Scientific Computing I

Winter semester 2022/2023
Prof. Dr. Carsten Burstedde
Uta Seidler and Denis Düsseldorf

UNIVERSITÄT BONN

Exercise sheet 1.

Submission on **27.10.2022**.

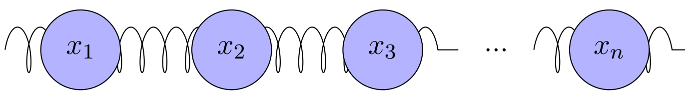
Exercise 1. (Oscillations of crystals - Wave equation)

(0 Points)

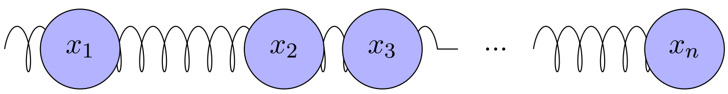
In this exercise we want to model the oscillations happening inside of crystals. Ultimately, this will lead us to the wave equation.
A crystal is made out of atoms, and these atoms are positioned in a grid-like structure. Ideally, the distance between two neighboring atoms is equal everywhere in the structure. Oscillatory states of the atoms may be induced as a result of external stimuli. We will first consider a one-dimensional crystalline structure that consists of n points having a mass m each, that are located in a row. Neighboring mass points are connected via elastic springs having spring-constant D, meaning that the change in energy is proportional (with proportionality constant D) to the change in distance between the points connected by the spring,

$$\Delta F = D \Delta x. \tag{1}$$

By $x_i(t)$ we denote the deflection (vertical displacement) of mass point i at time t. The



Initial state $t = 0$



Deflected state $t > 0$

force acting on x_i, F_i, is given by

$$F_i = F_{i,i+1} + F_{i,i-1}, \tag{2}$$

where $F_{i,i\pm1}$ is the force that $x_{i\pm1}$ exerts on x_i, which according to (1) amounts to

$$F_{i,i\pm1} = D(x_{i\pm1} - x_i). \tag{3}$$

a) Let $v_i(t) = \frac{\mathrm{d}}{\mathrm{d}t} x_i(t)$ be the velocity of mass point i. Use Newton's law,

$$\text{Force} = \frac{\mathrm{d}}{\mathrm{d}t}(\text{mass} \cdot \text{velocity}), \tag{4}$$

to derive the relation

$$\forall i = 2, \dots, n-1 : \quad \frac{\mathrm{d}^2}{\mathrm{d}t^2} x_i = \omega_0^2 (x_{i+1} - 2x_i + x_{i-1}), \tag{5}$$

with $\omega_0^2 = \frac{D}{m}$.

b) Suppose that the deflection for the first and last mass points are given as

$$x_1(t) = x_{1,0}(t), \quad x_n(t) = x_{n,0}(t), \quad t \geq 0. \tag{6}$$

Denote by a the distance between two consecutive mass points. Since there are many atoms are located in the crystalline structure, we strive to make the transitions $a \to 0$ and $n \to \infty$, while the total length of the sample structure $L = na$ remains constant. By passing to the limits, we can represent the deflection of any point x from the crystalline structure at rest by a deflection function u via

$$x_i(t) = u(x,t), \quad \text{where } x = ia. \tag{7}$$

Rewrite the differential equation obtained from a) so that it applies to the deflection function u. Then, perform a Taylor expansion of order 2 of $u(x \pm a, t)$ for any (x,t) in the first argument. Insert the Taylor expansion into (5).

c) Finally, pass to the limit of the longitudinal distance parameter, $a \to 0$, to obtain the well-known wave equation

$$\forall (x,t) \in (0,L) \times (0,\infty): \quad \frac{\partial^2}{\partial t^2} u(x,t) = c^2 \frac{\partial^2}{\partial x^2} u(x,t), \tag{8}$$

Identify an expression for c and show that, ignoring the boundary conditions, a solution is given by

$$u(x,t) = y(\pm(ct - x)) \tag{9}$$

for any sufficiently differentiable univariate function $y = y(q)$.

Find a non-trivial solution for the homogeneous boundary conditions $u(0,t) = u(L,t) = 0$.

d) In reality, a rectangular piece of matter is made up of many parallel such systems replicated, say every distance b, in the y and z dimensions. The mass of one particle is thus related to the material density ρ,

$$m = ab^2\rho. \tag{10}$$

For a block of material pulled parallel to the x direction we find experimentally that a displacement $u(x)$ prompts an elastic force per perpendicular area scaled by the elasticity modulus μ,

$$F = \mu \,\text{area}\, \frac{\partial u}{\partial x}, \qquad \text{thus} \qquad \mu = \frac{D\Delta u}{\text{area}\,\Delta u/a} = \frac{Da}{b^2}. \tag{11}$$

For example, we measure:

material	$\rho/\frac{\text{kg}}{\text{m}^3}$	$\mu/\frac{\text{N}}{\text{m}^2}$
rubber	1060	$4 \cdot 10^6$
steel	8050	$2 \cdot 10^{11}$
saphhire	3980	$345 \cdot 10^9$

Express c (aka. the speed of sound) by invariant physical constants and compute it for each of the materials tabulated above.

Exercise 2. (Green's identities)

(6 Points)

Recall the divergence theorem:
Let $\Omega \subset \mathbb{R}^d$ be an open and bounded subset with smooth boundary ∂D. For a continuously differentiable vector field $F\colon \Omega \to \mathbb{R}^d$, it holds

$$\int_\Omega \operatorname{div} F(x)\,\mathrm{d}x = \int_{\partial\Omega} F(x)\cdot n(x)\,\mathrm{d}s\,,$$

where $n(x)$ is the outer normal vector.
Use the divergence theorem to show the following identities for $u, v \in C^2(D)$:

a) $\int_\Omega \Delta u(x)\,\mathrm{d}x = \int_{\partial\Omega} \nabla u(x)\cdot n(x)\,\mathrm{d}s$

b) $\int_\Omega v(x)\Delta u(x)\,\mathrm{d}x + \int_\Omega \nabla u(x)\cdot\nabla v(x)\,\mathrm{d}x = \int_{\partial\Omega} v(x)\nabla u(x)\cdot n(x)\,\mathrm{d}s$

c) $\int_\Omega (u(x)\Delta v(x) - v(x)\Delta u(x))\,\mathrm{d}x = \int_{\partial\Omega}(u(x)\nabla v(x) - v\nabla u(x))\cdot n(x)\,\mathrm{d}s$

Exercise 3. (Rotational symmetry)

(6 Points)

Let Ω be a domain in $\mathbb{R}^d$ with $d \geq 1$ and let S be a linear orthogonal coordinate transformation on $\mathbb{R}^d$, i.e., $S^T S = I$. Show that $v := (u \circ S)$ satisfies

$$-\Delta v = -\Delta(u \circ S) = 0$$

provided that $u : \Omega \to \mathbb{R}$ solves $-\Delta u = 0$ on Ω.