Solving the 1D and 2D diffusion equation
FYS4150 - Project 5

Karl Henrik Fredly
Universitetet i Oslo
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In this project, we will look at several different ways of solving the diffusion equation in both one and two dimensions. We will also look at a diffusion equation with a source term describing the heat production in the lithosphere. We will find that the Crank-Nicolson scheme outperforms both the explicit and implicit scheme in one dimension. It achieves a mean squared error of $2.8e-11$ with a step length $\Delta x = 0.01$, while the other two methods sit at around $3.3e-9$. For solving the 2D diffusion equation, we compared the explicit and implicit scheme. The implicit scheme requires an inefficient iterative method, and was slower and got a twice as large mean squared error as the explicit scheme in our testing. The lithosphere model let us analyze how radioactive enrichment affects the heat production in the lithosphere. Our main finding was that a decaying radioactive enrichment in the mantle 1Gy ago would lead to a large temperature increase across the entire lithosphere until around present day when the temperature would fall again throughout the lithosphere.

- Github repository with code and results:
https://github.com/KarlHenrik/ComputationalPhysicsMaster/tree/master/FYS4150/Project5

I. INTRODUCTION

The diffusion equation describes the behavior of many particles in Brownian motion. This has many applications, from simulating how a gas spreads to modeling the spread of temperature in a material. The use of finite difference methods to solving partial differential equations like the diffusion equation is another powerful tool which lets us better understand the physical world around us, especially with the great processor power of today.

In the methods section, we will present the diffusion equation in one and two dimensions, each with its own initial and boundary conditions to solve for. We will show how to solve the equations analytically, with the explicit scheme, the implicit scheme, and in one dimension, the Crank-Nicolson scheme as well. We will also describe the lithosphere model, and how to deal with the source term and scaling of the equation.

In the results section we present the results of our numerical solutions to these equations, including plots and measures of the mean squared error from the analytical solution for all of the methods.

In the discussion we discuss how the different solvers compare given our results, and interpret the physical ramifications of the results from the lithosphere model. Finally we summarize and conclude the report, with some possibilities for further improvements.

All code used to calculate the results in this report can be found in our github repository [1]. For this project we implemented the explicit, implicit and Crank-Nicolson scheme in 1D. We also implemented the explicit scheme in 2D and the implicit scheme in 2D which implements the Jacobi algorithm with parallelization.

II. METHODS

A. One-dimensional diffusion equation

The first equation we are going to solve is the diffusion equation in one dimension, with no source term:

$$\frac{\partial^2 v(x,t)}{\partial x^2} = \frac{\partial v(x,t)}{\partial t} \tag{1}$$

For our specific problem, we define

$$\begin{aligned} & x \in [0,1], \quad t > 0 \\ & v(x,0) = 0 \quad 0 < x < L \\ & v(0,t) = 0 \\ & v(1,t) = 1 \end{aligned} \tag{2}$$

These conditions model the temperature change in a rod with length 1, when it starts with a temperature 0 everywhere but the end at $x = 1$, where the temperature is 1 constantly. The end at $x = 0$, is set to have a constant temperature of 0. $v(x,t)$ is then the temperature at position x on the rod at time t.

We want the time-dependent part of $v(x,t)$ to be 0 at the boundaries however, so we write it as

$$v(x,t) = u(x,t) + f(x) \tag{3}$$

where $u(x,t)$ is 0 at $x = 0$ and $x = 1$, and $f(x)$ is 0 at $x = 0$ and 1 at $x = 1$, so that $v(x,t)$ fulfills the boundary conditions. We assume that $u(x,t)$ also obeys the diffusion equation. We then get

$$\frac{\partial^2 u(x,t)}{\partial x^2} = \frac{\partial u(x,t)}{\partial t} \tag{4}$$

This gives a constraint to $f(x)$ due to 1:

$$\begin{aligned}\frac{\partial^2(u(x,t)+f(x))}{\partial x^2} &= \frac{\partial(u(x,t)+f(x))}{\partial t}\\ \frac{\partial^2 u(x,t)}{\partial x^2}+\frac{\partial^2 f(x)}{\partial x^2} &= \frac{\partial u(x,t)}{\partial t}\\ \frac{\partial^2 f(x)}{\partial x^2} &= 0\end{aligned} \tag{5}$$

Given the boundaries of $f(x)$, and 4, we find that

$$f(x) = x \tag{6}$$

The initial condition for $u(x,t)$ then becomes $u(x,0) = -f(x) = -x$, for $0 < x < 1$. The general solution to equation 4 can be found by separation of variables. We write $u(x,t) = X(x)T(t)$ which when put into equation 4 gives

$$\frac{X''}{X} = \frac{T'}{T} \tag{7}$$

Since the equation must hold for all x and t, both sides must equal a separation constant we call $-\lambda^2$. This gives us the two expressions

$$\begin{aligned}X'' + \lambda^2 X &= 0\\ T' + \lambda^2 T &= 0\end{aligned} \tag{8}$$

with general solutions

$$\begin{aligned}X(x) &= A\sin\lambda x + B\cos\lambda x\\ T(t) &= Ce^{-\lambda^2 t}\end{aligned} \tag{9}$$

Since $u(0,t) = u(1,t) = 0$, $B = 0$ and $\lambda = n\pi$ where n is an integer. To fit the initial condition $u(x,0) = -x$, one must then find the infinite number of $X(x)$ terms with different A and n values that together equal $-x$ in the range $[0,1]$. We set C equal to 1 since we are free to change the Cs or As in unison. We call the coefficients A for each n the Fourier coefficients A_n.

The solution to 4 is then given by

$$u(x,t) = \sum_{n=1}^{\infty} A_n sin(n\pi x)e^{-n^2\pi^2 t} \tag{10}$$

This gives the analytical solution to the equation (via equation 3), which we will use to assess the numerical methods. Note that this analytical solution is dependant on numerical methods to find and use the Fourier coefficients, which makes it slightly inaccurate in practice.

B. One-dimensional schemes

We will be solving the equation with three finite difference schemes. The explicit scheme, the implicit scheme and the Crank-Nicolson scheme.

Since we will be dealing with finite differences, we no longer use the continuous variables x and t, but rather the discrete values values x_i and t_i which come in steps of Δx and Δt respectively. To make our equations more compact we use the notation $u_{i,j} = u(x_i, t_j)$ and $u_{i+1,j+1} = u(x_i + \Delta x, t_j + \Delta t)$.

In the explicit and implicit scheme, we use the following approximation for the second derivative

$$\frac{\partial^2 u(x_i,t_j)}{\partial x^2} \approx u_{xx}(x_i,t_j) = \frac{u_{i+1,j} - 2u_{i,j} + u_{i-1,j}}{\Delta x^2} \tag{11}$$

with a truncation error $\mathcal{O}(\Delta x^2)$.

In the explicit scheme, we use the following approximation for the time derivative

$$\frac{\partial u(x_i,t_j)}{\partial t} \approx \frac{u_{i,j+1} - u_{i,j}}{\Delta t} \tag{12}$$

Since we know the value of $u_{i,j} = u(x_i,t_j)$ for all x_i at the time $t_j = 0$ from the initial conditions, we can iteratively find the values $u_{i,j+1} = u(x_i, t_j + \Delta t)$ for all subsequent time steps by putting equation 11 and 12 into equation 1, and rewriting so that we get:

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

where $\alpha = \frac{\Delta t}{\Delta x^2}$. All of the terms on the right hand side are known for $t_i = 0$, which means the left hand side gives all the values for $t = 0 + \Delta t$. These values can again be used to find the values at the next timestep and so on. This is the explicit scheme. It has a truncation error of $\mathcal{O}(\Delta x^2 + \Delta t)$.

The explicit scheme can be written in terms of a matrix-vector multiplication:

$$\begin{aligned}U_{j+1} &= AU_j\\ &= \begin{bmatrix}(1-2\alpha) & \alpha & 0 & 0\dots\\ \alpha & (1-2\alpha) & \alpha & 0\dots\\ \dots & \dots & \dots & \dots\\ 0\dots & 0\dots & \alpha & (1-2\alpha)\end{bmatrix}\begin{bmatrix}u_{1,j}\\ u_{2,j}\\ \dots\\ u_{n,j}\end{bmatrix}\end{aligned} \tag{14}$$

so that the values U_{j+1} can be found by repeated matrix multiplications:

$$U_{j+1} = AU_j = \dots = A^{j+1}U_0 \tag{15}$$

Since we want U_j to approach a definite value, A needs to have a spectral radius less than 1. This gives the constraint for stability: $\alpha = \frac{\Delta t}{\Delta x^2} \leq 1/2$ [2].

The implicit scheme circumvents this constraint by using a different approximation for the time derivative:

$$\frac{\partial u(x_i,t_j)}{\partial t} \approx \frac{u_{i,j} - u_{i,j-1}}{\Delta t} \tag{16}$$

This, together with equation 1 and 11 leads to:

$$u_{i,j-1} = -\alpha u_{i+1,j} + (1+2\alpha)u_{i,j} - \alpha u_{i-1,j} \tag{17}$$

We can write this as a tridiagonal matrix equation:

$$\begin{aligned}U_{j-1} &= AU_j \\ &= \begin{bmatrix}(1+2\alpha) & -\alpha & 0 & 0\dots \\ -\alpha & (1+2\alpha) & -\alpha & 0\dots \\ \dots & \dots & \dots & \dots \\ 0\dots & 0\dots & -\alpha & (1+2\alpha)\end{bmatrix}\begin{bmatrix}u_{1,j} \\ u_{2,j} \\ \dots \\ u_{n,j}\end{bmatrix}\end{aligned} \tag{18}$$

This time, only the left hand side is known, but since it is a tridiagonal matrix equation it can be solved efficiently by forward and backward substitution as discussed in a previous project [3]. This is how the solution is calculated in the implicit scheme. In contrast to the explicit scheme, the matrix A is positive definite, which means that the matrix A^{-1} which drives the time evolution in this case, has a spectral radius less than 1. This means there is no criteria on Δx or Δt for stability. However, the truncation error is still $\mathcal{O}(\Delta x^2 + \Delta t)$.

The Crank-Nicolson scheme approximates the derivatives around the time $t + \Delta t/2$. This leads to the truncation error of the method being $\mathcal{O}(\Delta x^2 + \Delta t^2)$ [2]. We get the following approximation for the second derivative:

$$\frac{\partial^2 u(x_i, t_j)}{\partial x^2} \approx \frac{u_{xx}(x_i, t_{j+1})}{2} + \frac{u_{xx}(x_i, t_j)}{2} \tag{19}$$

and the time derivative

$$\frac{\partial u(x,t)}{\partial t} \approx \frac{u_{i,j+1} - u_{i,j}}{\Delta t} \tag{20}$$

Equation 19, 20 and 1 gives us

$$\frac{u_{xx}(x_i, t_{j+1})}{2} + \frac{u_{xx}(x_i, t_j)}{2} = \frac{u_{i,j+1} - u_{i,j}}{\Delta t} \tag{21}$$

which we can expand and reorganize to get

$$\begin{aligned}&\alpha u_{i+1,j} + (2 - 2\alpha)u_{i,j} + \alpha u_{i-1,j} \\ &= -\alpha u_{i+1,j+1} + (2 + 2\alpha)u_{i,j+1} - \alpha u_{i-1,j+1}\end{aligned} \tag{22}$$

The left hand side of this equation holds only known values. The right hand side contains three (two at the ends) unknowns for each t_j. This then becomes essentially the same problem as the tridiagonal matrix equation for the implicit scheme, equations 17 and 18. We therefore solve equation 22 in exactly the same way, with forward and backward substitution as in a previous project [3].

The tridiagonal matrix equation can also be solved by inversion of the matrix, which gives us a matrix which turns u at one time step into u at the next time step. It can be shown that this matrix always has a spectral radius less than 1, which means that the Crank-Nicolson scheme is stable for all Δx and Δt [2].

In our code implementation we take the boundary conditions into account directly by expanding(and thus breaking) the matrix equation slightly so that the first and last equations have an extra known value(the boundary value). We chose to code this approach due to its flexibility, but we chose to explain the typical approach in the report due to it being better at showing where the stability constraint comes from.

C. Two-dimensional diffusion equation

The two dimensional diffusion equation is given by

$$\frac{\partial^2 u(x,y,t)}{\partial x^2} + \frac{\partial^2 u(x,y,t)}{\partial y^2} = \frac{\partial u(x,t)}{\partial t} \tag{23}$$

For our specific problem, we define (chosen to give a nice analytical solution since we were free to choose)

$$\begin{aligned}&x, y \in [0,1], \qquad t > 0 \\ &u(x,y,0) = sin(\pi x)sin(\pi y) \qquad 0 < x, y < 1 \\ &u(0,y,t) = u(1,y,t) = u(x,0,t) = u(x,1,t) = 0\end{aligned} \tag{24}$$

The analytical solution is found in a similar way to the one dimensional equation. We must find the stationary state when the time derivative of u is 0, and subtract it from u to get 0 at all boundaries. Then we solve the diffusion equation for whatever remains [4].

In this case however, u is 0 at all boundaries, which means the stationary state of u is 0 everywhere. This means we can solve 23 directly.

We again use separation of variables and write $u(x,y,t) = X(x)Y(y)T(t)$. Using the same trick as in equation 7 and 8 we get the three expressions

$$\begin{aligned}X'' + \lambda_x^2 X &= 0 \\ Y'' + \lambda_y^2 Y &= 0 \\ T' + (\lambda_x^2 + \lambda_y^2)T &= 0\end{aligned} \tag{25}$$

The solution to these three functions with the conditions of the problem are(Y and T have no scaling constant, since we let A_{mn} decide the scaling of the total function)

$$\begin{aligned}X(x) &= A_{mn} sin(\lambda_x x) \\ Y(y) &= sin(\lambda_y y) \\ T(t) &= e^{-(\lambda_x^2 + \lambda_y^2)t}\end{aligned} \tag{26}$$

where $\lambda_x = m\pi$ and $\lambda_y = n\pi$, where m and n are integers. One must then find the Fourier coefficients A_{mn} that fit $u(x,y,0)$ to the initial condition of the problem. In our case, we only need one A_{mn} for $m = n = 1$, where $A_{mn} = 1$.

The analytical expression for $u(x,y,t)$ then becomes

$$\begin{aligned}u(x,y,t) &= \sum_{m=1}^{\infty}\sum_{n=1}^{\infty} A_{mn} sin(m\pi x) sin(n\pi y) e^{-n^2\pi^2 t} \\ &= sin(\pi x) sin(\pi y) e^{-2\pi^2 t}\end{aligned} \tag{27}$$

D. Two-dimensional schemes

The explicit scheme in two dimensions follows the same idea as the one in one dimension. We define

$$\frac{\partial^2 u(x,y,t)}{\partial x^2} \approx \frac{u(x - \Delta x, y, t) - 2u(x,y,t) + u(x + \Delta x, t, y)}{\Delta x^2} \tag{28}$$

with a truncation error of $\mathcal{O}(\Delta x^2)$. The second derivative wrt. y is of course completely equivalent. The approximation to the time derivative is given by

$$\frac{\partial u(x,y,t)}{\partial t} \approx \frac{u(x,y,t+\Delta t) - u(x,y,t)}{\Delta t} \tag{29}$$

with a truncation error of $\mathcal{O}(\Delta t)$. By putting these into equation 23, we get

$$\begin{aligned} &u(x,y,t+\Delta t) = u(x,y,t) + \alpha[u(x+\Delta x,y,t)+ \\ &u(x-\Delta x,y,t) + u(x,y+\Delta y,t) + u(x,y-\Delta y,t) - 4u(x,y,t)] \end{aligned} \tag{30}$$

All of the terms on the right hand side are known when calculating the values at the time $0+\Delta t$ (since the right hand side is then the values at $t=0$), which means we can find all values $u(x,y,\Delta t)$, and then $u(x,y,2\Delta t)$ and so on, just like the one dimensional case. The scheme has a stability criterion $\Delta t \leq \frac{\Delta x^2}{2} + \frac{\Delta y^2}{2}$.

The implicit scheme in two dimensions requires an iterative method to calculate a time step forward, due to the number of unknowns being too large in the equations that come from the iterative scheme. We will be implementing Jacobi's algorithm. In the implicit scheme the time derivative is approximated by

$$\frac{\partial u(x,y,t)}{\partial t} \approx \frac{u(x,y,t) - u(x,y,t-\Delta t)}{\Delta t} \tag{31}$$

with a truncation error of $\mathcal{O}(\Delta t)$. This, together with the spacial derivatives defined in equation 28 gives us the equation for the implicit scheme when put into equation 23:

$$\begin{aligned} u(x,y,t) = \frac{1}{1+4\alpha}[\alpha(u(x-\Delta x,y,t) + u(x+\Delta x,y,t)+ \\ u(x,y-\Delta y,t) + u(x,y+\Delta y,t)) + u(x,y,t-\Delta t)] \end{aligned} \tag{32}$$

On the right hand side, there are four values of u at the time t which we don't know. The Jacobi algorithm circumvents this problem by ignoring it until it goes away. The algorithm starts by guessing all the values $u(x,y,t) = u(x,y,t-\Delta t)$, then it updates all the values $u(x,y,t)$ by setting them equal to the right hand side of equation 32. We have now updated all of our guesses, and have completed one iteration of the algorithm. We then update all the values again using equation 32, but now with our updated guesses on the right hand side instead. This continues until the values $u(x,y,t)$ change less than some threshold during an iteration, or the maximum number of iterations have been reached [2]. Since we are updating every value $u(x,y,t)$ using only known unchanging values for each iteration, the Jacobi algorithm lends itself well to parallelization. Simply let each thread handle a given set of x values. The implicit scheme in two dimensions also doesn't have a stability criterion for the step lengths.

E. Temperature distribution in the lithosphere

Finally, we will apply our solvers to the diffusion equation with a source term. We will study a model of the Earth's lithosphere (crust and upper mantle). Radioactive decay produces heat at different rates in different parts of the lithosphere. Additionally, subduction can enrich the mantle with extra radioactive elements which produce extra heat until they have decayed.

With this heat source and the properties of the lithosphere taken into account, the temperature of the lithosphere $u(x,t)$ at the depth x(we are only interested in changes in temperature in depth) and time t is described by the equation

$$k\frac{\partial^2 u(x,t)}{\partial x^2} + Q(x,t) = \rho c_p \frac{\partial u(x,t)}{\partial t} \tag{33}$$

where we have the density of the lithosphere $\rho = 3.5 * 10^3 kg/m^3$, the thermal conductivity $k = 2.5\frac{W}{mC}$, the specific hear capacity $c_p = 1000\frac{J}{kgC}$. The heat source $Q(x,t)$ has a constant heat production in the upper crust(0-20km) of $1.4\mu W/m^3$, in the lower crust(20-40km) of $0.35\mu W/m^3$ and in the mantle(40-120km) of $0.05\mu W/m^3$.

The radioactive enrichment of the mantle leads to an extra heat production of $0.5\mu W/m^3$ in the mantle. We assume that this enrichment is caused 40% by U, 40% by Th and 20% by K, which means that over time, the extra heat production is given by

$$Q_+(t) = 0.5 * (0.4e^{-\lambda_U t} + 0.4e^{-\lambda_{Th} t} + 0.2e^{-\lambda_K t})\mu W/m^3 \tag{34}$$

where the different λ are the decay constants of each element given by $ln(2)/t_{1/2}$, where $t_{1/2}$ is the half-life of the element. The elements U, Th and K have the half-lives 4.47 Gy, 14.0 Gy and 1.25 Gy respectively.

With the source term and the constants explained, it remains only to show how the Crank-Nicolson scheme changes when we include a source term and constants. We start by collecting all physical constants in a constant D.

$$\begin{aligned} \frac{k}{\rho c_p}\frac{\partial^2 u(x,t)}{\partial x^2} + \frac{Q(x,t)}{\rho c_p} &= \frac{\partial u(x,t)}{\partial t} \\ D\frac{\partial^2 u(x,t)}{\partial x^2} + Q_0(x,t) &= \frac{\partial u(x,t)}{\partial t} \end{aligned} \tag{35}$$

where $Q_0(x,t)$ is defined to include the constant $1/\rho c_p$. The Crank-Nicolson scheme now includes an extra term, and a different factor for all of the terms from the double derivative approximation:

$$\begin{aligned} &\alpha u_{i+1,j} + (2-2\alpha)u_{i,j} + \alpha u_{i-1,j} + \Delta t Q_0(x_i,t_j) \\ &= -\alpha u_{i+1,j+1} + (2+2\alpha)u_{i,j+1} - \alpha u_{i-1,j+1} \end{aligned} \tag{36}$$

where $\alpha = D\frac{\Delta t}{\Delta x^2}$.

Before we solve equation 33 however, we need initial conditions, and we need to scale the equations. The heat at the surface(x=0) is a constant 8°C, and the heat at the bottom of our model, in the mantle(x=120km), is a constant 1300°C. The temperature in between starts at the steady state when no heat production is taken into account, which means a linear temperature change as seen for the simple 1D problem, since that problem is the exact same with some simple scaling. We will assume the radioactive enrichment happened 1Gy ago, and simulate the heat change up to present day and 9Gy in the future. This makes it sensible to use the unit Gy for time, units of 120km for depth (m_s for meters scaled), and a temperature scale where 0 corresponds to 8°C and 1300°C corresponds to 1 (T_s for temperature scaled). Each unit temperature then has the size $1T_s = 1292C$, and the scale is shifted down, so that $0T_s = 8C$.

The change of units leads to different values of the physical constants. The value of D will become

$$\begin{aligned} D = \frac{k}{\rho c_p} &= 7.14 * 10^{-7} \frac{J}{mCs} \frac{kgC}{J} \frac{m^3}{kg} = 7.14 * 10^{-7} m^2 \frac{1}{s} \\ &= 7.143 * 10^{-7} * \frac{m_s^2}{120000^2} * \frac{31556926 * 10^9}{Gy} \\ &= 1.565 \frac{m_s^2}{Gy} \end{aligned} \tag{37}$$

the heat production $Q_0(x, t)$ will also have its units changed, which means we must scale its output to change to the new units

$$\begin{aligned} \frac{1}{\rho c_p} \mu W/m^3 &= 2.8571 * 10^{-13} \frac{J}{sm^3} \frac{kgC}{J} \frac{m^3}{kg} = 2.8571 * 10^{-13} C \frac{1}{s} \\ &= 2.8571 * 10^{-13} * \frac{T_s}{1292} \frac{31556926 * 10^9}{Gy} \\ &= 6.9785 \frac{T_s}{Gy} \end{aligned} \tag{38}$$

With the physical units of our problem all having values going from 0 to 1, our program won't have to deal with very large numbers, and the solution should be easy to compare with results from other problems. We will scale the final computed results up again however, since we are most interested in the physical implications of the results when looking at plots.

III. RESULTS

A. One-dimensional diffusion equation

We solved the diffusion equation in one dimension with the explicit, implicit and Crank-Nicolson scheme for two different step sizes. We recorded the solution at two different times, and compared with the analytical solution. Figure 1, 2 and 3 show the three solutions for the step size $\Delta x = 0.1$.

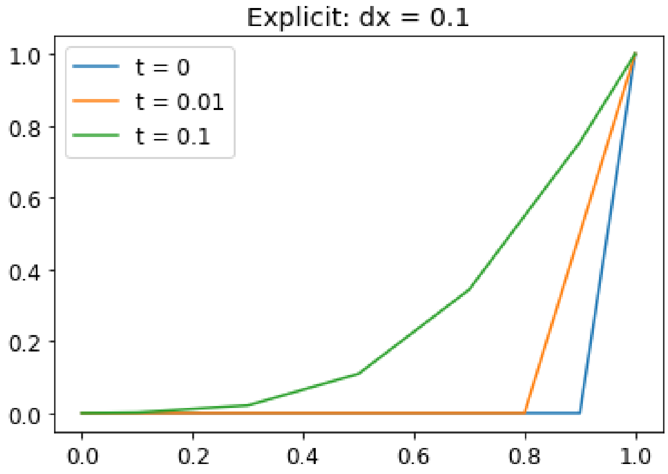

Figure 1. The 1D diffusion equation solved with the explicit scheme with $\Delta x = 0.1$ and $Deltat = \Delta x^2/2$. The initial condition is shown together with the solution at two later times.

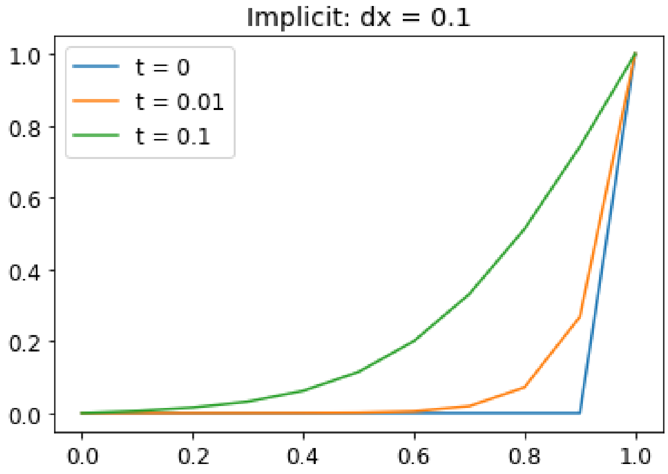

Figure 2. The 1D diffusion equation solved with the implicit scheme with $\Delta x = 0.1$ and $Deltat = \Delta x^2/2$. The initial condition is shown together with the solution at two later times.

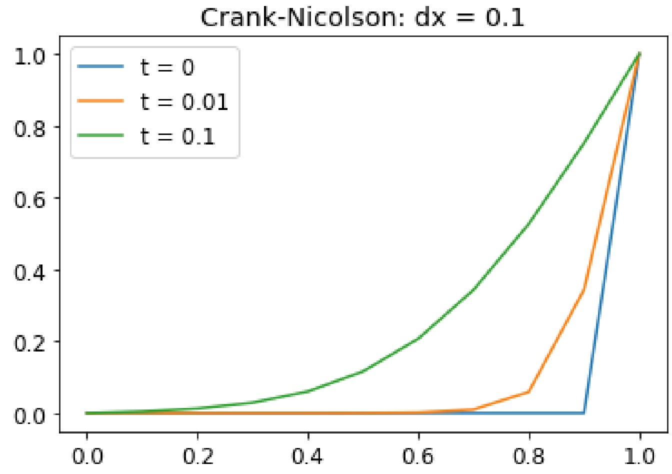

Figure 3. The 1D diffusion equation solved with the Crank-Nicolson scheme with $\Delta x = 0.1$ and $Deltat = \Delta x^2/2$. The initial condition is shown together with the solution at two later times.

Figure 4 shows the solution using the Crank-Nicolson scheme with the step size $\Delta x = 0.01$.

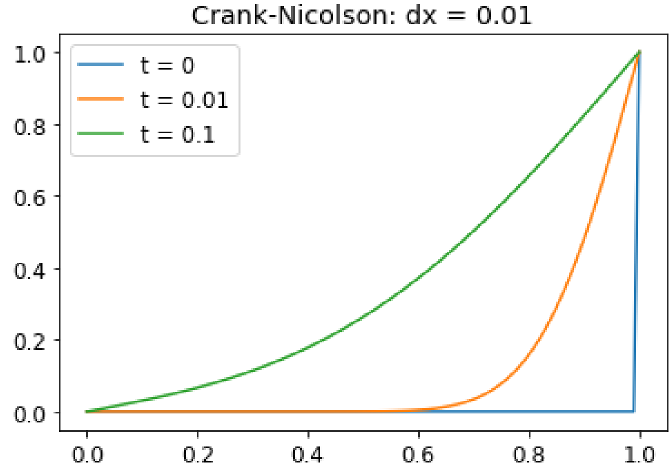

Figure 4. The 1D diffusion equation solved with the explicit scheme with $\Delta x = 0.01$ and $Deltat = \Delta x^2/2$. The initial condition is shown together with the solution at two later times.

The performance of these different methods with different step sizes at the two times are shown in table I.

	$\Delta x = 0.1$		$\Delta x = 0.01$	
	t = 0.01	t = 0.1	t = 0.01	t = 0.1
Explicit	2.394e-03	1.004e-02	1.132e-07	3.282e-09
Implicit	4.753e-03	1.186e-02	6.874e-08	2.364e-09
Crank-Nicolson	2.624e-03	1.089e-02	2.395e-09	2.767e-11

Table I. The mean squared error of the solution to the 1D diffusion equation using the three different schemes with two different step lengths. We used $\Delta t = \Delta x^2/2$. At the first time point the solution is quite curved, while at the second time point the solution is much closer to a linear function.

Table II shows the value of the expected truncation error in different situations.

	$\Delta x = 0.1$	$\Delta x = 0.01$
$\Delta x^2 + \Delta t$	1.500e-02	1.500e-04
$\Delta x^2 + \Delta t^2$	1.003e-02	1.000e-04
(2D) $2\Delta x^2 + \Delta t$	2.250e-02	2.250e-04

Table II. The value of the expected truncation error at with different step sizes and formulas for the truncation error. The first formula is for the 1D explicit and implicit schemes. The second is for the 1D Crank-Nicolson scheme. For these two, $\Delta t = \Delta x^2/2$, while for the formula for the truncation in the 2D explicit and implicit scheme $\Delta t = \Delta x^2/4$.

B. Two-dimensional diffusion equation

We solved the diffusion equation in two dimensions with the explicit and implicit scheme for two different step sizes. We recorded the solution at two different times, and compared with the analytical solution. Figures 5, 6 and 7 show the initial condition, the solution at $t = 0.01$ and the solution at $t = 0.05$ using the implicit scheme with a step size $\Delta x = \Delta y = 0.01$ and $\Delta t = \Delta x^2/4$.

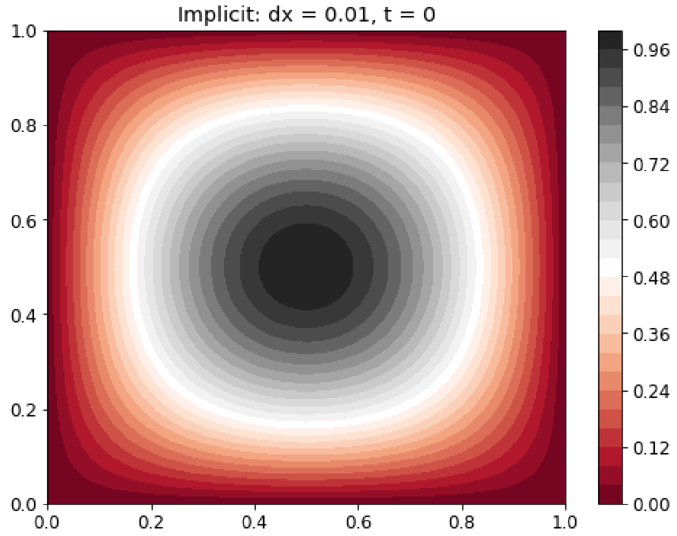

Figure 5. The initial condition to the 2D diffusion equation we solve.

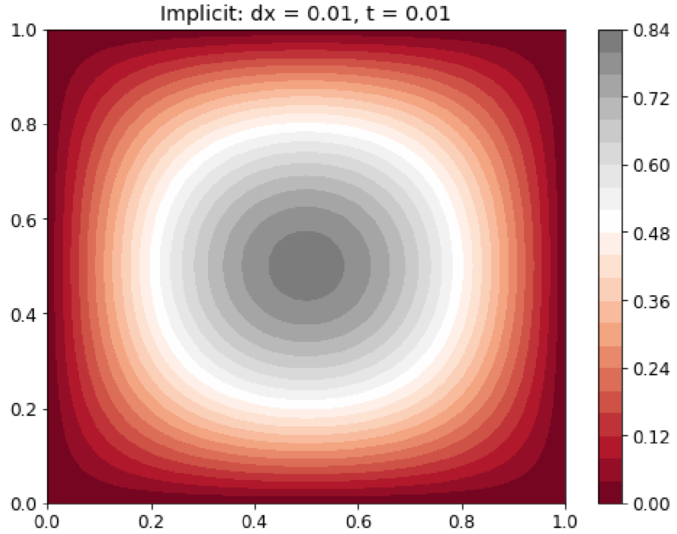

Figure 6. The 2D diffusion equation solved with the implicit scheme with $\Delta x = \Delta y = 0.01$ and $\Delta t = \Delta x^2/4$. This figure shows the solution at a time $t = 0.05$.

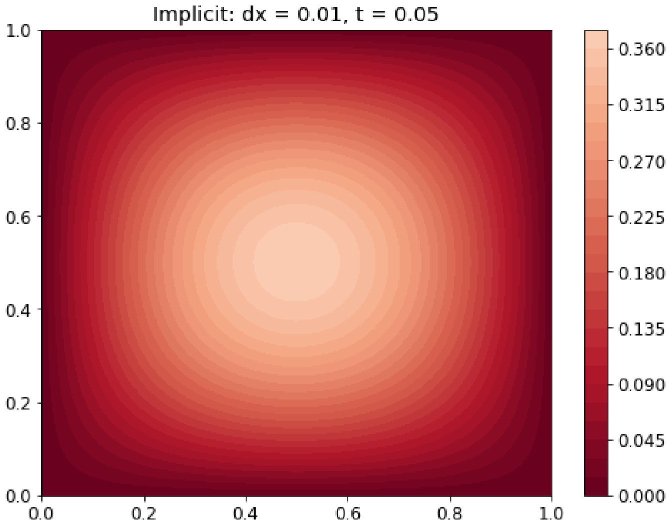

Figure 7. The 2D diffusion equation solved with the implicit scheme with $\Delta x = \Delta y = 0.01$ and $\Delta t = \Delta x^2/4$. This figure shows the solution at a time $t = 0.05$.

The performance of the two methods at the two different times using the two step lengths is shown in table III.

	$\Delta x = \Delta y = 0.1$		$\Delta x = \Delta y = 0.01$	
	t = 0.01	t = 0.05	t = 0.01	t = 0.05
Explicit	3.203e-04	1.999e-03	1.741e-10	8.984e-10
Implicit	4.293e-04	2.762e-03	6.966e-10	3.586e-09

Table III. The mean square error of the solution to the 2D diffusion equation using the two different schemes with two different step lengths. We used $\Delta t = \Delta x^2/4$. The the first time point, the solution is quite close to the 2D sinusoidal at the start, while the solution at the second time point is much flatter.

C. Temperature distribution in the lithosphere

We simulated the heat of the Earths lithosphere from 1Gy to today and into the future. The model we used came in three levels of complexity and realism. The first model assumed a constant heat production that was higher closer to the surface. The solution to the diffusion equation given by this model is shown in figure 8. We used the Crank-Nicolson scheme to solve these equations.

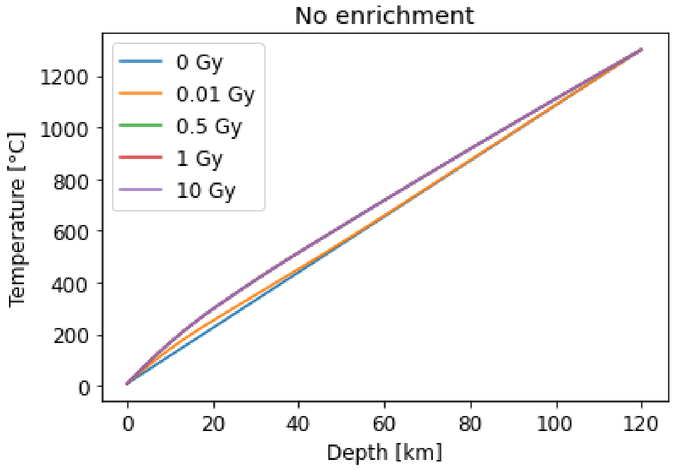

Figure 8. The solution to the diffusion equation describing the heat in the Earths lithosphere with a constant depth dependant heat production. Solved with the Crank-Nicolson scheme.

The second model assumed an enrichment of radioactive material into the mantle which caused extra constant heat production in the mantle. The solution to the diffusion equation given by this model is shown in figure 9.

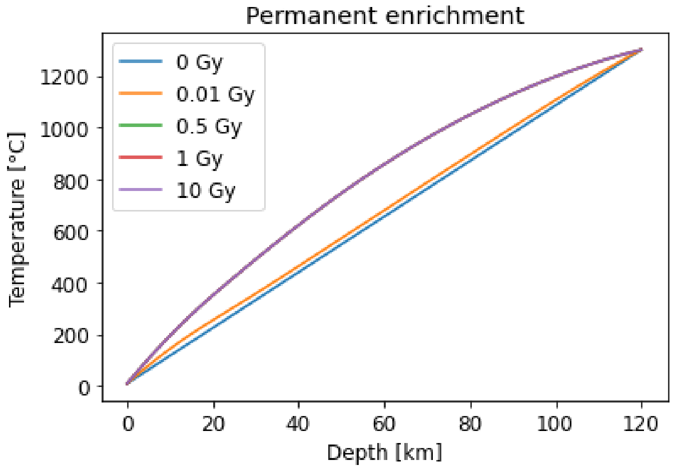

Figure 9. The solution to the diffusion equation describing the heat in the Earths lithosphere with a constant depth dependant heat production and extra heat production in the mantle. Solved with the Crank-Nicolson scheme.

The third and final model assumes that the radioactive enrichment to the mantle decays over time, which means the extra heat production in the mantle decreases over time. The solution to the diffusion equation given by this model is shown in figure 10.

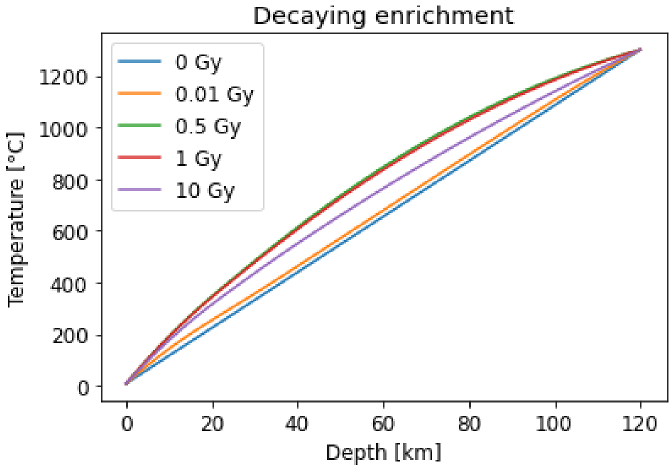

Figure 10. The solution to the diffusion equation describing the heat in the Earths lithosphere with a constant depth dependant heat production and extra decaying heat production in the mantle. Solved with the Crank-Nicolson scheme.

IV. DISCUSSION

The 1D solvers performed as expected. The explicit scheme and the implicit scheme took turns outperforming each other, but neither of them were much better at accuracy than the other. Figure 1 and 2 shows that the implicit method gives a much smoother plot for large step lengths, although it lead to a larger error in this case.

The Crank-Nicolson scheme was mostly better than the two other 1D schemes, especially for smaller time steps when its lower truncation error gives it a big advantage. If we compare table II and table I however, we see that the error for small step lengths is much smaller than the expected truncation error, which tells us that truncation error estimates aren't completely telling of the performance of a numerical method.

In two dimensions, the explicit scheme outperformed the implicit scheme, as shown in table III. The implicit scheme might be preferable in a case where a larger time step is needed, but in this case the use of the implicit scheme and Jacobi method lead to worse performance. More iterations and a smaller tolerance might make the Jacobi method perform better, but at that point it might be better again to use the explicit scheme with a smaller time step both in terms of accuracy and speed. Again, the errors were much smaller than the expected truncation errors. Figures 5, 6 and 7 show the temperature gradually evening out to 0 as expected.

Figure 8 shows the temperature change in the lithosphere with only a constant depth dependant heat source which is bigger near the surface. We see that the temperature becomes static already before 0.5Gy, which means the heat production reached equilibrium with the heat loss near the lower end. Since the most heat is produced near the surface, we see the largest bulge over the temperature gradient with no source near the surface.

Figure 9 shows the temperature change with a larger heat source in the mantle due to radioactive enrichment. Even though the heat source is still biggest near the surface, the large area with heat production and the distance to the cold surface leads to a much taller and wider increase in temperature compared to the temperature with no source.

Figure 10 shows the temperature change with a larger decaying heat source in the mantle due to radioactive enrichment. Here we see that the temperature quickly matched that of figure 9, but after just 1Gy starts decreasing again. After 10Gy the temperature is closer to the steady state in figure 8 with no extra source, but with a wider bulge due to there still being some heat production throughour the mantle. Given that this is supposed to model the heat production in the mantle given enrichment 1Gy ago, this means that we would expect the temperature to just have started decreasing from its maximum value throughout the lithosphere.

V. CONCLUSION

We found that for solving the 1D diffusion equation the explicit and implicit scheme were on an even footing. They both had a mean square error of around $3.3e-9$ with a step length of $\Delta x = 0.01$, but the Crank-Nicolson scheme was best with a mean square error of $2.8e-11$. For a larger step length, the Crank-Nicolson was only slightly better.

For solving the 2D diffusion equation, the explicit scheme had around a twice as small mean square error as the implicit scheme. The implicit sheme also relies on an expensive iterative method, so unless a very large time step is required, the explicit scheme is the best.

We modeled the heat production in the lithosphere with different heat productions at different depths, from 1Gy ago to 9Gy in the future. We simulated and analyzed a model with permanent radioactive enrichment, decaying radioactive enrichment, and no enrichment. In all three models we saw a distinct result. With no enrichment, the temperature increased the most compared to the steady temperature near the surface, due to the heat production being highest there. With permanent enrichment, we saw a large increase in temperature throughout the entire lithosphere, especially in the middle of the mantle, even though the heat production still was largest near the surface. This was due to the extra heat production being further away from the cold surface. In the final model we included a decaying heat production, which lead to a large temperature increase throughout the lithosphere, like in the previous model. But at around 1Gy, or today, the temperature started decreasing throughout the lithosphere.

Future improvements to our testing of diffusion equation solvers could include an analysis of how the different schemes perform for much smaller of much larger step sizes. One could also look at how the initial conditions affect the performance of the different schemes, such as smooth initial conditions vs. more ”spiky” initial conditions, like the ones often seen in real observations.

[1] “Github repository with code and results: github.com/KarlHenrik/ComputationalPhysicsMaster/tree/master/FYS4150/Project5,” (17.12.2020).

[2] M. Hjorth-Jensen, *Computational Physics, Lecture Notes Fall 2015* (Department of Physics, University of Oslo, August 2015) pp. 306–322.

[3] “Project 1: https://github.com/KarlHenrik/ComputationalPhysicsMaster/blob/master/FYS4150/Project1/Latex/Project1.pdf,” (17.12.2020).

[4] R. C. Daileda, “The two dimensional heat equation: http://ramanujan.math.trinity.edu/rdaileda/teach/s12 /m3357/lectures/lecture$_{36s}hort.pdf$,” (6.3.2012).