Diffusion

Sebastian Amundsen, Marcus Berget and Andreas Wetzel

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1 Introduction

In this report we want to test three algorithms for solving partial differentiation equations using finite difference schemes. Specifically we want to solve the heat equation in one dimension using three different methods, where we compare our numerical results to an analytical solution. Secondly, we wish to simulate the temperature distribution in the lithosphere. This is to be done in two dimensions using the Forward Euler algorithm.

2 Theory

2.1 Heat equation

The general heat equation can be written as,

$$\frac{\partial T(\mathbf{x},t)}{\partial t} = \frac{k}{C\rho}\nabla^2 T(\mathbf{x},t). \tag{1}$$

where $\mathbf{x}$ is the spatial vector, t is time, c_p is the specific heat capacity, ρ is the density and k is the thermal conductivity. We can then gather all the constants in the diffusion constant, $D = \frac{k}{C\rho}$. For the first part of the project we will just set the diffusion constant equal to one. The heat equation in one dimension then becomes,

$$\frac{\partial T(x,t)}{\partial t} = \frac{\partial^2 T(x,t)}{\partial x^2}, \tag{2}$$

or

$$T_{xx} = T_t. \tag{3}$$

2.2 Numerical methods for solving the heat equation

We set the initial conditions of equation (2) at $t = 0$ to,

$$T(x,0) = 0, \quad 0 < x < L \tag{4}$$

where $L = 1$ is the length of the x-region of interest. We set the boundary conditions to

$$T(0,t) = 0, \quad t \geq 0, \tag{5}$$

and

$$T(L,t) = 1, \quad t \geq 0. \tag{6}$$

Equation (2) with the mentioned initial conditions and boundary conditions can be solved numerically using the forward Euler method, the backward Euler method and the implicit Crank-Nicholson scheme.

2.2.1 Explicit forward Euler method

We proceed with equation (2) and the mentioned initial/boundary conditions. We define the step length for the spatial variable x,

$$\Delta x = \frac{1}{n+1}. \tag{7}$$

The position after i steps and time after j steps are then given by,

$$t_j = j\Delta t, \quad j \geq 0,$$
$$x_i = i\Delta x, \quad 0 \leq i \leq n+1.$$

By using the forward formula to approximate the derivatives we obtain

$$T_t = \frac{T_{i,j+1} - T_{i,j}}{\Delta t} \tag{8}$$

and

$$T_{xx} = \frac{T_{i+1,j} - 2T_{i,j} + T_{i-1,j}}{\Delta x^2}. \tag{9}$$

Defining the value $\alpha = \Delta t/\Delta x^2$, the one-dimensional heat equation can be rewritten as

$$T_{i,j+1} = \alpha T_{i-1,j} + (1-2\alpha)T_{i,j} + \alpha T_{i+1,j}. \tag{10}$$

We can then see than since the initial conditions are known, one could use equation (10) to find the temperature in the next time step, which one could use to the find the temperature after two time steps, and so on. This algorithm is an explicit scheme, since the temperature in the next time step is explicitly given.

2.2.2 Implicit backward Euler method

Here, we do just as for the forward Euler method, but instead of using the forward formula to approximate the first derivative, we use the backward formula,

$$T_t = \frac{T_{i,j} - T_{i,j-1}}{\Delta t}. \tag{11}$$

The spatial second derivative becomes just as for the explicit scheme,

$$T_{xx} = \frac{T_{i+1,j} - 2T_{i,j} + T_{i-1,j}}{\Delta x^2}. \tag{12}$$

Again, by defining $\alpha = \Delta t/\Delta x^2$ we obtain

$$T_{i,j-1} = -\alpha T_{i-1,j} + (1+2\alpha)T_{i,j} - \alpha T_{i+1,j}. \tag{13}$$

The only unknown quantity in equation 13 is $T_{i,j-1}$, which means that we can rewrite the equation as a matrix A:

$$A = \begin{bmatrix} 1+2\alpha & -\alpha & 0 & \cdots & 0 \\ -\alpha & 1+2\alpha & -\alpha & \cdots & 0 \\ \vdots & \ddots & \ddots & \ddots & \vdots \\ \vdots & \vdots & \ddots & \ddots & -\alpha \\ 0 & 0 & \cdots & -\alpha & 1+2\alpha \end{bmatrix} \tag{14}$$

We can reformulate the problem as a matrix vector multiplication:

$$AV_j = V_{j-1} \tag{15}$$

We can then write the problem as:

$$\begin{aligned} V_j &= A^{-1}V_{j-1} = A^{-1}(A^{-1}V_{j-2}) \\ &= A^{-1}(A^{-1}(A^{-1}V_{j-3})) = A^{-j}V_0 \end{aligned} \tag{16}$$

2.2.3 Crank-Nicholson scheme

The Crank-Nicholson scheme is given by

$$T_t = \frac{T(x_i, t_j + \Delta t) - T(x_i, t_j)}{\Delta t} \tag{17}$$

and

$$T_{xx} = \frac{1}{2}\Bigg(\frac{T(x_i+\Delta x, t_j) - 2T(x_i, t_j) + T(x_i - \Delta x, t_j) +}{\Delta x^2} \\ \frac{T(x_i+\Delta x, t_j+\Delta t) - 2T(x_i, t_j+\Delta t) + T(x_i - \Delta x, t_j+\Delta t)}{\Delta x^2}\Bigg) \tag{18}$$

We then combine equation 17 and 18, where the left side is given by $t_j + \Delta t$ and the right by t_j:

$$\begin{aligned} &-\alpha T(x_i - \Delta x, t_j + \Delta t) + (2+2\alpha)T(x_i, t_j + \Delta t) \\ &-\alpha T(x_i + \Delta x, t_j + \Delta t) = \alpha T(x_i - \Delta x, t_j) + (2-2\alpha)T(x_i, t_j) \\ &+\alpha T(x_i + \Delta x, t_j) \end{aligned} \tag{19}$$

Where we have used that $\alpha = \frac{D\Delta t}{\Delta x^2}$. We can write this as a tridiagonal matrix system:

$$(2I + \alpha B)V_j = (2I - \alpha B)V_{j-1} \tag{20}$$

We can rewrite equation 20 as:

$$V_j = (2I + \alpha B)^{-1}(2I - \alpha B)V_{j-1} \tag{21}$$

Where I is the identity matrix and B is given by:

$$B = \begin{bmatrix} 2 & -1 & 0 & \cdots & 0 \\ -1 & 2 & -1 & \cdots & 0 \\ \vdots & \ddots & \ddots & \ddots & \vdots \\ \vdots & \vdots & \ddots & \ddots & -1 \\ 0 & 0 & \cdots & -1 & 2 \end{bmatrix}$$

The truncation error for the Crank Nicholson scheme goes as $O(\Delta t^2)$ and is stable for all combinations of Δx and Δy.

2.3 Analytical solution for one dimensional heat equation

It is beneficial to have a analytical solution which we can compare our numerical methods to. For the one dimensional diffusion equation we have the analytical expression:

$$u(x,t) = x/L + \sum_{n=1}^{\infty} \frac{2(\pi n \cos(\pi n) - \sin(\pi n))}{\pi^2 n^2} \sin(n\pi x/L) e^{-n^2\pi^2 t/L} \tag{22}$$

Where g(x) is a function of position. The calculations are given in appendix B.

3 Method

3.1 One dimensional model

We start by implementing our numerical methods in one dimension. We begin by initializing our boundary and initial conditions. We will be testing our algorithms with different spatial steps given $\Delta x = 1/10$ and $\Delta x = 1/100$, where Δt will be dictated by the stability limit of the explicit scheme. This limit is given $\alpha < 0.5$. We therefore need to adjust the duration of each time step and the number of time steps we are using to fulfill this explicit limit. We wish to study the algorithms during two different occasions. There will be an equilibrium time before our solution becomes stable. It is relevant to study the system during this equilibrium time t_1 and when the system is close to stationary t_2. This will be done for each spatial step Δx. The truncation error should go according to Table 1.

3.1.1 Comparison between numerical and analytical model

We can test the stability and precision of our numerical algorithms by comparing our numerical approximations to our analytical solution given equation 22. We need to set N to something less than ∞ due to numerical limitations. We set N=1000. We compare our numerical and analytical results both visually by using plots and by studying the relative root mean square error (RRMSE). This will give us insight to how well our numerical approximations represent the one dimensional heat equation. We can then choose which of the three methods (Forward Euler, Backward Euler and Crank-Nicholson) best fit our analytical solution. The relative root mean square error is given by:

$$RRMSE = \sqrt{\frac{\frac{1}{n}\sum_{i=1}^{n}(u_{ana} - u_{num})^2}{\sum_{i=1}^{n} u_{ana}^2}} \tag{23}$$

Where u_{ana} is the analytical solution and u_{num} is the numerical approximation [4]. We will also be plotting the difference between the analytical solution and the values given the algorithms. This is to be done for both $\alpha > 0.5$ and $\alpha < 0.5$, which hopefully will showcase the stability of the implicit methods. To obtain the different values for α we adjust the duration of each time step in our simulation. The boundary given time steps Δt and spatial steps Δx for the explicit method is:

$$\Delta t \leq \Delta x^2/2 \tag{24}$$

We wish to study the case where this boundary is fulfilled and when it is unsatisfied.

4 Implementation

5 Results

5.1 One dimensional model

The analytical solution for different time occasions (t_1 and t_2) and spatial steps are given in Figure 1. The simulation time for each of the different algorithms are given in Table 2.

The deviation from the analytical solution for the three methods are given in Figure 3 and 5 for $\Delta x = 1/10$. The deviation for $\Delta x = 1/100$ is given in Figure 4 and 6. The RRMSE values are given in Table 3.

6 Discussion

6.1 One dimensional model

There is little variance between the three algorithms when looking at the one dimensional case (see Figure 2). The RRMSE values for $t_1 = 0.01$ were smallest for the Backward Euler method and highest for the Forward Euler method, when looking at $\Delta x = 1/10$. For $t_1 = 0.01$ and $\Delta x = 1/10$ the RRMSE values were highest for the Crank Nicholson scheme and smallest for the Backward Euler scheme. This is surprising given the fact that the Crank Nicholson algorithm has an higher order of truncation error than both the backward and forward method (Table 1). One explanation could be the amount of FLOPS for each method. The Crank Nicholson method has more calculations than both the other algorithms, which makes room for round off errors. It is also possible that either the algorithms, the analytical solution or the RRMSE method are not implemented correctly.

The differences in RRMSE were not detectable for t_2 (4). This is to be expected given that all three algorithms should move towards the same final solution (as long as the boundary condition for the explicit method is satisfied). We can see that the increased spatial resolution (decreasing Δx) leads to better precision for all the methods, due to the error becoming smaller for $\Delta x = 1/100$ than for $\Delta x = 1/10$. This is true for both t_1 and t_2.

The forward Euler method has the shortest simulation time by far, which make it time efficient when solving large simulations (Table 2). When $alpha < 0.5$ the deviation from the analytical solution is indistinguishable for the three methods when we are looking at Figure 3 and 4. Based on these factors, it seems that Forward Euler method is the best algorithm for solving the one dimensional problem as long as the boundary condition is fulfilled.

However, when $\alpha > 0.5$ the error for the explicit method (Forward Euler) "skyrockets" (Figure 5 and Figure 6). For the implicit schemes we dont have the same problem. The implicit solvers maintain stable at all values for α. It is therefore necessary to choose the numerical method based on the problem you wish to solve. The Forward Euler method might not be suitable when we are required to use larger time-steps in our simulation.

7 Concluding remarks

A Appendix

A.1 Figures

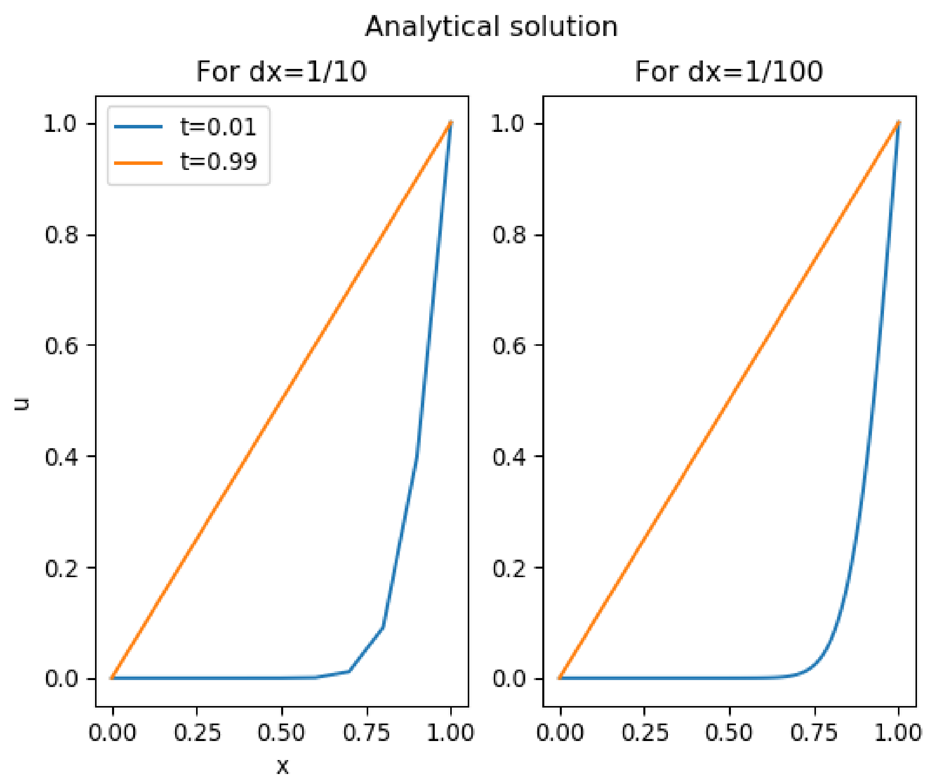

Figure 1: .

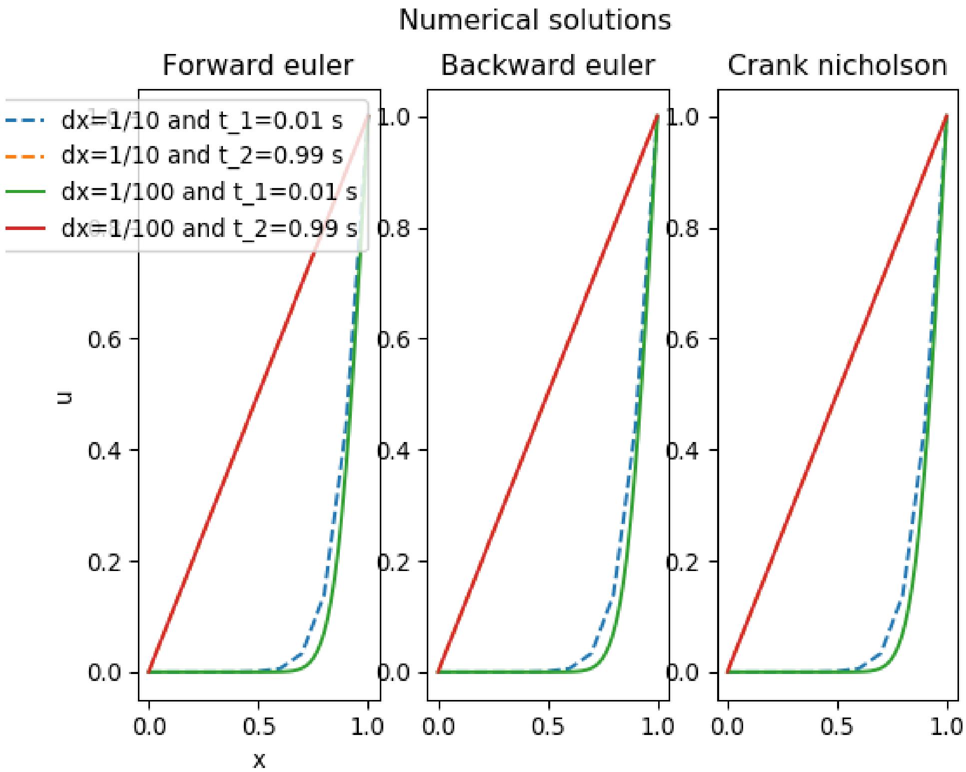
Numerical solutions
Forward euler
Backward euler
Crank nicholson
dx=1/10 and t_1=0.01 s
dx=1/10 and t_2=0.99 s
dx=1/100 and t_1=0.01 s
dx=1/100 and t_2=0.99 s
u
x
0.0
0.2
0.4
0.6
0.8
1.0
0.5

Figure 2: .

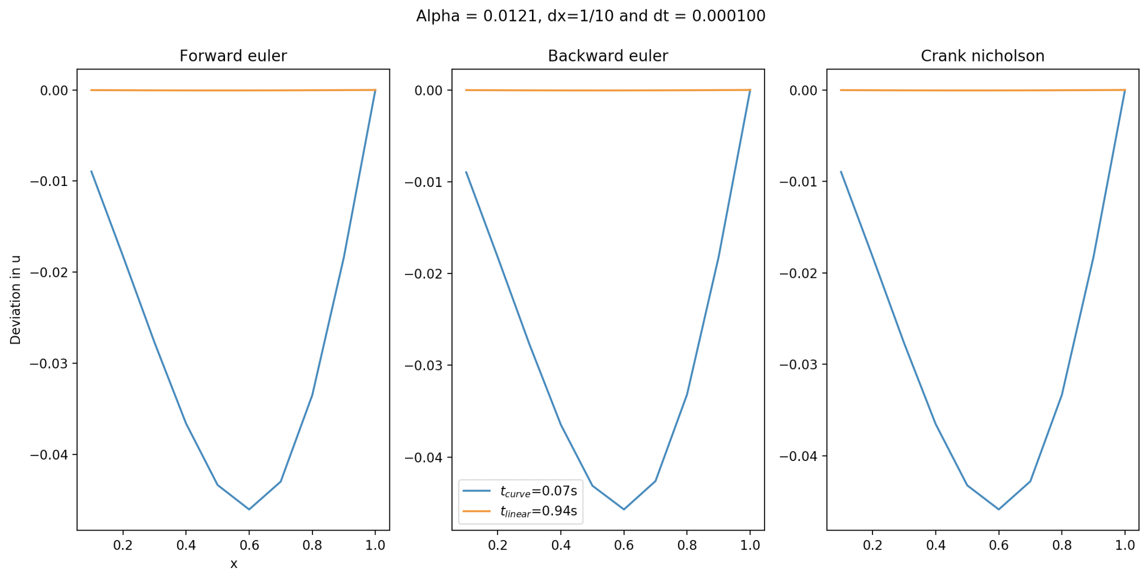

Figure 3: Deviation from analytical solution for $\alpha < 0.5$.

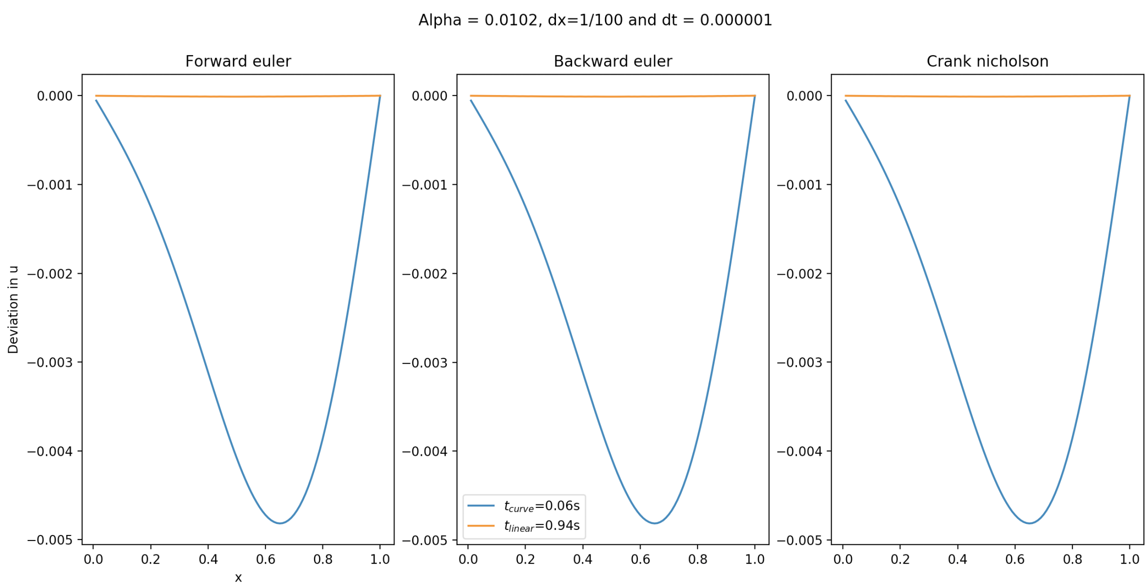

Figure 4: Deviation from analytical solution for $\alpha < 0.5$.

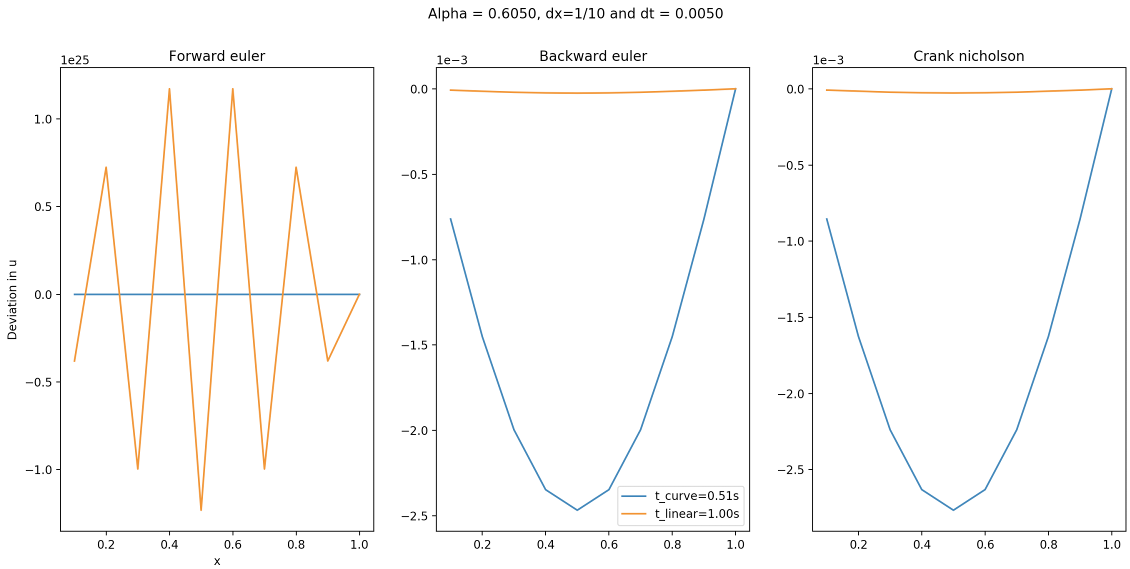

Figure 5: Deviation from analytical solution for $\alpha > 0.5$.

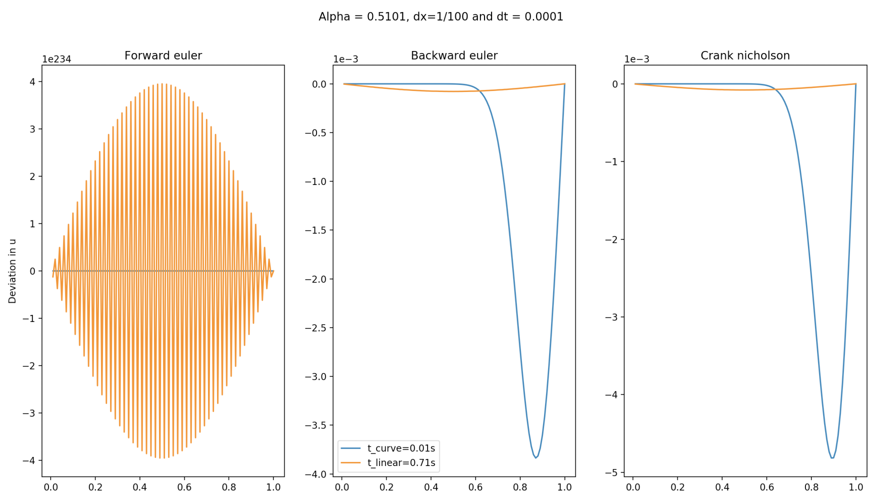

Figure 6: Deviation from analytical solution for $\alpha > 0.5$.

A.2 Tables

Table 1: Theoretical truncation errors.

Scheme:	Truncation error	Stability requirments
Crank Nicholson	$O(\Delta x^2)$ and $O(\Delta t^2)$	Stable for all
Backward Euler	$O(\Delta x^2)$ and $O(\Delta t)$	Stable for all
Froward Euler	$O(\Delta x^2)$ and $O(\Delta t)$	$\Delta t \leq 1/2 \Delta x^2$

Table 2: Simulation time for algorithms (1D case).

Scheme:	$\Delta x = 1/10$	$\Delta x = 1/100$
Crank Nicholson	0.019732s	14.9372s
Backward Euler	0.021026s	14.5824s
Froward Euler	0.00865s	3.58414s

Table 3: RRMSE for the different algorithms for $t_1 = 0.01$.

Scheme:	$\Delta x = 1/10$	$\Delta x = 1/100$
Crank Nicholson	0.034560	0.0038095
Backward Euler	0.034521	0.0038079
Froward Euler	0.034599	0.0038086

Table 4: RRMSE for the different algorithms for $t_2 = 0.99$.

Scheme:	$\Delta x = 1/10$	$\Delta x = 1/100$
Crank Nicholson	9.5847294×10^{-5}	6.7524668×10^{-5}
Backward Euler	9.5847294×10^{-5}	6.7524668×10^{-5}
Froward Euler	9.5847294×10^{-5}	6.7524668×10^{-5}

B Appendix

The one dimensional diffusion equation has an analytical expression for the continuous problem.

$$\nabla^2 u(x,t) = \frac{\partial u(x,t)}{\partial t} \tag{25}$$

The initial condition is $u(x,0) = g(x)$, when $0 < x < L$. We also have $u(0,t) = 0$ and $u(L,t) = 0$, when $t \leq 0$. We use separation of variables when solving 25:

$$u(x,t) = F(x)G(t) \tag{26}$$

This gives us one function only depending on position x and one only depending on time t. We get the set of equations:

$$\frac{\partial u}{\partial t} = F\frac{\partial G}{\partial t}$$

and

$$\frac{\partial^2 u}{\partial x^2} = G\frac{\partial^2 F}{\partial x^2}$$

We can now use the relation given equation 2:

$$\begin{aligned} F\frac{\partial G}{\partial t} &= G\frac{\partial^2 F}{\partial x^2} \\ \frac{1}{G}\frac{\partial G}{\partial t} &= \frac{1}{F}\frac{\partial^2 F}{\partial x^2} \end{aligned} \tag{27}$$

We set the equations equal to a negative constant $-\lambda^2$. This gives us the solutions:

$$\begin{aligned} G &= Ae^{-\lambda^2 t} \\ F &= B\cos(\lambda x) + C\sin(\lambda x) \end{aligned}$$

We can now use equation 26 to find the general solution u:

$$\begin{aligned} u = GF &= Ae^{-\lambda^2 t}[B\cos(\lambda x) + C\sin(\lambda x)] \\ &= e^{-\lambda^2 t}[C_1\cos(\lambda x) + C_2\sin(\lambda x)] \end{aligned} \tag{28}$$

The boundary conditions gives us the solution:

$$u(x,t) = A_n \sin(n\pi x/L)e^{-n^2\pi^2 t/L} \tag{29}$$

We have infinitely many solutions to this equation, due to the n factor. We can use a superposition of these solutions since the diffusion equation is linear:

$$u(x,t) = \sum_{n=1}^{\infty} A_n \sin(n\pi x/L)e^{-n^2\pi^2 t/L} \tag{30}$$

We decide the coefficient A_n by using the initial condition:

$$u(x,0) = g(x) = \sum_{n=1}^{\infty} A_n \sin(n\pi x/L) \tag{31}$$

Which gives us that:

$$A_n = \frac{2}{L}\int_0^L g(x)\sin(n\pi x/L)dx$$

We need to find the function g(x). We should obtain an equilibrium temperature when the time goes to infinity. This can be written as:

$$\lim_{t\to\infty} u(x,t) = u_E(x)$$

Where $u_E(x)$ is the equilibrium temperature. We can look at how this function behaves given the boundary conditions:

$$\frac{d^2u_E}{dx^2} = 0 \qquad u_E(0) = 0 \qquad u_E(L) = 1$$

This gives us the general solution:

$$u_E(x) = k_1x + k_2$$

Where k_1 and k_2 are constants. We get the function $u_E(x) = x/L$. Now we define a new function $v(x,t) = u(x,t) - u_E(x)$, where $u(x,t)$ is the solution to equation 30, which we wish to solve for:

$$u(x,t) = v(x,t) + u_E(x) \tag{32}$$

We need to know the boundary and initial conditions for $v(x,t)$:

$$\begin{aligned} v(x,0) &= u(x,0) - u_E(x) = 0 - x/L = -x/L \\ v(0,t) &= u(0,t) - u_E(0) = 0 - 0 = 0 \\ v(L,t) &= u(L,t) - u_E(L) = 1 - 1 = 0 \end{aligned}$$

We use the same method as earlier and find the solution for v(x,t):

$$v(x,t) = \sum_{n=1}^{\infty} B_n \sin{(n\pi x/L)} e^{-n^2\pi^2 t/L} \tag{33}$$

Where the coefficient B_n is given by:

$$B_n = \frac{2}{L}\int_0^L g(x)\sin{(n\pi x/L)}dx \tag{34}$$

Now we can use the fact that g(x)=v(x,0)=-x/L and equation 32:

$$u(x,t) = x/L + \sum_{n=1}^{\infty} \frac{2}{L}\int_0^L (-x/L)\sin{(n\pi x/L)}dx \sin{(n\pi x/L)} e^{-n^2\pi^2 t/L} \tag{35}$$

We solve the integral and find the final solution:

$$\begin{aligned} &\int_0^L (-x/L)\sin{(n\pi x/L)}dx = \frac{L(\pi n\cos{(\pi n)} - \sin{(\pi n)})}{\pi^2 n^2} \\ &\Rightarrow u(x,t) = x/L + \sum_{n=1}^{\infty} \frac{2(\pi n\cos{(\pi n)} - \sin{(\pi n)})}{\pi^2 n^2} \sin{(n\pi x/L)} e^{-n^2\pi^2 t/L} \end{aligned}$$

We now have a analytical expression for heat diffusion in one dimension [1][3].

References

[1] Jensen, M.H., 2015, Computational Physics Lecture Notes Fall 2015

[2] Jensen, M.H., 2017, Computational Physics Lectures: Statistical physics and the Ising Model

[3] Dawkins, Paul., 2018, Heat Equation With Non-Zero Temperature Boundaries

[4] Despotovic, M, et al., 2016, Evaluation of empirical models for predicting monthly mean horizontal diffuse solar radiation

[5] Daileda, R., 2012, The two dimensional heat equation