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# **Project 5: The diffusion equation**

FYS3150 - Computational physics

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### Abstract

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# 1 Mathematical theory

## 1.1 Forward Euler

### 1.1.1 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:

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

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:

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

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 propotional to  $h^2$ . The order of  $h$  is not reduced, as this error is not accumulated.

### 1.1.2 Stability analysis

## 1.2 Backward Euler

**1.2.1 Derivation and error analysis****1.2.2 Stability analysis****1.3 Crank-Nicolson****1.3.1 Derivation and error analysis****1.3.2 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).