## APPLICATIONS OF MATHEMATICS

## IN ENGINEERING AND SCIENCE

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## Static analysis of a 3-bar truss structure

Keywords: Mechanics, static analysis, solution of linear equations.

Truss structures are commonly used in structural engineering and architecture due to their superior stiffness and strength for a given amount of material. A truss structure that consists of straight members connected by means of pin joints, and supported at both ends by means of hinged joints or rollers, such that they cannot transfer moments, is described as being statically determinate. Thus, loading subjected to a truss structure results in either tensile or compressive forces in the members, together with reaction forces at the supports. Examples of truss structures are seen in Figure 1 which illustrates the supporting truss structure for the roof in Hamburg Airport.


Figure 1: Truss structure support of roof in Hamburg Airport.

In the following a small illustrative example of a 3-bar planar truss defined by Figure 2 is treated where the static equilibrium equations are set up using free body diagrams. This approach is possible because the structure is statically determined. The 3-bar truss is subjected to a vertical load $F$ of value 1000 N in node 1 and a static analysis of the structure can determine the unknown internal bar forces $\left(N_{12}, N_{13}, N_{23}\right)$ and reaction forces $\left(R_{2 x}, R_{2 y}, R_{3 y}\right)$. Internal bar forces in tension are considered positive.

The static equilibrium equations express the fact that the sum of the $x$ - and $y$-components of the forces at each of the three joints must be equal to zero. Thus, the governing equations are:

$$
\begin{array}{ll}
x \text {-components of forces at joint 1: } & \sum F_{x}=0: \\
y \text {-components of forces at joint 1 }: \sum F_{y}=0: & -\cos \alpha N_{12}+\cos \beta N_{13}=0 \\
x \text {-components of forces at joint 2: } \sum \sum F_{x}=0: & \cos \alpha N_{12}+\sin \beta N_{13}-1000=0 \\
y \text {-components of forces at joint 2: } 2 F_{2 x}=0: & \sin \alpha N_{12}+R_{2 y}=0 \\
x \text {-components of forces at joint 3: } 3 F_{x}=0: & -N_{23}-\cos \beta N_{13}=0 \\
y \text {-components of forces at joint 3: } \sum \sum F_{y}=0: & \sin \beta N_{13}+R_{3 y}=0
\end{array}
$$



Figure 2: A 3-bar truss with internal and external forces.

This is a linear system of equations with 6 unknowns, and it can be written in matrix form as

$$
\left[\begin{array}{cccccc}
-\cos \alpha & 0 & \cos \beta & 0 & 0 & 0 \\
-\sin \alpha & 0 & -\sin \beta & 0 & 0 & 0 \\
\cos \alpha & 1 & 0 & 1 & 0 & 0 \\
\sin \alpha & 0 & 0 & 0 & 1 & 0 \\
0 & -1 & -\cos \beta & 0 & 0 & 0 \\
0 & 0 & \sin \beta & 0 & 0 & 1
\end{array}\right]\left[\begin{array}{l}
N_{12} \\
N_{23} \\
N_{13} \\
R_{2 x} \\
R_{2 y} \\
R_{3 y}
\end{array}\right]=\left[\begin{array}{c}
0 \\
1000 \\
0 \\
0 \\
0 \\
0
\end{array}\right]
$$

A Matlab program TrussExample.m for the solution of the 3-bar truss example is given below:

```
% File TrussExample.m for the solution of 3-bar truss problem
% Solves the system of equations AX = B, where
% X is a column vector of unknown forces, of the form
%
% X [N_12 N_23 N_13 R_2x R_2y R_3y]'
sin_a = 4/5;
cos_a = 3/5;
sin_b = 3/5;
cos_b = 4/5;
% Coefficient matrix
A = [ -cos_a 0 cos_b 0 0 0
    -sin_a 0 -sin_b 0 0 0
        cos_a 1 0 1 0 0
        sin_a 0 0 0 1 0
            0
            0 0 sin_b 0 0 1 ];
% Right-hand side, external forces
B = [0 1000 0 0 0 0]';
% Solve for the unknown forces
X = A\B; % Use Matlab's built-in slash operator for solving the system of equations
% Display the results in a nice format
disp('Solution:')
disp(' N_l2 N_23 N_l3 R_2x R_2y R_3y') % display labels
disp(X') % Display the transpose of X
```

Running the Matlab program, the following result is obtained:

```
Solution:
    N_l2 
```

The above approach is applicable to statically determined structures. Stresses in the bars can be computed based on the bar forces divided by cross sectional areas, and knowing the allowable stresses for the materials used, it is possible to choose appropriate cross sectional areas of the bars. In general, structural analysis of trusses of any type can be carried out using a matrix method such as the direct stiffness method, the flexibility method or the finite element method. The use of a matrix based approach as illustrated above makes it possible to treat systems with many variables in a general, structured way.

## Further reading:

Brockman, J.B.: "Introduction to Engineering: Modeling and Problem Solving", John Wiley \& Sons, ISBN 978-0-471-43160-2, 2009, pp. 484-487. The book gives an introduction to modeling in engineering, and many of the problems considered are solved using Matlab.
Analysis of mechanical structures like truss structures are covered by very many text books.

## Steady-state heat conduction

Keywords: Thermal problems, steady state analysis, governing equations, linear second order partial differential equations, Gauss' divergence theorem.

In physics, a conservation law states that a particular measurable property of an isolated physical system does not change as the system evolves. Such a conservation law/continuity equation is a differential equation that describes the transport of some kind of conserved quantity. Since mass, energy, momentum, electric charge and other natural quantities are conserved, a vast variety of physics may be described with continuity equations.

In the following the derivation of a conservation law will be illustrated for heat conduction problems where the objective is to find a steady-state temperature distribution in a given domain, for example in a pump housing as illustrated by Figure 3.


Figure 3: Example of temperature distribution in pump housing.
The general heat equation is derived from Fourier's law and conservation of energy. Fourier's law states that the flow rate of heat energy is proportional to the negative temperature gradient across the surface, i.e. for 1D problems

$$
\begin{equation*}
q_{x}=-k_{c} \frac{d T}{d x} \tag{1}
\end{equation*}
$$

and for general 3D problems

$$
\mathbf{q}=-k_{c} \nabla T, \quad \text { or } \quad\left[\begin{array}{c}
q_{x}  \tag{2}\\
q_{y} \\
q_{z}
\end{array}\right]=-k_{c}\left[\begin{array}{c}
\frac{\partial I}{\partial x} \\
\frac{\partial T}{\partial y} \\
\frac{\partial T}{\partial z}
\end{array}\right]
$$

Here $\mathbf{q}$ is the heat flow vector, $k_{c}$ is the thermal conductivity of the material and $T$ is the temperature. The component of the heat flow vector in the $x$-direction is named $q_{x}$, and similarly in the two other directions. In some text books you will find the notation $\operatorname{grad} T$ instead of $\nabla T$ for the temperature gradient vector. Boldface notation is used here, i.e. the vector $\vec{q}$ is written as $\mathbf{q}$.

Next we study the flux of the vector field $\mathbf{q}$. Consider the closed surface $S$ that defines the volume $V$ in Figure 4. The unit vector $\mathbf{n}$ is the outward normal to the surface element $d A$ and $\mathbf{q}$ is the heat flow vector at the surface element.

The heat flow through the surface element $d A$ is the area times the component of $\mathbf{q}$ perpendicular to $d A$. This component $q_{n}$ is given by the following dot product

$$
\begin{equation*}
q_{n}=\mathbf{q} \cdot \mathbf{n} \tag{3}
\end{equation*}
$$



Figure 4: Closed surface $S$ that defines the volume $V . \mathrm{q}$ is the heat flow vector at the surface element.

The heat flow out through $d A$ is $\mathbf{q} \cdot \mathbf{n} d A$. If we integrate over the whole surface $\mathbf{S}$, we obtain the flux:

$$
\begin{equation*}
\text { Total heat flow outward through } S=\text { Flux of } \mathbf{q} \text { through surface } S=\int_{S} \mathbf{q} \cdot \mathbf{n} d A \tag{4}
\end{equation*}
$$

In case of a situation where some material has been heated and no further heat energy is generated or absorbed, the conservation of heat yields

$$
\begin{equation*}
\int_{S} \mathbf{q} \cdot \mathbf{n} d A=-\frac{d Q}{d t} \tag{5}
\end{equation*}
$$

where $Q$ is the heat inside the body.
Consider in Figure 5 the small cube of dimensions $d x \times d y \times d z$ and center point with coordinates $(x, y, z)$. We want to find the flux of the vector field $\mathbf{q}$ through the surface of the cube. First consider the two faces 1 and 2 used for describing the flux through the volume in the $x$-direction.


Figure 5: Heat flow through cube of dimensions $d x \times d y \times d z$ and center point with coordinates $(x, y, z)$.

The flux outward of face 1 , which has its normal in the negative $x$-direction, is given as

$$
\begin{equation*}
-\int\left(q_{x}-\frac{\partial q_{x}}{\partial x} \frac{d x}{2}\right) d y d z \tag{6}
\end{equation*}
$$

Similarly, the flux outward of face 2 , which has its normal in the $x$-direction, is given as

$$
\begin{equation*}
\int\left(q_{x}+\frac{\partial q_{x}}{\partial x} \frac{d x}{2}\right) d y d z \tag{7}
\end{equation*}
$$

Summing the fluxes in the $x$-direction we obtain

$$
\begin{equation*}
\int\left(q_{x}+\frac{\partial q_{x}}{\partial x} \frac{d x}{2}-\left(q_{x}-\frac{\partial q_{x}}{\partial x} \frac{d x}{2}\right)\right) d y d z=\int \frac{\partial q_{x}}{\partial x} d x d y d z \tag{8}
\end{equation*}
$$

Similar summing of fluxes is done in $y$ - and $z$-directions. The total flux through all faces is the sum of the terms, and we obtain

$$
\begin{equation*}
\int_{S, \text { cube }} \mathbf{q} \cdot \mathbf{n} d A=\int_{V, \text { cube }}\left(\frac{\partial q_{x}}{\partial x}+\frac{\partial q_{y}}{\partial y}+\frac{\partial q_{z}}{\partial z}\right) d V \tag{9}
\end{equation*}
$$

The sum of the derivatives is defined as the divergence of $\mathbf{q}$. This is written as $\nabla \cdot \mathbf{q}$ or div $\mathbf{q}$. We now have a connection between the divergence of $q$ and the flux of $q$ out of the volume. This relation is called Gauss' divergence theorem and states, that the integral of the normal component of any vector over any closed surface can also be written as the integral of the divergence of the vector over the volume enclosed by the surface:

$$
\begin{equation*}
\int_{S} \mathbf{q} \cdot \mathbf{n} d A=\int_{V} \nabla \cdot \mathbf{q} d V \tag{10}
\end{equation*}
$$

Inserting the definition of the heat flow vector $\mathbf{q}$ from Fourier's law, see Equation2, and considering the steady state situation, where the flux out of the volume of material is zero (conservation of energy, i.e., $d Q / d t=0$ ), the governing conservation equation (in integral form) is

$$
\begin{equation*}
\int_{V} k_{c} \nabla \cdot \nabla T d V=0, \text { i.e. } \int_{V} k_{c}\left(\frac{\partial^{2} T}{\partial x^{2}}+\frac{\partial^{2} T}{\partial y^{2}}+\frac{\partial^{2} T}{\partial z^{2}}\right) d V=0 \tag{11}
\end{equation*}
$$

This is valid for any volume, and by shrinking the size of the cube we thus also have the following governing equation in differential (strong) form:

$$
\begin{equation*}
\frac{\partial^{2} T}{\partial x^{2}}+\frac{\partial^{2} T}{\partial y^{2}}+\frac{\partial^{2} T}{\partial z^{2}}=0 \tag{12}
\end{equation*}
$$

The governing PDE just derived is the so-called Laplace equation, also called the diffusion equation, and it represents a conservation law valid for the steady-state distribution of any quantity where the rate of flow is proportional to the gradient.

Thus, any conservation law/continuity equation can be expressed in an "integral form" (in terms of a flux integral), which applies to any finite region, or in a "differential form" (in terms of the divergence operator) which applies at a point.

## Further reading:

Feynman, R.; Leighton, R.; Sands, M.: "The Feynman Lectures on Physics (3 volumes set), 1964, 1966. ISBN 0-8053-9045-6 (2006, the definitive edition (2nd printing)), Volume 2, Chapter 3.

## The Euler Column

Keywords: Statics, Euler column, Bernoulli Euler beam, buckling, ordinary second order linear differential equations, eigenvalues, eigenfunctions.

In Engineering, columns are structural members that are sensitive to buckling, when compressive axial loads are applied, see Figure 1. A column is actually a beam loaded with a compressive force. The so-called buckling load gives the load bearing capacity for relatively slender columns where buckling occurs before yielding (material failure). For buckling analysis, a so-called second order theory is applied in the deformed state.


Figure 6: At left is shown a column in a real life structure and at right the corresponding static model.

An initial straight beam with length, $L$, is loaded with a compressive axial force, $P$, see Figure 1. The beam is simply supported, thus boundary conditions are specified so that it is fixed in one end but allowed to deform axially in the other end. In both ends it is allowed to rotate (the symbols in Figure 1 define this). The buckling load is obtained by analyzing if a state of equilibrium can exist in a deformed state. The transverse deformation at position $x$ is denoted $v(x)$, see Figure 2. By cutting the beam (column) into two, adding the so-called section forces and stating that one of the two parts of the beam should be in equilibrium, moment equilibrium gives:

$$
\begin{equation*}
M(x)=-P v(x) \tag{13}
\end{equation*}
$$

By assuming linear elasticity, the bending moment, $M$, can be related to the curvature of the beam, $\kappa$, by the bending stiffness, $E I$. Furthermore, by assuming Bernoulli-Euler beam theory the curvature can be approximated by the second order derivative of the transverse displacement, $v$ :

$$
\begin{equation*}
M(x)=E I \kappa(x) \quad, \quad \kappa(x)=\frac{d^{2} v(x)}{d x^{2}} \tag{14}
\end{equation*}
$$



Figure 7: At left is shown the column in the deformed state and at right equilibrium is applied on one part of the column by adding section forces.

By combining the relations above, the following ordinary linear second order homogeneous differential equation is obtained (the constant $\alpha^{2}$ is selected in order to ensure a positive coefficient):

$$
\begin{equation*}
\frac{d^{2} v(x)}{d x^{2}}+\alpha^{2} v(x)=0 \quad, \quad \alpha^{2}=\frac{P}{E I} \tag{15}
\end{equation*}
$$

The form of the differential equation suggests an eigenvalue problem. The differential equation can be solved for the eigenvalues and eigenfunctions by applying a solution on the form $e^{r x}$ resulting in:

$$
\begin{equation*}
v(x)=e^{r x} \quad, \quad \frac{d v(x)}{d x}=r e^{r x} \quad, \quad \frac{d^{2} v(x)}{d x^{2}}=r^{2} e^{r x} \tag{16}
\end{equation*}
$$

By inserting this in the differential equation one obtains:

$$
\begin{align*}
& r^{2} e^{r x}+\alpha^{2} e^{r x}=0 \\
& \Downarrow  \tag{17}\\
& r^{2}+\alpha^{2}=0
\end{align*}
$$

Two complex roots $r_{1}=-\alpha i$ and $r_{2}=\alpha i$ exist corresponding to the linear independent solutions $e^{-\alpha i x}$ and $e^{\alpha i x}$ and the corresponding real independent solutions are $\sin \alpha x$ and $\cos \alpha x$. The complete solution is then:

$$
\begin{equation*}
v(x)=c_{1} \sin \alpha x+c_{2} \cos \alpha x \tag{18}
\end{equation*}
$$

The condition that the column does not deform transversely at the ends can be used as boundary conditions to obtain the constants $c_{1}$ and $c_{2}$ :

$$
\begin{array}{lll}
v(0)=0 & \Rightarrow \quad c_{2}=0 \\
v(L)=0 & \Rightarrow \quad c_{1}=0 \quad \vee \quad \sin \alpha L=0 \tag{19}
\end{array}
$$

The only non-trivial solution exists for:

$$
\begin{equation*}
\sin \alpha L=0 \quad \Rightarrow \alpha L=\frac{n \pi}{L} \quad, \quad n=1,2, \ldots \tag{20}
\end{equation*}
$$

By inserting this into the definition of $\alpha$, one obtains the eigenvalues:

$$
\begin{equation*}
P_{n}=n^{2} \pi^{2} \frac{E I}{L^{2}} \quad, \quad n=1,2, \ldots \tag{21}
\end{equation*}
$$

Corresponding to eigenfunctions giving the transverse deformation:

$$
\begin{equation*}
v_{n}(x)=c_{1} \sin \frac{n \pi x}{L} \quad, \quad n=1,2, \ldots \tag{22}
\end{equation*}
$$

The $P_{n}$ are so-called critical loads where a state of equilibrium can exist in the deformed state found before. It can be observed that only the form of $v_{n}(x)$ can be determined, as the constant $c_{1}$ can



Figure 8: At left is shown the critical loads as function of maximum transverse displacement and at right the corresponding deformation shapes.
not be determined, see Figure 3. Thus, the deformation can be arbitrary large and the column will buckle in practice. In reality the column will buckle when $P_{1}$ is reached, which is termed the Euler critical load given by:

$$
\begin{equation*}
P_{e}=P_{1}=\pi^{2} \frac{E I}{L^{2}} \tag{23}
\end{equation*}
$$

When the load is applied gradually, the column will remain straight until the Euler load, $P_{e}$, is reached and the column will buckle (fail) and the deformation becomes infinite. Higher critical loads can be of practical relevance by constraining the transverse deformation of the column. E.g. if the column is supported in the transverse direction at the middle, $x=L / 2$, it will buckle for the load $P_{2}$. In reality a column is not perfect straight and for many practical applications a transverse load is applied, e.g. wind loading on the facade of a building. In these cases it turns out that equilibrium is governed by an inhomogeneous linear second order differential equation.

To summarize, equilibrium of a beam/column loaded in axial compression is governed by an ordinary homogeneous second order differential equation. The solution in terms of eigenvalues and eigenfunctions is an infinite number of buckling loads and corresponding deformed shapes. In the case of a simply supported column, only the lowest buckling load is of practical relevance.

## Further reading:

Williams, M.S.; Todd, J.D.: "Structures, theory and analysis", Palgrave Macmilan, ISBN 0-333-67760-9, 2000.

## Vibrations in $\mathrm{CO}_{2}$ molecules: coupled oscillators

Keywords: Coupled oscillations, eigenvalue problems, eigenmodes.

The vibrations in molecules are very important fingerprints that allow you to identify the contents of various liquids and gases using spectroscopy. They show up because electromagnetic radiation ("light") is absorbed when the oscillation frequency of the radiation matches that of the molecular vibration. Such vibrational resonances are typically found in the infrared part of the electromagnetic spectrum. Hence, as an example, radiation is absorbed in the earth's atmosphere at characteristic frequencies determined by the molecules found in the atmosphere. These are mainly water molecules $\mathrm{H}_{2} \mathrm{O}$ but also carbon dioxide $\mathrm{CO}_{2}$ contributes to the absorption. In fact, the absorption is precisely what is thought to be responsible for the global warming following increased concentrations of $\mathrm{CO}_{2}$.

In this brief note, we show how the characteristic vibration frequencies are calculated from a matrix eigenvalue problem. We consider the slightly more general molecule in the figure below. Here, three masses are connected via two springs. The masses are denoted $m_{1}, m_{2}$ and $m_{3}$ and the two springs are assumed identical with spring constants $k$.


To describe the vibrational motion, we now set up Newton's second law for each mass. We only consider motion along the $x$-axis that describes so-called stretch vibrations. The displacement of a mass from the equilibrium position is denoted $x_{i}$ with $i=1,2$ or 3 . The spring force depends on the relative displacements. Hence, if $x_{2}$ is larger than $x_{1}$ the force on $m_{1}$ points to the right, i.e. is positive with our choice of coordinate system. Generally, the force acting on $m_{1}$ can be written as $-k\left(x_{1}-x_{2}\right)$. Using similar arguments, we find that the equations of motion for the three masses are

$$
\begin{aligned}
& m_{1} \ddot{x}_{1}=-k\left(x_{1}-x_{2}\right) \\
& m_{2} \ddot{x}_{2}=-k\left(x_{2}-x_{1}\right)-k\left(x_{2}-x_{3}\right) \\
& m_{3} \ddot{x}_{3}=-k\left(x_{3}-x_{2}\right) .
\end{aligned}
$$

Here, the double over-dots mean the second time-derivative, i.e. the acceleration. We now look for characteristic vibrations called normal modes. A normal mode is found when all masses oscillate with a common frequency. Thus, the solutions of the equations above must be of the form $x_{1}(t)=$ $A_{1} \cos (\omega t)+B_{1} \sin (\omega t)$ and similarly for the other two masses. It follows that for all displacements $\ddot{x}_{i}=-\omega^{2} x_{i}$ since the second derivative of both cosine and sine terms lead to factors of $-\omega^{2}$. We now divide the first equation above by $m_{1}$ and the second by $m_{2}$ etc. We also use $\ddot{x}_{i}=-\omega^{2} x_{i}$ in each line and then rewrite the system of equations as a single matrix equation

$$
\omega^{2}\left[\begin{array}{l}
x_{1} \\
x_{2} \\
x_{3}
\end{array}\right]=k\left[\begin{array}{rrr}
\frac{1}{m_{1}} & -\frac{1}{m_{1}} & 0 \\
-\frac{1}{m_{2}} & \frac{2}{m_{2}} & -\frac{1}{m_{2}} \\
0 & -\frac{1}{m_{3}} & \frac{1}{m_{3}}
\end{array}\right]\left[\begin{array}{l}
x_{1} \\
x_{2} \\
x_{3}
\end{array}\right] .
$$

It is seen that the square of the characteristic frequencies are found as eigenvalues of a matrix containing the masses and the spring constant. These eigenvalues are quite complicated generally.

However, in the case of $\mathrm{CO}_{2}$ we obviously have $m_{1}=m_{3}=m_{O}$ and $m_{2}=m_{C}$, where $m_{O}$ and $m_{C}$ are the atomic oxygen and carbon masses, respectively. The characteristic determinant equation therefore becomes

$$
\left|\begin{array}{ccc}
\frac{1}{m_{O}}-\lambda & -\frac{1}{m_{O}} & 0 \\
-\frac{1}{m_{C}} & \frac{2}{m_{C}}-\lambda & -\frac{1}{m_{C}} \\
0 & -\frac{1}{m_{O}} & \frac{1}{m_{O}}-\lambda
\end{array}\right|=0
$$

where $\lambda=\omega^{2} / k$. Computing the determinant leads to the condition

$$
\lambda\left(1-m_{O} \lambda\right)\left(2 m_{O}+m_{C}-m_{O} m_{C} \lambda\right)=0
$$

so that the roots are $0,1 / m_{O}$, and $\left(2 m_{O}+m_{C}\right) / m_{O} m_{C}$. It follows that the three normal mode frequencies are

$$
\omega_{1}=0, \quad \omega_{2}=\sqrt{\frac{k}{m_{O}}}, \quad \omega_{3}=\sqrt{\frac{k\left(2 m_{O}+m_{C}\right)}{m_{O} m_{C}}} .
$$

The value of the spring constant is $k=1600 \mathrm{~N} / \mathrm{m}$ and the masses are $m_{C}=12 u$ and $m_{O}=16 u$, where $u=1.66 \cdot 10^{-27} \mathrm{~kg}$ is the mass unit. Plugging in numbers we find

$$
\omega_{1}=0 \mathrm{rad} / \mathrm{s}, \omega_{2}=2.45 \cdot 10^{14} \mathrm{rad} / \mathrm{s}, \omega_{3}=4.70 \cdot 10^{14} \mathrm{rad} / \mathrm{s}
$$

The zero eigenvalue is not really a vibration at all but rather the case, in which the whole molecule moves left or right. The eigenvectors belonging to the last two frequencies are $\vec{c}_{2}=(1,0,-1)$ and $\vec{c}_{3}=\left(1,-2 \frac{m_{0}}{m_{C}}, 1\right)$, respectively. They show that the second mode is a symmetric stretch mode, in which the carbon is fixed and if the first oxygen moves left the second moves right and vice versa. The third modes is an asymmetric stretch mode for which the two oxygens always move in the same direction and oppositely to the carbon. Note that the centre of mass remains stationary.


Symmetric stretch


Asymmetric stretch


Bending mode

We finish with a brief note on the greenhouse effect connected to global warming. The physics behind this phenomenon is that the earth radiates heat into the atmosphere approximately as a big black-body radiator with a temperature of roughly $T=273 \mathrm{~K}$. Wien's displacement law tells you that the frequency spectrum of such a black body peaks at an angular frequency that is proportional to the temperature and given by $T \cdot 3.7 \cdot 10^{11} \mathrm{rad} / \mathrm{sK}$. Hence, the peak is found approximately at a frequency of $10^{14} \mathrm{rad} / \mathrm{s}$. This is quite close to the $\omega_{2}$ found above is so $\mathrm{CO}_{2}$ in the atmosphere are likely to absorb some of the heat radiation that would otherwise escape into space. In fact, there is a second type of vibrations called bending modes, in which atoms move mostly perpendicular to the molecular axis ( $x$-axis) rather than parallel. The bending mode in $\mathrm{CO}_{2}$ has a frequency of $\omega_{2}=1.25 \cdot 10^{14} \mathrm{rad} / \mathrm{s}$, which sits very close to the centre of the black body spectrum and so this mode is the dominant one for the greenhouse effect.

## Further reading:

Oscillations in general: R. Wolfson, Essential University Physics, Vol. 1, Chapter 13, 2. Ed., Pearson (2012).

Vibrational spectroscopy: P. Atkins and J. de Paula, Physical Chemistry Chapter 16, 7. Ed., Oxford (2002).

Greenhouse effect: D.J. Wilson and J. Gea-Banacloche, American Journal of Physics, Vol. 80, page 306 (2012).

## Dynamic models of feed-back control systems - an example

Keywords: Linear differential equations, coupled 1st order differential equations, eigenvalues

Automatic control plays an important role in engineering - and feedback control systems are used everywhere in our daily life: Some simple examples include speed pilots in cars, room temperature control in domestic homes and pump systems circulating fresh water, but the use of automatic control in vehicles, industrial products, energy systems etc. is virtually unlimited. A modern wind turbine, for example, is equipped with many control systems that regulate e.g. the wind turbine speed, the power production, and the pitch angle.


Figure 9: Closed-loop control system.
As illustrated in Figure 9 , the basic objective of a closed-loop control system is to regulate the output from a system, like the speed of a car driving on a road. In order to do so, the system output must be measured continuously; this is done by a sensor, which outputs e.g. the actual speed. Now, in order to change the speed if it deviates from the wanted speed (the setpoint), the compensator changes the engine torque (which is considered to be the system input): If the actual speed is too low, the speed pilot compensator asks the engine to deliver more torque in order to accelerate the car; if the speed is too high, the speed compensator should reduce the engine torque in order to slow down the car.

## System analysis - without compensator

The analysis of physical systems is always based on the physical laws describing the behavior. A very large class of physical systems is mathematically modeled by differential equations. For example, mechanical systems are governed by Newton's laws of motion whereas electric systems may be described by Kirchhoff's laws. A DC motor is an example of an electro-mechanical device, which converts electric power to mechanical power; first-generation electric vehicles was, in fact, using DC motors. A DC motor may be modeled by the circuit shown in Figure 10 .


Figure 10: Model of DC motor.
$u$ is the applied voltage, $i$ is the current, $e$ is the induced back-emf. Also $\tau$ is the torque and $\omega$ is the shaft speed. $R$ is the winding resistance, $L$ is the inductance.

Mathematically, the equations are [1]:

$$
\begin{align*}
& u=r i+L \frac{d i}{d t}+e  \tag{24}\\
& e=K \omega  \tag{25}\\
& \tau=K i=B \omega+J \frac{d \omega}{d t} \tag{26}
\end{align*}
$$

where $K$ is the back-emf constant, $B$ is the mechanical friction constant and $J$ is the inertia of the rotating parts. If we consider the voltage $u$ as the system input and the speed $\omega$ as the system output, we can derive the following second order differential equation from the equations above:

$$
\begin{equation*}
\frac{L J}{K} \frac{d^{2} \omega}{d t^{2}}+\left(\frac{R J}{K}+\frac{L B}{K}\right) \frac{d \omega}{d t}+\left(\frac{R B}{K}+K\right) \omega=u \tag{27}
\end{equation*}
$$

The intrinsic behavior of the DC motor depends on the parameters ( $R, L, K, B$ and $J$ ). For a particular forcing function $u(t)$ the output $\omega(t)$ may be determined by solving (27).

Alternatively, the DC motor model (24)-(26) may be described by two coupled first-order equations:

$$
\frac{d}{d t}\left[\begin{array}{c}
i  \tag{28}\\
\omega
\end{array}\right]=\left[\begin{array}{cc}
-R / J & -K / L \\
K / J & -B / J \omega
\end{array}\right]\left[\begin{array}{c}
i \\
\omega
\end{array}\right]+\left[\begin{array}{c}
1 / L \\
0
\end{array}\right] u
$$

which has the advantage that the current may be calculated as well.
To illustrate Figure 11 shows the speed for a sudden change of the voltage input $u(t)$. It may be seen that the speed oscillates heavily; the frequency of oscillation may be found by analytical solution of either (27) or (28). In this example the eigenvalues are $-0.5 \pm \mathrm{j} 3.1$ leading to a poorly damped oscillation having the frequency equal to 0.5 Hz . For practical purposes the large intrinsic oscillations should be removed.


Figure 11: DC motor response - without compensator.

## Compensator design - and closed loop response

By means of a compensator, it is possible to alter the behavior of the system. The basic idea is to use the error signal (defined in Figure 9) as the input to another differential equation, which in turn outputs the plant input. Specifically, for the DC motor example, we may choose

$$
\begin{equation*}
u=K_{p}\left(\omega_{\text {set }}-\omega\right)+K_{d} \frac{d\left(\omega_{\text {set }}-\omega\right)}{d t} \tag{29}
\end{equation*}
$$

where $K_{p}$ and $K_{d}$ are constants, which must be determined.
Assuming that $\omega_{\text {set }}$ is constant, the closed-loop differential equation now becomes

$$
\begin{equation*}
\frac{L J}{K} \frac{d^{2} \omega}{d t^{2}}+\left(\frac{R J}{K}+\frac{L B}{K}+K_{d}\right) \frac{d \omega}{d t}+\left(\frac{R B}{K}+K+K_{p}\right) \omega=K_{p} \omega_{s e t} \tag{30}
\end{equation*}
$$

or in matrix form:

$$
\frac{d}{d t}\left[\begin{array}{c}
i  \tag{31}\\
\omega
\end{array}\right]=\left[\begin{array}{cc}
-\left(R / J+K_{p}\right) & -\left(K / L+K_{d}\right) \\
K / J & -B / J
\end{array}\right]\left[\begin{array}{c}
i \\
\omega
\end{array}\right]+\left[\begin{array}{c}
K_{p} / L \\
0
\end{array}\right] \omega_{\text {set }} \Rightarrow \frac{d \mathbf{x}}{d t}=\mathbf{A x}+\mathbf{B} \omega_{\text {set }}
$$

From (31), it may be seen that the eigenvalues of the system matrix $\mathbf{A}$ is a function of $K_{p}$ and $K_{d}$ and this fact may be used to shape the response of the closed loop. Basically, we specify the eigenvalues $p_{1}$ and $p_{2}$ of the closed-loop system matrix (31) and then we calculate the required $K_{p}$ and $K_{d}$ in such a way that eig $(\mathbf{A})=\left[p_{1} p_{2}\right]^{T}$.

Using this idea of feeding back the instantaneous speed $\omega(t)$ to a compensator, which in turn calculates the DC motor voltage, it is possible to get a speed response as shown in Figure 12 below. Notice that the large oscillations are removed and the output settles at its steady-state value faster than for the open loop system (Figure 11). In this case the eigenvalues of (31) are real ( $-1 \pm \mathrm{j} 0$ and $-20+\mathrm{j} 0$ ).


Figure 12: DC motor response in a closed-loop control system with a compensator.

## Further reading:

Katsuhiko Ogata, "Modern Control Engineering," 5th Edition, Pearson, 2010

## Analysis of electric AC circuits

Keywords: Differential equations, linear algebra, trigonometry, complex numbers, Euler's identity

We live in an electrified world: electro-technology is used everywhere, and living today without electricity is virtually impossible even for the shortest duration of time. Electric power is generated both at central power plants and by dispersed units such as wind turbine farms or large solar cell arrays, and by means of large and complex electric networks the power is transmitted/distributed from production units to consumers. Electro-technology is also a fundamental prerequisite for the way we today distribute and store information: electronic circuits are used everywhere in our society to convey information. Living without electro-technology is not an option.

From an electrical engineering point of view, detailed knowledge of electro-technology is of vital importance, and a very important tool is circuit analysis. A good understanding of this topic enables us to analyze and to design electric circuits and systems, irrespective of whether we consider transmission of power in the hundreds of megawatt scale - or we consider low-level signals within integrated electronics.

Circuit analysis uses mathematics to analyze the network, and as an example, consider the network shown in Figure 13below. This network consists of three elements: a voltage source $u(t)$, a resistor $R$ and an inductance $L$. This simple circuit may model e.g. an electric furnace, an electric motor, a loud-speaker, etc.


Figure 13: $R L$ series circuit.
Using Kirchhoff's laws, the resistive-inductive circuit fulfills the equation

$$
\begin{equation*}
L \frac{d i(t)}{d t}+R i(t)=u(t) \tag{32}
\end{equation*}
$$

which is a first-order differential equation. In electrical engineering the forcing function $u(t)$ is often a sinusoidal function:

$$
\begin{equation*}
u(t)=U_{a} \cos (\omega t) \tag{33}
\end{equation*}
$$

where $U_{a}$ is the amplitude and $\omega$ is the angular frequency for the voltage. For example, the electric outlet in our homes has $U_{a}=\sqrt{2} \cdot 230 \mathrm{~V}$ and $\omega=2 \pi f=100 \pi \mathrm{rad} / \mathrm{s}$.
The question is now: how do we find the current $i(t)$ ?

## Solution using trigonometric identities

Since the input (the forcing function) is on the form (33), we may guess that the current (the forced response, stationary solution) is given by

$$
\begin{equation*}
i(t)=I_{a} \cos (\omega t+\varphi) \tag{34}
\end{equation*}
$$

Hence, we need to find the constants $I_{a}$ and $\varphi$ so that (32) is fulfilled.
Using $\cos (\alpha+\beta)=\cos \alpha \cos \beta-\sin \alpha \sin \beta$, we get

$$
\begin{equation*}
i(t)=I_{a} \cos (\omega t) \cos \varphi-I_{a} \sin (\omega t) \sin \varphi=I_{a 1} \cos (\omega t)+I_{a 2} \sin (\omega t), \tag{35}
\end{equation*}
$$

where $I_{a 1}=I_{a} \cos \varphi$ and $I_{a 2}=-I_{a} \sin \varphi$.
Substitution of (35) into (32) yields

$$
\begin{equation*}
L \frac{d}{d t}\left(I_{a 1} \cos (\omega t)+I_{a 2} \sin (\omega t)\right)+R\left(I_{a 1} \cos (\omega t)+I_{a 2} \sin (\omega t)\right)=U_{a} \cos (\omega t) \tag{36}
\end{equation*}
$$

which implies

$$
\begin{equation*}
L\left(-\omega I_{a 1} \sin (\omega t)+\omega I_{a 2} \cos (\omega t)\right)+R\left(I_{a 1} \cos (\omega t)+I_{a 2} \sin (\omega t)\right)=U_{a} \cos (\omega t) \tag{37}
\end{equation*}
$$

Equating coefficients gives

$$
\left[\begin{array}{cc}
-\omega L & R  \tag{38}\\
R & \omega L
\end{array}\right]\left[\begin{array}{c}
I_{a 1} \\
I_{a 2}
\end{array}\right]=\left[\begin{array}{c}
0 \\
U_{a}
\end{array}\right]
$$

and this linear set of equations may be used to find $I_{a 1}$ and $I_{a 2}$. Completing the algebra leads to

$$
\begin{equation*}
i(t)=\frac{U_{a}}{R^{2}+(\omega L)^{2}}(R \cos (\omega t)+\omega L \sin (\omega t)) \tag{39}
\end{equation*}
$$

To get (39) on the format (34), we use the identity $\cos (\alpha-\beta)=\cos \alpha \cos \beta+\sin \alpha \sin \beta$ and after some calculations we finally get

$$
\begin{equation*}
i(t)=\frac{U_{a}}{\sqrt{R^{2}+(\omega L)^{2}}} \cos \left(\omega t-\arctan \left(\frac{\omega L}{R}\right)\right) \tag{40}
\end{equation*}
$$

Note how the current amplitude $I_{a}$ and the phase angle $\varphi$ may be read seen from (40).
This example shows that finding the solution (in this case the current in the circuit) requires a lot of tedious calculations, even for a very simple electric circuit. More complex circuits will require a lot more work using this procedure, but fortunately - as illustrated below - an alternative method using complex numbers and complex functions is available.

## Solution using complex forcing function

The starting point is Euler's identity $e^{j \omega t}=\cos \omega t+j \sin \omega t$, where $j$ denotes the complex unit. Suppose for a moment that the voltage source in Figure 13 is the (unrealizable) complex-valued voltage defined by

$$
\begin{equation*}
\mathbf{u}(t)=U_{a} e^{j \omega t} \tag{41}
\end{equation*}
$$

Boldface symbols indicate a complex quantity. Later, we use that $\operatorname{Re}(\mathbf{u}(t))=U_{a} \cos \omega t$, but here we treat voltage and current as complex functions of time even though this is not physically possible. (In the real world, voltages and currents are always scalar quantities.)

If we apply the complex voltage (41) to the right hand side of (32), we can find the forced response. The current is now a complex function on the format

$$
\begin{equation*}
\mathbf{i}(t)=I_{a} e^{j(\omega t+\varphi)} \tag{42}
\end{equation*}
$$

Substitution of the complex voltage (41) and ditto current (42) into (32) gives

$$
\begin{equation*}
L \frac{d}{d t}\left(I_{a} e^{j(\omega t+\varphi)}\right)+R\left(I_{a} e^{j(\omega t+\varphi)}\right)=U_{a} e^{j \omega t} \tag{43}
\end{equation*}
$$

which after differentiation leads to

$$
\begin{equation*}
j \omega L I_{a} e^{j(\omega t+\varphi)}+R I_{a} e^{j(\omega t+\varphi)}=U_{a} e^{j \omega t} \tag{44}
\end{equation*}
$$

All terms have a common factor $e^{j \omega t}$, and dividing all terms with this factor gives

$$
\begin{equation*}
j \omega L I_{a} e^{j \varphi}+R I_{a} e^{j \varphi}=(j \omega L+R) I_{a} e^{j \varphi}=U_{a} \tag{45}
\end{equation*}
$$

Since the modulus of $e^{j \varphi}$ is 1 , we immediately get from (45) that

$$
\begin{equation*}
I_{a}=\left|\frac{U_{a}}{R+j \omega L}\right|=\frac{U_{a}}{\sqrt{R^{2}+(\omega L)^{2}}} \tag{46}
\end{equation*}
$$

Now, because $\angle(R+j \omega L)=\angle\left(e^{-j \varphi}\right)=-\varphi$, we find

$$
\begin{equation*}
\varphi=-\arctan \left(\frac{\omega L}{R}\right) \tag{47}
\end{equation*}
$$

Substitution of (46) and (47) into (42), the complex-valued forced response to the complex-valued input voltage becomes

$$
\begin{equation*}
\mathbf{i}(t)=\frac{U_{a}}{\sqrt{R^{2}+(\omega L)^{2}}} e^{j\left(\omega t-\arctan \left(\frac{\omega L}{R}\right)\right)} \tag{48}
\end{equation*}
$$

which may be reformulated as

$$
\begin{equation*}
\mathbf{i}(t)=\frac{\mathbf{u}(t)}{\sqrt{R^{2}+(\omega L)^{2}} \cdot e^{j \arctan \left(\frac{\omega L}{R}\right)}}=\frac{\mathbf{u}(t)}{R+j \omega L} \tag{49}
\end{equation*}
$$

By equating the real part on both sides of (48), the actual real current in the circuit in Figure 13 is given by

$$
\begin{equation*}
i(t)=\frac{U_{a}}{\sqrt{R^{2}+(\omega L)^{2}}} \cos \left(\omega t-\arctan \left(\frac{\omega L}{R}\right)\right) \tag{50}
\end{equation*}
$$

which corresponds to (40) derived earlier.

## Concluding remarks

In (49) it is convenient to define $\mathbf{Z}=R+j \omega L=\sqrt{R^{2}+(\omega L)^{2}} e^{j \varphi}$ as the complex impedance of the series connection of the resistor and the inductor shown in Figure 13, Then, (49) is on the form $\mathbf{u}(t)=\mathbf{Z} \mathbf{i}(t)$ and hence for the purpose of ac circuit analysis (49) extends Ohm's Law $u=R i$ for resistive circuits to also include circuits having inductors as well as resistors.

As illustrated by this small example, the principle of using complex-valued voltage and current functions and complex impedance's is a very powerful tool for analysis of electric circuits. Basically what happens is that a time-domain differential equation is transformed to an equivalent algebraic equation containing complex coefficients, but the latter is in general much easier to solve.

In addition all the mathematical tools related to complex numbers and complex functions may used to gain further engineering insight into a circuit's characteristics.

## Further reading:

J. David Irwin and R. Mark Nelms, "Basic Engineering Circuit Analysis", Wiley, 2005

## Matrix formulation of chemical problems

Keywords: Matrices, mass balance, first order reaction, system of differential equations, entropy, chemical equation.

## Balance of chemical equations

One of the most frequent tasks, in both laboratory and chemistry class, is obtaining a set of stoichiometric coefficients to 'balance' a chemical equation. This task is a necessary first step towards solving most school problems. As has been pointed out, the expression "balancing a chemical equation" is a contradiction of terms. A chemical equation is fundamentally a conservation statement about atomic species and, thus, it should already be balanced. Usually, students obtain coefficients by a trial and error method. This effort yields no profit and loses a lot of time. When a moderate number of chemical species ( 8 or more) are involved in a given skeletal equation, the task is nearly impossible to solve by trial and error. Thus, some special methods are necessary. Up to best of our knowledge, three main methods can be used which are: the oxidation-number method; the ion-electron method; and the matrix method. However, there are a lot of limitations to use the first and second method to balance some systems, and due to this matrices play a key role in chemical reactions. For example we have used matrices concept to balance the following chemical equation

$$
a \mathrm{FeCl}_{2}+b \mathrm{Na}_{3}\left(\mathrm{PO}_{4}\right) \rightarrow c \mathrm{Fe}_{3}\left(\mathrm{PO}_{4}\right)_{2}+d \mathrm{NaCl}
$$

where $a, b, c$, and $d$ are the stoichiometric coefficients.
Writing the balance for each ion we get the following homogeneous equations:

$$
\begin{array}{lllll}
\mathrm{Fe}: & 1 a & +0 b & -3 c & -0 d=0 \\
\mathrm{Cl}: & 2 a & +0 b & +0 c & -1 d=0 \\
\mathrm{Na}: & 0 a & +3 b & +0 c & -1 d=0 \\
\left(\mathrm{PO}_{4}\right): & 0 a & +1 b & -2 c & -0 d=0
\end{array}
$$

For this reaction, it is better to treat the phosphate ion $\left(\mathrm{PO}_{4}\right)^{-3}$ as an element, and not break it into two individual elements. The coefficient matrix for the homogeneous linear equation system above is

$$
\left[\begin{array}{rrrr}
1 & 0 & -3 & 0 \\
2 & 0 & 0 & -1 \\
0 & 3 & 0 & -1 \\
0 & 1 & -2 & 0
\end{array}\right],
$$

and a few row operations gives the reduced row echelon form

$$
\left[\begin{array}{rrrr}
1 & 0 & 0 & -\frac{1}{2} \\
0 & 1 & 0 & -\frac{1}{3} \\
0 & 0 & 1 & -\frac{1}{6} \\
0 & 0 & 0 & 0
\end{array}\right] .
$$

Hence, the smallest positive integer solution is $a=3, b=2, c=1$, and $d=6$.

## Chemical reaction kinetics

In 1975, L. Papula presented a method to obtain the kinetic equations of a consecutive reaction scheme involving only irreversible fist-order steps at University of Stuttgart, Germany. The method was based on matrix algebra. In fact, matrix algebra offers an elegant way of solving differential equations for chemical engineering systems, especially in the field of chemical reactions.


Figure 14: Continuous stirred-tank reactor for first order reaction like $X \rightarrow Y$
We can also use matrices to find the chemical reaction kinetics. For example in a first order reaction, consider $X \rightarrow Y$ which has occurred in chemical reactor like Figure 14, let the molecular concentrations of $X$ and $Y$ at time $t$ be $C_{X}(t)$ and $C_{Y}(t)$. The rates of formation of $X$ and $Y$ are $C_{X}{ }^{\prime}(t)$ and $C_{Y}{ }^{\prime}(t)$. Then this reaction obeys the following system of homogeneous linear differential equations of the first order with constant coefficient

$$
\left[\begin{array}{l}
C_{X}^{\prime} \\
C_{Y}^{\prime}
\end{array}\right]=\left[\begin{array}{rr}
-k & 0 \\
k & 0
\end{array}\right]\left[\begin{array}{l}
C_{X} \\
C_{Y}
\end{array}\right]
$$

or alternatively $\vec{C}^{\prime}=A \vec{C}$ where

$$
\vec{C}=\left[\begin{array}{l}
C_{X} \\
C_{Y}
\end{array}\right], \quad A=\left[\begin{array}{rr}
-k & 0 \\
k & 0
\end{array}\right] .
$$

By diagonalizing the matrix $A$ we get

$$
\vec{C}_{1}^{\prime}=\left[\begin{array}{rr}
0 & 0 \\
0 & -k
\end{array}\right] \vec{C}_{1} \text { where } \vec{C}=\left[\begin{array}{rr}
0 & 1 \\
1 & -1
\end{array}\right] \vec{C}_{1} .
$$

The solution for $\vec{C}_{1}$ is

$$
\vec{C}_{1}=\left[\begin{array}{c}
A \\
B e^{-k t}
\end{array}\right],
$$

where $A$ and $B$ are arbitrary constants. Thus the solution for $\vec{C}$ becomes

$$
\vec{C}=\left[\begin{array}{c}
B e^{-k t} \\
A-B e^{-k t}
\end{array}\right] .
$$

Finally, using initial conditions $C_{X}(0)=a, C_{Y}(0)=b$ we obtain

$$
C_{X}=a e^{-k t} \text { and } C_{y}=a+b-a e^{-k t} .
$$

[^0]
## Matrices and chemical systems

## Example 1:

A firm wishes to market bags of lawn fertilizer which contain $25 \%$ nitrogen, $7 \%$ phosphoric acid, and $8 \%$ potash. The firm has four chemical precursors C1, C2, C3, C4 which are to be combined to make the fertilizer. The percentage of each ingredient in a pound of these chemicals is given in Table 1. How much of each chemical should be mixed to obtain 100 pounds of fertilizer meeting

|  | C1 | C2 | C3 | C4 |
| :--- | ---: | ---: | ---: | ---: |
| Nitrogen | 20 | 25 | 0 | 3 |
| Phosphoric Acid | 12 | 5 | 6 | 7 |
| Potash | 0 | 5 | 15 | 10 |

Table 1: Percentage of chemicals
these criteria? Let $x_{i}$ be the number of pounds of chemical Ci used. Then since the total adds up to 100 pounds we have $x_{1}+x_{2}+x_{3}+x_{4}=100$. Now $x_{1}$ pounds of chemical C1 contains $0.20 x_{1}$ pounds of nitrogen, $x_{2}$ pounds of C 2 contains $0.25 x_{2}$ pounds of nitrogen, $x_{3}$ pounds of C 3 contains 0 pounds of nitrogen, and $x_{4}$ pounds of C 4 contains $0.30 x_{4}$ pounds of nitrogen. Since there should be $0.25 \cdot 100=25$ pounds of nitrogen in the mixture we obtain

$$
0.20 x_{1}+0.25 x_{2}+0 x_{3}+0.30 x_{4}=25 .
$$

Similar expressions can be derived for phosphoric acid and potash giving us all together a system of linear equations with augmented matrix

$$
\left[\begin{array}{llll|r}
1 & 1 & 1 & 1 & 100 \\
0.2 & 0.25 & 0 & 0.3 & 25 \\
0.12 & 0.05 & 0.06 & 0.07 & 7 \\
0 & 0.05 & 0.15 & 0.1 & 8
\end{array}\right]
$$

Using Gaussian elimination we get

$$
\left[\begin{array}{rrrr|r}
1 & 0 & 0 & 0 & 11.74 \\
0 & 1 & 0 & 0 & 25.08 \\
0 & 0 & 1 & 0 & 8.57 \\
0 & 0 & 0 & 1 & 54.60
\end{array}\right]
$$

from which the solution can be read of directly.

## Example 2:

Consider a linear chain of N atoms. Each of the atoms can be in one of three states A, B or C, except that an atom in state A cannot be adjacent to an atom in state C. Let us find the entropy per atom for this system as $N \rightarrow \infty$. To solve this problem it is useful to define the set of three dimensional column vectors $\vec{V}^{(j)}$ such that the three elements are the total number of allowed configurations of a j-atom chain having the jth atom in state A, B or C. For example,

$$
\vec{V}^{(1)}=\left[\begin{array}{l}
1 \\
1 \\
1
\end{array}\right], \quad \vec{V}^{(2)}=\left[\begin{array}{l}
2 \\
3 \\
2
\end{array}\right], \quad \vec{V}^{(3)}=\left[\begin{array}{l}
5 \\
7 \\
5
\end{array}\right], \ldots
$$

The vector $\vec{V}^{(j+1)}$ can be found from $\vec{V}^{(j)}$ using the matrix equation $\vec{V}^{(j+1)}=M \vec{V}^{(j)}$ where for this example

$$
M=\left[\begin{array}{lll}
1 & 1 & 0 \\
1 & 1 & 1 \\
0 & 1 & 1
\end{array}\right]
$$

The matrix $M$ is the so-called transfer matrix for the system. The atoms can be in state A if the atoms before is in stage A and B - but not C - producing the first row of $M$. The atom can be in state B independently of the previous states producing the second row of $M$. Finally, the atom can be in state C if the atoms before is in stage B and C producing the third row of $M$.

As an illustration let us find $\vec{V}^{(4)}$ :

$$
\vec{V}^{(4)}=M \vec{V}^{(3)}=\left[\begin{array}{lll}
1 & 1 & 0 \\
1 & 1 & 1 \\
0 & 1 & 1
\end{array}\right]\left[\begin{array}{l}
5 \\
7 \\
5
\end{array}\right]=\left[\begin{array}{l}
12 \\
17 \\
12
\end{array}\right]
$$

Further let us list all states for the case of $N=3$ to verify that we get the same result as calculated using the transfer matrix. Remembering that $\vec{V}^{(3)}$ gives us the number of sequences that end in a given state we should organize our list in the same manner. States like AAC are not allowed because A and C are neighbours.

| States ending in A | States ending in B | States ending in C |
| :---: | :---: | :---: |
| AAA | AAB | ABC |
| ABA | ABB | BBC |
| BAA | BAB | BCC |
| BBA | BBB | CBC |
| CBA | BCB | CCC |
|  | CBB |  |
|  | CCB |  |
| 5 states | 7 states | 5 states |

Table 2: The components of $\vec{V}^{(3)}$.

We will now use Boltzmann's entropy formula $S=k \ln W$ to find the entropy per atom for this chain as $N$ goes to infinity; $k$ is Boltzmann's constant $1.38062 \cdot 10^{-23}$ joule/kelvin.

It can be shown that the number of configurations is $W=\operatorname{tr}\left(M^{N}\right)$. Now for large $N, \operatorname{tr}\left(M^{N}\right) \simeq$ $\left(\lambda_{\max }\right)^{N}$, where $\lambda_{\max }$ is the largest eigenvalue of $M$. So $W \simeq k \ln \left(\left(\lambda_{\max }\right)^{N}\right)$. We get:

$$
\lim _{N \rightarrow \infty} \frac{S}{N}=\lim _{N \rightarrow \infty} \frac{1}{N} k \ln (W)=\lim _{N \rightarrow \infty} \frac{k}{N} \ln \left(\left(\lambda_{\max }\right)^{N}\right)=\lim _{N \rightarrow \infty} \frac{k}{N} N \ln \left(\lambda_{\max }\right)=k \ln \left(\lambda_{\max }\right) .
$$

The eigenvalues of $M$ are $1-\sqrt{2}, 1$, and $1+\sqrt{2}$, so $\lambda_{\max }=1+\sqrt{2}$. Hence the limiting entropy per atom is $k \ln (1+\sqrt{2})$.

## Further reading:

Rawlings, J. B., Ekerdt, J. G. "Chemical reactor analysis and design fundamentals," Nob Hill Publishing, Madison, WI, 2004.

## Catenary

Keywords: Shape of transmission lines, plane curves, arch length, first order separable differential equations, hyperbolic functions


Figure 15: Transmission lines crossing Limfjorden near Nordjyllandsværket.
The problem we want to deal with: What is the shape of a transmission line?
To make things simple we assume that a transmission line acts as a homogeneous flexible inextensible string hanging from two points only under the influence of gravity.


$$
\begin{gathered}
\boldsymbol{S}_{1}=-k_{1}\left(\boldsymbol{i}+f^{\prime}(x) \boldsymbol{j}\right) \\
\boldsymbol{S}_{2}=k_{2}\left(\boldsymbol{i}+f^{\prime}(x+h) \boldsymbol{j}\right) \\
\boldsymbol{T}=-(\rho \Delta s) g \boldsymbol{k} \\
\rho \text { is the density per unit length } \\
g \text { is the gravity acceleration }
\end{gathered}
$$

Figure 16: String forces and gravity acting on a part of the string.

Note that the string forces acts in direction of the curve tangents.
Projection on the $x$-axis gives

$$
-k_{1}+k_{2}=0 \quad \Rightarrow \quad k_{1}=k_{2}=k \quad \text { for all } x,
$$

[^1]and projection on the $y$-axis gives
$$
-k f^{\prime}(x)+k f^{\prime}(x+h)=-\rho g \Delta s \quad \Rightarrow \quad \frac{f^{\prime}(x+h)-f^{\prime}(x)}{h}=\frac{\rho g}{k} \frac{\Delta s}{h} .
$$

Letting $h \rightarrow 0$ in the last equation leads to

$$
f^{\prime \prime}(x)=\frac{1}{a} \frac{d s}{d x}, \quad a=\frac{k}{\rho g},
$$

where $d s$ is the arch length element. Substituting $\sqrt{1+f^{\prime}(x)^{2}} d x$ for $d s$ gives

$$
f^{\prime \prime}(x)=\frac{1}{a} \sqrt{1+f^{\prime}(x)^{2}},
$$

a second order differential equation. By setting $u(x)=f^{\prime}(x)$, the second order equation can be split into two first order differential equations

$$
u^{\prime}(x)=\frac{1}{a} \sqrt{1+u(x)^{2}} \quad \text { and } \quad f^{\prime}(x)=u(x) .
$$

The first equation in a slightly different notation

$$
\frac{d u}{d x}=\frac{1}{a} \sqrt{1+u^{2}}
$$

can be recognised as a separable equation, hence

$$
\frac{d u}{\sqrt{1+u^{2}}}=\frac{1}{a} d x .
$$

To solve this equation we need a bit of knowledge of hyperbolic functions. These functions have been introduced in 'Kompendium i lineær algebra' to illustrate some theoretical aspects of linear algebra, see pages $4,5,28,29$, and 31 .

Here we will make use of the fundamental relation between the hyperbolic cosine and the hyperbolic sine

$$
\cosh ^{2} x-\sinh ^{2} x=1,
$$

which is easily proven from the definitions of cosh and sinh. Regarding differentiation of cosh and sinh see 'Kompendium i lineær algebra' page 29.

Going back to the separated equation we introduce the substitution

$$
u=\sinh t \quad \Rightarrow \quad d u=\cosh t d t
$$

on the left side. The inverse substitution is

$$
t=\operatorname{arsinh} u
$$

(The inverse functions to cosh and sinh are called area functions.) Now

$$
u=\sinh t \quad \Rightarrow \quad \sqrt{1+u^{2}}=\sqrt{1+\sinh ^{2} t}=\sqrt{\cosh ^{2} t}=\cosh t
$$

hence

$$
\frac{d u}{\sqrt{1+u^{2}}}=\frac{\cosh t d t}{\cosh t}=d t
$$

and the solution of the differential equation follows as

$$
t=\frac{1}{a} x+c \quad \Rightarrow \quad \operatorname{arsinh} u=\frac{1}{a} x+c \quad \Rightarrow \quad u(x)=\sinh \left(\frac{1}{a} x+c\right) .
$$

Using the initial condition $u(0)=0$, the arbitrary constant $c$ becomes 0 . Thus

$$
u(x)=\sinh \frac{x}{a} .
$$

To solve the second differential equation $f^{\prime}(x)=u(x)$ we only need to find an antiderivative to $u(x)$ :

$$
f(x)=\int \sinh \frac{x}{a} d x=a \int \sinh \frac{x}{a} d\left(\frac{x}{a}\right)=a \cosh \frac{x}{a}+c
$$

Using the initial condition $f(0)=a$ we get $c=0$.
Finally we can conclude that the shape of a transmission line is identical with that of a hyperbolic cosine

$$
f(x)=a \cosh \frac{x}{a},
$$

which in this context is called a catenary (Latin catena chain).
Note that this result is valid for arbitrary choices of supporting points, i.e., with masts in different heights, the transmission lines between masts will always form catenaries.

## Appendix

Looking up the antiderivative

$$
\int \frac{1}{\sqrt{x^{2}+1}} d x
$$

in a table of integrals we find

$$
\ln \left(x+\sqrt{x^{2}+1}\right) .
$$

Anything wrong in the calculation above? To answer that let us find the inverse function to the hyperbolic sine:

$$
y=\sinh x \quad \Leftrightarrow \quad y=\frac{e^{x}-e^{-x}}{2}=\frac{e^{2 x}-1}{2 e^{x}} \quad \Leftrightarrow \quad e^{2 x}-2 y e^{x}-1=0
$$

The last equation is a quadratic equation in $e^{x}$, which we can solve:

$$
e^{x}=\frac{\left.2 y_{(-)}^{+}\right) \sqrt{4 y^{2}+4}}{2}=y \stackrel{+}{(-)} \sqrt{y^{2}+1} \quad \Rightarrow \quad x=\ln \left(y+\sqrt{y^{2}+1}\right)
$$

Interchanging the variables $x$ and $y$ we obtain the identity

$$
\operatorname{arsinh} x=\ln \left(x+\sqrt{x^{2}+1}\right) .
$$

## Further reading:

Edwards \& Penney, Calculus Early Transcendentals, 7th ed., Section 6.9 and Section 8.3.
Adams \& Essex, Calculus A Complete Course, 7th ed., Section 3.6 and Section 17.2.
Wikipedia, http://en.wikipedia.org/wiki/Catenary


[^0]:    *Paula, L., "Mathematik für Chemikero," F. Enke-Verlag, Stuttgart, 1975.

[^1]:    ${ }^{\dagger}$ In Danish: Kædelinie

