

**UiO : Department of Physics**  
University of Oslo

# **Project 5: The diffusion equation**

FYS3150 - Computational physics

**Kristine Baluka Hein**  
**Anders Johansson**



# Contents

<b>1</b>	<b>Introduction</b>	<b>3</b>
<b>2</b>	<b>Mathematical theory</b>	<b>3</b>
2.1	Discretisation . . . . .	3
2.2	Forward Euler . . . . .	3
2.2.1	Derivation and error analysis . . . . .	3
2.2.2	Stability analysis . . . . .	4
2.3	Backward Euler . . . . .	4
2.3.1	Derivation and error analysis . . . . .	4
2.3.2	Stability analysis . . . . .	4
2.4	Crank-Nicolson . . . . .	4
2.4.1	Derivation and error analysis . . . . .	4
2.4.2	Stability analysis . . . . .	4
	<b>References</b>	<b>5</b>

## Abstract

Hei.

# 1 Introduction

## 2 Mathematical theory

We will now take a look into how we can numerically approximate the given problem. As there exists many different approaches, we have chosen to look at three different methods, namely Forward Euler, Backward Euler and Crank-Nicolson.

### 2.1 Discretisation

### 2.2 Forward Euler

#### 2.2.1 Derivation and error analysis

The Forward Euler scheme is an explicit scheme based on Taylor polynomials. To find an approximation of the time derivative of  $u$  at point  $(x_i, t_j)$ , a first order Taylor polynomial around  $x_i, t_j$  is used to calculate  $u(x_i, t_{j+1})$  is used:

$$u_{i,j+1} = u_{i,j} + \Delta t \frac{\partial u_{i,j}}{\partial t} + \frac{1}{2}(\Delta t)^2 \frac{\partial^2 u(x_i, \tilde{t})}{\partial t^2} \Rightarrow \frac{\partial u_{i,j}}{\partial t} = \frac{u_{i,j+1} - u_{i,j}}{\Delta t} + \frac{1}{2}\Delta t \frac{\partial^2 u(x_i, \tilde{t})}{\partial t^2} \quad (1)$$

where  $\tilde{t} \in (t_j, t_{j+1})$  and the last term is the truncation error, which is proportional to  $\Delta t$ .

Similarly, the three point approximation to the second derivative (derived in [1]) with its error is used to approximate the second derivative of  $u$  at point  $(x_i, t_j)$  with respect to position:

$$\frac{\partial^2 u_{i,j}}{\partial x^2} = \frac{u_{i+1,j} + u_{i-1,j} - 2u_{i,j}}{h^2} - \frac{1}{12}h^2 \frac{\partial^4 u(\tilde{x}, t_j)}{\partial x^4} \quad (2)$$

where the last term is the truncation error, which for this approximation is proportional to  $h^2$ . The observation  $\tilde{x} \in (x_{i-1,j} + x_{i+1,j})$  is shown in the referenced report.

Inserting these two expressions into the diffusion equation gives

$$\frac{u_{i,j+1} - u_{i,j}}{\Delta t} + \frac{1}{2}\Delta t \frac{\partial^2 u(x_i, \tilde{t})}{\partial t^2} = \frac{u_{i+1,j} + u_{i-1,j} - 2u_{i,j}}{h^2} - \frac{1}{12}h^2 \frac{\partial^4 u(\tilde{x}, t_j)}{\partial x^4}$$

The goal is to find the value of  $u$  at the next time step, i.e.  $u_{i,j+1}$ . Multiplying by  $\Delta t$  on both sides of the equation and moving one term to the right, we get

$$u_{i,j+1} = u_{i,j} + \frac{\Delta t}{h^2}(u_{i+1,j} + u_{i-1,j} - 2u_{i,j}) + \frac{1}{2}(\Delta t)^2 \frac{\partial^2 u(x_i, \tilde{t})}{\partial t^2} - \Delta t \cdot \frac{1}{12}h^2 \frac{\partial^4 u(\tilde{x}, t_j)}{\partial x^4}$$

The quantity  $\Delta t/h^2$  can be defined as  $\alpha$ , which, with a slight reorganisation yields the final expression

$$u_{i,j+1} = (1 - 2\alpha)u_{i,j} + \alpha(u_{i+1,j} + u_{i-1,j}) + \frac{1}{2}(\Delta t)^2 \frac{\partial^2 u(x_i, \tilde{t})}{\partial t^2} - \Delta t \cdot \frac{1}{12}h^2 \frac{\partial^4 u(\tilde{x}, t_j)}{\partial x^4}$$

The two error terms are proportional to  $(\Delta t)^2$  and  $\Delta t \cdot h^2$ . As per usual, the global error is one order lower, as the error is accumulated. This gives one error term proportional to  $\Delta t$  and one proportional to  $h^2$ . The order of  $h$  is not reduced, as this error is not accumulated.

### 2.2.2 Stability analysis

## 2.3 Backward Euler

The idea of backward Euler is similar to the forward Euler. Actually, the only difference lies in how we approximate the time derivative of  $u$ .

### 2.3.1 Derivation and error analysis

We can also use Taylor polynomials of  $u(x_i, t_{j-1})$  to write an approximation of the time derivative of  $u$  around  $x_i, t_j$ :

$$u_{i,j-1} = u_{i,j} - \Delta t \frac{\partial u_{i,j}}{\partial t} + \frac{1}{2}(\Delta t)^2 \frac{\partial^2 u(x_i, \tilde{t})}{\partial t^2} \implies \frac{\partial u_{i,j}}{\partial t} = \frac{u_{i,j} - u_{i,j-1}}{\Delta t} + \frac{1}{2} \Delta t \frac{\partial^2 u(x_i, \tilde{t})}{\partial t^2}$$

where  $\tilde{t}$  and the second term are the same as defined in section 2.2.1 on the preceding page. Equation (2) on the previous page can be reused as an approximation to the second derivative.

With these approximations, the diffusion equation can be written as

$$\begin{aligned} \frac{u_{i,j} - u_{i,j-1}}{\Delta t} &= \frac{u_{i+1,j} - 2u_{i,j} + u_{i-1,j}}{h^2} \\ u_{i,j} - u_{i,j-1} &= \alpha(u_{i+1,j} - 2u_{i,j} + u_{i-1,j}) \\ -\alpha u_{i-1,j} + (1 + 2\alpha)u_{i,j} - \alpha u_{i+1,j} &= u_{i,j-1} \end{aligned}$$

### 2.3.2 Stability analysis

## 2.4 Crank-Nicolson

### 2.4.1 Derivation and error analysis

### 2.4.2 Stability analysis

## References

- [1] Anders Johansson. “Project 1”. In: *FYS3150, Computational Physics* (Sept. 2016), pp. 4–6. URL: [https://github.com/anjohan/Offentlig/blob/master/FYS3150/Oblig1/Johansson\\_Anders\\_FYS3150\\_Oblig1.pdf](https://github.com/anjohan/Offentlig/blob/master/FYS3150/Oblig1/Johansson_Anders_FYS3150_Oblig1.pdf).