

Various discretization methods exist. In this appendix we will limit the discussion to the discretization of a partial differential equation using the finite difference method. The origin of this method can be found in the early works of the mathematicians Euler and Kutta, and is similar to the Runge-Kutta family of numerical methods employed in solving ODEs. For PDEs, the finite difference methods consist in approximating the differential operator in an equation using differential quotients to replace the derivatives in the equation. By doing so we are partitioning the domain in space and time. The difference between the differential operator and differential quotient is a measure for the error of the numerical solution compared to the analytical solution; this is often known as the *truncation error*.

In essence, Figure Figure A.1 describes the workflow of discretizing a PDE using the finite difference method.

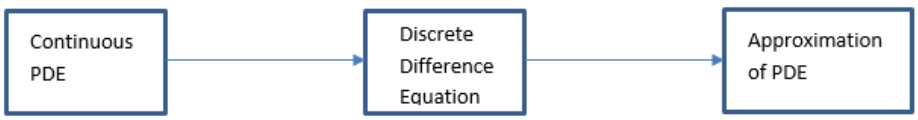


Figure A.1: General workflow of discretization methods

**Example**

Suppose we wish to approximate $u$ at a point $x$. Assuming $u(x)$ is a smooth differentiable function, we can assess the derivative of $u$ around $x$ for step size $h$ as follows:

$$\frac{\partial u}{\partial x} = \lim_{h \to 0} \frac{u(x+h) - u(x)}{h}. \tag{A.1}$$

As one would expect, as $h$ becomes smaller the approximation on the right hand side of the equation becomes more accurate. Equation A.1 illustrates the basic concept behind the finite difference schemes, which we shall further explain later.

## A.2 Generating the mesh

Discretizing the domain means we will end up with a series of points in space and time which are evenly spaced. Suppose we are interested in the temperature distribution over time in a rod along its length $L$, which we shall call the $x$-direction, then we would obtain the following:

$$0 \leq x \leq L \tag{A.2}$$

$$x_i = (i-1)\Delta x \qquad \text{for } i = 1, 2, \cdots, N, \tag{A.3}$$

where $n$ represents the amount of grid points. Based on $L$ and $N$, we can then determine $\Delta x$:

$$\Delta x = \frac{L}{N-1}. \tag{A.4}$$

Similar equations hold for discretizing time:

$$0 \leq t \leq t_{\text{final}} \tag{A.5}$$

$$t_k = (k-1)\Delta t \qquad \text{for } k = 1, 2, \cdots, K, \tag{A.6}$$

where $K$ denotes the number of time steps, and $\Delta t$ refers to the size of the time step given by

$$\Delta t = \frac{t_{\text{final}}}{K-1}. \tag{A.7}$$

The above can be visualized in a grid known as a mesh, as shown in Figure A.2. In this figure, the horizontal axis represents the $x$-direction of the rod (along its length $L$), and the vertical axis represents steps through time. For each time step, we calculate all grid points $i$. In other words, at $t = 0$, we start in the bottom left corner and initialize the solution vector with the green rectangles, as these should be known, because we need to start at some determined value (*initial value*). Now, we move to the second row and start calculating the

blue grid points based on the finite different scheme; row $k$ is assessed using row $k-1$. As calculation of a grid point often depends on its neighbors in the $x$-direction in the previous time step, we need to specify the values at the boundaries of the mesh. These are called the *boundary conditions* (indicated by the red rectangles), and need to be specified at both $x = 0$ and $x = L$, for each time $t > 0$.

## A.3 First order forward difference

In this section we will cover the first order forward difference scheme, which is derived from a Taylor series expansion $u(x)$ around a point $x_i$:

$$\left.\frac{\partial u}{\partial x}\right|_{x_i} \approx \frac{u_{i+1} - u_i}{\Delta x} - \frac{\Delta x}{2}\left.\frac{\partial^2 u}{\partial x^2}\right|_{x_i} - \frac{\Delta x^2}{3!}\left.\frac{\partial^3 u}{\partial x^3}\right|_{x_i} + \cdots . \tag{A.8}$$

Replacing the higher order terms using the mean value theorem, we obtain the following:

$$\left.\frac{\partial u}{\partial x}\right|_{x_i} \approx \frac{u_{i+1} - u_i}{\Delta x} + \frac{\Delta x^2}{2}\left.\frac{\partial^2 u}{\partial x^2}\right|_{\epsilon}, \tag{A.9}$$

where the terms to the right of the difference in $u$ over $\Delta x$ in Equation A.9 represent the *truncation error*, which results from truncating (cutting off, or neglecting) the higher order terms in Equation A.8. In general, we de not know what $\epsilon$ is and also cannot compute the second order term of $u$ with respect to $x$ as the function $u(x,t)$ is not known. To deal with

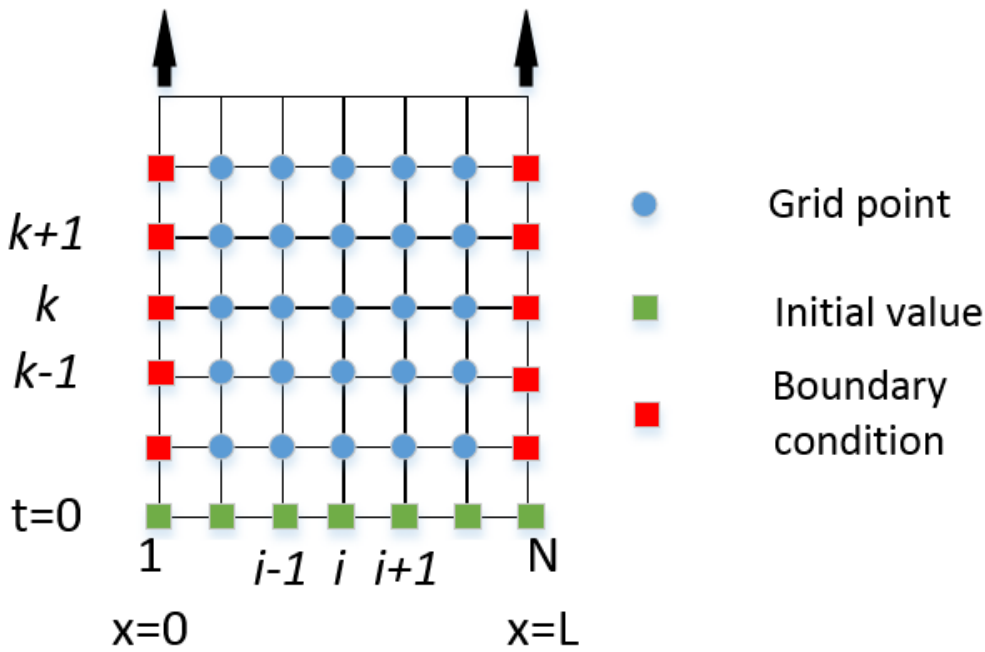


Figure A.2: Mesh of the heat equation example

the truncation error, the term $\mathcal{O}(\Delta x^2)$ is often used. The $\mathcal{O}$ represents the dependence of the truncation error on the mesh, which we determine prior to simulation:

$$\frac{\Delta x^2}{2} \left.\frac{\partial^2 u}{\partial x^2}\right|_{\epsilon} = \mathcal{O}(\Delta x^2). \tag{A.10}$$

Rewriting Equation A.9 then yields

**Definition: First order backward difference equation**

$$\left.\frac{\partial u}{\partial x}\right|_{x_i} = \frac{u_{i+1} - u_i}{\Delta x} + \mathcal{O}(\Delta x). \tag{A.11}$$

Note that $\Delta x^2$ was replaced with $\Delta x$ as the right hand side of Equation A.10 is not meant as a strict equality; it shows the dependence of the order of magnitude of the error, and how is approaches zero as function of the meshing.

Equation A.11 is called the forward difference equation because it utilizes the nodes $i$ and $i + 1$.

## A.4 First order backward difference

If we replace the use of $\Delta x$ in Equation A.8 with $-\Delta x$, then we obtain the backward difference equation:

$$\left.\frac{\partial u}{\partial x}\right|_{x_i} \approx \frac{u_i - u_i - 1}{\Delta x} + \frac{\Delta x}{2} \left.\frac{\partial^2 u}{\partial x^2}\right|_{x_i} - \frac{\Delta x^2}{3!} \left.\frac{\partial^3 u}{\partial x^3}\right|_{x_i} + \cdots . \tag{A.12}$$

$$u_{i-1} = u_i - \Delta x \left.\frac{\partial u}{\partial x}\right|_{x_i} + \frac{\Delta x^2}{2} \left.\frac{\partial^2 u}{\partial x^2}\right|_{x_i} - \frac{(\Delta x)^3}{3!} \left.\frac{\partial^3 u}{\partial x^3}\right|_{x_i} + \cdots . \tag{A.13}$$

Again, truncating the higher order terms and using $\mathcal{O}$ notation, we obtain

**Definition: First order backward difference equation**

$$\left.\frac{\partial u}{\partial x}\right|_{x_i} = \frac{u_i - u_i - 1}{\Delta x} + \mathcal{O}(\Delta x), \tag{A.14}$$

where we can see why it is called the backward difference, as it depends on evaluating nodes $i$ and $i - 1$. Note that the truncation error for both the forward and backward difference equation is the same.

## A.5 First order central difference

The central difference equation is actually a combination of both the forward and backward difference equations.The main idea is to reduce the truncation error; in the central difference equation, this error approaches zero much faster as we decrease $\Delta x$, as we will show below.

First, recall the Taylor series expansions for $u_{i+1}$ and $u_{i-1}$:

$$u_{i+1} = u_i + \Delta x \left.\frac{\partial u}{\partial x}\right|_{x_i} + \frac{\Delta x^2}{2} \left.\frac{\partial^2 u}{\partial x^2}\right|_{x_i} + \frac{(\Delta x)^3}{3!} \left.\frac{\partial^3 u}{\partial x^3}\right|_{x_i} + \cdots , \tag{A.15}$$

$$u_{i-1} = u_i - \Delta x \left.\frac{\partial u}{\partial x}\right|_{x_i} + \frac{\Delta x^2}{2} \left.\frac{\partial^2 u}{\partial x^2}\right|_{x_i} - \frac{(\Delta x)^3}{3!} \left.\frac{\partial^3 u}{\partial x^3}\right|_{x_i} + \cdots . \tag{A.16}$$

Subtracting Equation A.15 from A.16 yields

$$u_{i+1} - u_{i-1} = 2\Delta x \left.\frac{\partial u}{\partial x}\right|_{x_i} + \frac{2(\Delta x)^3}{3!} \left.\frac{\partial^3 u}{\partial x^3}\right|_{x_i} + \cdots . \tag{A.17}$$

If we solve for $\left.\frac{\partial u}{\partial x}\right|_{x_i}$, we get

$$\left.\frac{\partial u}{\partial x}\right|_{x_i} = \frac{u_{i+1} - u_{i-1}}{2\Delta x} - \frac{(\Delta x)^3}{3!} \left.\frac{\partial^3 u}{\partial x^3}\right|_{x_i} + \cdots , \tag{A.18}$$

which, with the $\mathcal{O}$ notation, leads to the central difference equation:

**Definition: First order central difference equation**

$$\left.\frac{\partial u}{\partial x}\right|_{x_i} = \frac{u_{i+1} - u_{i-1}}{2\Delta x} + \mathcal{O}(\Delta x^2). \tag{A.19}$$

As you can see, the truncation error will approach zero much faster than for the forward and back equations, Equation A.11 and A.14, respectively. However, there is a disadvantage to the first order central differenc equation, as it does not contain the grid point $i$. Depending on the problem, this might cause complications, but further discussion is beyond the scope of this introductory document.

## A.6 Second order central difference

Similar to the first order central difference, the second order central difference equation involves Equation A.15 and A.16 with the appropriate Taylor expansion. Contrary to the first order difference equation, we are now interested in estimating the *second order* derivative of the function. To this end, we write both Taylor expansions up to fourth order:

$$u_{i+1} = u_i + \Delta x \left.\frac{\partial u}{\partial x}\right|_{x_i} + \frac{\Delta x^2}{2} \left.\frac{\partial^2 u}{\partial x^2}\right|_{x_i} + \frac{(\Delta x)^3}{3!} \left.\frac{\partial^3 u}{\partial x^3}\right|_{x_i} + \frac{\Delta x^4}{4!} \left.\frac{\partial^4 u}{\partial x^4}\right|_{x_i} + \cdots , \tag{A.20}$$

$$u_{i-1} = u_i - \Delta x \left.\frac{\partial u}{\partial x}\right|_{x_i} + \frac{\Delta x^2}{2} \left.\frac{\partial^2 u}{\partial x^2}\right|_{x_i} - \frac{\Delta x^3}{3!} \left.\frac{\partial^3 u}{\partial x^3}\right|_{x_i} + \frac{\Delta x^4}{4!} \left.\frac{\partial^4 u}{\partial x^4}\right|_{x_i} + \cdots . \tag{A.21}$$

Instead of subtracting the two Taylor series from each other, we add them together, resulting in the following expression:

$$u_{i+1} + u_{i-1} = 2u_i + \Delta x^2 \left.\frac{\partial^2 u}{\partial x^2}\right|_{x_i} + \frac{\Delta x^4}{4!} \left.\frac{\partial^4 u}{\partial x^4}\right|_{x_i} + \cdots . \tag{A.22}$$

Rearranging yields

$$\left.\frac{\partial^2 u}{\partial x^2}\right|_{x_i} = \frac{u_{i+1} - 2u_i + u_{i-1}}{\Delta x^2} - \frac{\Delta x^2}{4!} \left.\frac{\partial^4 u}{\partial x^4}\right|_{x_i} + \cdots . \tag{A.23}$$

We can see that, after rearranging, the first error term in Equation A.23 contains $\Delta x^2$. Hence, we conclude that the second order central difference equation has error $\mathcal{O}(\Delta x^2)$, so we can write

**Definition: Second order central difference equation**

$$\left.\frac{\partial^2 u}{\partial x^2}\right|_{x_i} = \frac{u_{i+1} - 2u_i + u_{i-1}}{\Delta x^2} + \mathcal{O}(\Delta x^2). \tag{A.24}$$

## A.7 Conclusion

The difference equations discussed in this Appendix form the basics of many widely used numerical methods. Throughout this course, we apply both the first and second order difference equations, for example to approximate PDEs in heat diffusion problems.

To summarize, the derivation of all finite difference equations in this Appendix have followed the same procedure. First, derive the appropriate Taylor Expansion(s), depending on the order of the equation you want to estimate. Then, rewrite and solve for the PDE that you're estimating. Finally, determine the most dominant error term, containing the time step variable, $\Delta x^n$, and denote the order of the method as $\mathcal{O}(\Delta x^n)$. More information

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