Computational Physics - Project 1

Johannes Scheller, Vincent Noculak Lukas Powalla

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1 Introduction to Project 1

In physics, we often have to deal with differential equations o second order, which can be generally written in the from

$$\frac{d^2 y}{dx12} + k^2(x)y = f(x) \quad , \tag{1}$$

where we call f the inhomgeneous term and $k^2(x)$ is a real function. A special case of these cases is Poisson's equation, which reads in the one-dimensional, spherical case

$$\frac{1}{r^2}\frac{d}{dr}\left(r^2\frac{d\Phi}{dr}\right) = -4\pi\rho(\mathbf{r}) \quad . \tag{2}$$

Doing some substitutions, we can write this in the following, more general form:

$$-u''(x) = f(x) \tag{3}$$

In this project, we try to solve eq.(3) with the boundary conditions $u(0) = u(1) = 0$. Therefore, we have to discretize f and u. We approximate $u(x)$ as v_i, using a grid of n gridpoints $x_i = i \cdot h$. Thus, $h = 1/(n+1)$ is our steplength. We will also write $f_i = f(x_i) = f(hi)$.

Approximating the second derivative of u, we get

$$-\frac{v_{i+1} + v_{i-1} - 2v_i}{h^2} = f_i \tag{4}$$

Our goal is to solve this equation (4). Therefore, we will rewrite it as a set of linear equations in matrix form.

1.1 Rewriting the equation in matrix-form

Eq (4) can be written as a set of linear equations in matrix form. Therefore, we have to do the following steps:

$$\begin{aligned} -\frac{v_{i+1} + v_{i-1} - 2v_i}{h^2} &= f_i \\ -(v_{i+1} + v_{i-1} - 2v_i) &= h^2 \cdot f_i \qquad (5) \\ & \qquad (6) \end{aligned}$$

Assuming we have an $n \times n$-matrix $\mathbf{A}$ of the following form

$$\mathbf{A} = \begin{pmatrix} 2 & -1 & 0 & \dots & \dots & 0 \\ -1 & 2 & -1 & 0 & \dots & \dots \\ 0 & -1 & 2 & -1 & 0 & \dots \\ \dots & \dots & \dots & \dots & \dots & \dots \\ 0 & \dots & \dots & -1 & 2 & -1 \\ 0 & \dots & \dots & 0 & -1 & 2 \end{pmatrix} \quad , \tag{7}$$

then we can rewrite this matrix in index notation as

$$a_{ij} = \begin{cases} 2 & \text{if } i = j \\ -1 & \text{if } |i-j| = 1 \\ 0 & \text{else} \end{cases} \quad . \tag{8}$$

Using this, we can also rewrite the multiplication $\mathbf{w} = \mathbf{A} \cdot \mathbf{v}$ with an n-dimensional vector $\mathbf{v}$ in the following way:

$$w_i \underset{\text{def}}{=} \sum_{j=1}^{n} a_{ij} \cdot v_j \underset{(8)}{=} -v_{i-1} + 2v_i - v_{i+1} \tag{9}$$

By using this result and substituting $h^2 \cdot f_i \rightarrow \bar{b}$ in eq (5), we get to the following equation:

$$\mathbf{Av} = \bar{\mathbf{b}} \tag{10}$$

with matrix $\mathbf{A}$ as given above. This is a set of linear equations that we are going to solve with our programm. In this example, we will assume that $f(x)$ is given by $f(x) = 100\mathrm{e}^{-10x}$. Thus, the analytical solution of eq (3) is given by $u(x) = 1 - (1 - \mathrm{e}^{-10})x - \mathrm{e}^{-10x}$. We will later compare our numerical results to this solution.