

# FYS4150 - Project 1

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## Abstract

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## I. INTRODUCTION

THIS project will examine different techniques for approximating the solution to a differential equation where a continuous function is known. The equation describes an electrostatic potential  $\Phi$  generated by a localized charge density  $\rho(\vec{r})$  and is usually described - in three dimensions - by:

$$\nabla^2 \Phi = -4\pi\rho(\vec{r}) \quad (1)$$

If  $\rho(\vec{r})$  is spherical symmetric, eq. 1 may be written in a one-dimensional manner by substituting  $\phi(r) = r\Phi(r)$ :

$$\frac{d^2\phi(r)}{dr^2} = -4\pi r\rho(r) \quad (2)$$

By rewriting eq. 2 to a general form it reads:

$$-u''(x) = f(x) \quad (3)$$

In this specific case, the Poisson equation is solved by *Gaussian elimination* of a set of linear equations, both in a general manner and an optimized way of a specific matrix. The optimized method is later compared with another general method called *LU-decomposition*.

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\*A thank you or further information

## II. METHODS

The methods used in this projects are the following:

- Dirichlet boundary conditions
- Numerical derivation
- Gaussian elimination
- LU-decomposition

### i. Dirichlet boundary condition

Dirichlet boundary conditions - also referred to as fixed boundary condition - specifies the value of a given function on a surface  $T = f(r, t)$ . In a one-dimensional problem it translates to defining an interval of  $x$  -  $x \in [x_{min}, x_{max}]$  - and the function values  $f(x_{min}) = f_l$  and  $f(x_{max}) = f_h$  at the edges of the interval.

### ii. Numerical derivation

The derivative of a discrete function may be found by numerical derivation. The principle of numerical derivation is a result of Taylor expansion. By expanding a function from a point  $x$  with a step  $h$ , two equations

form depending on the direction:

$$f(x+h) = f(x) + hf'(x) + \frac{h^2}{2}f''(x) \dots \quad (4)$$

$$f(x-h) = f(x) - hf'(x) + \frac{h^2}{2}f''(x) \dots \quad (5)$$

By adding eq. 5 to eq. 4, a approximation for the second derivative is achieved.

$$f'' = \frac{f_+ - 2f + f_-}{h^2} + \frac{h^4}{6h^2}f^{IV} \quad (6)$$

Where  $f_+ = f(x+h)$ ,  $f = f(x)$ ,  $f_- = f(x-h)$  and  $f^{IV}$  is the fourth derivative of  $f(x)$ . By truncating the series at the fourth derivative a small mathematical error -  $\mathcal{O}$  - appears in the order of  $h^2$ . If a discrete funtion is introduced where  $f_i = f(x_i) = f(c_0 + ih)$ , eq. 6 may be rewritten to an algorithm for the nummerical second derivative.

$$f''_i = \frac{f_{i+1} - 2f_i + f_{i-1}}{h^2} \quad (7)$$

In eq. 7 the mathematical error  $\mathcal{O}(h^2)$  is neglected.

### iii. Gaussian elimination

Gaussian elimination is a method for simplifying a set of linear equations. It is easly visualized through a matrix notation of  $Ax = y$  where  $A$  and  $y$  is known.

$$\begin{bmatrix} a_{11} & a_{12} & a_{13} \\ a_{21} & a_{22} & a_{23} \\ a_{31} & a_{32} & a_{33} \end{bmatrix} \begin{bmatrix} x_1 \\ x_2 \\ x_3 \end{bmatrix} = \begin{bmatrix} y_1 \\ y_2 \\ y_3 \end{bmatrix} \quad (8)$$

Gaussian elimination is often divided into two main parts, forward and backward substitution.

#### iii.1 Forward substitution

The forward substitution is focusing to

### iv. LU-decompostition

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