Partial Differential Equations
The Diffusion Equation

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Abstract

Contents

1 Introduction

In this project we want to study the numerical stability of different methods for solving partial differential equations (PDEs) and apply them to real world applications. First we will start off with the general one-dimensional diffusion equation and compare the numerical methods to the analytical solution to observe which method are the superior one. Then, by using the knowledge from the one-dimensional case, we will move to the two-dimensional case and further investigate the numerical methods accuracy to the closed form answer.

Finally, with all our experience with the general diffusion equation, we will attempt to study the heat diffusion found in the lithosphere.

These methods we will discuss are the explicit forward Euler algorithm

2 Theoretical Methods & Technicalities

2.1 Diffusion Equation in One Dimension

We start of with the one-dimensional PDE known as the diffusion equation

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

with initial conditions, i.e., the conditions at $t = 0$,

$$u(x,0) = 0 \qquad 0 < x < L$$

with $L = 1$ the length of the x-region of interest. The boundary conditions are

$$u(0,t) = 0 \qquad t \geq 0,$$

and

$$u(L,t) = 1 \qquad t \geq 0.$$

Luckily, it exists analytical solutions for this problem, and when doing scientifical research numerically, it is an invaluable resource to have analytical solutions to compare the numerical results with.

The analytical solution to this problem is

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

where the full derivation of this problem can be found in Appendix A.

2.1.1 Forward Euler - Explicit Scheme

One method of solving such a problem is the explicit forward Euler method. It starts by discretizing the time by a forward formula

$$\frac{\partial u}{\partial t} = u_t \approx \frac{u(x,t+\Delta t) - u(x,t)}{\Delta t} = \frac{u(x_i, t_j + \Delta t) - u(x_i, t_j)}{\Delta t}$$

with a truncation error which goes as $O(\Delta t)$,

and discretizing the position using a centered difference

$$\frac{\partial^2 u}{\partial x^2} = u_{xx} \approx \frac{u(x+\Delta x, t) - 2u(x,t) + u(x-\Delta x, t)}{\Delta x^2} = \frac{u(x_i + \Delta x, t_j) - 2u(x_i, t_j) + u(x_i - \Delta x, t_j)}{\Delta x^2}$$

with a local approximation error off $O(\Delta x^2)$.

These equations can be further simplified as

$$u_t \approx \frac{u_{i,j+1} - u_{i,j}}{\Delta t}$$
$$u_{xx} \approx \frac{u_{i+1,j} - 2u_{i,j} + u_{i-1,j}}{\Delta x^2}$$

and the one-dimensional diffusion equation can then be rewritten in its discretized version as

$$\frac{u_{i,j+1} - u_{i,j}}{\Delta t} = \frac{u_{i+1,j} - 2u_{i,j} + u_{i-1,j}}{\Delta x^2}.$$

By defining a parameter $\alpha = \frac{\Delta t}{\Delta x^2}$, results in the forward Euler explicit scheme

$$u_{i,j+1} = \alpha u_{i-1,j} + (1 - 2\alpha)u_{i,j} + \alpha u_{i+1,j}. \tag{3}$$

This system of equations can be rewritten in terms of a matrix-vector multiplication, by defining a matrix $\boldsymbol{A}$

$$\boldsymbol{A} = \begin{bmatrix} 1-2\alpha & \alpha & 0 & 0 & \dots & 0 \\ \alpha & 1-2\alpha & \alpha & 0 & \dots & 0 \\ 0 & \alpha & 1-2\alpha & \alpha & 0 & 0 \\ \dots & \dots & \dots & \dots & \dots & \dots \\ 0 & \dots & \dots & \alpha & 1-2\alpha & \alpha \\ 0 & \dots & \dots & \dots & \alpha & 1-2\alpha \end{bmatrix}$$

$$U_{j+1} = \boldsymbol{A}U_j \tag{4}$$

where the vector U_j is

$$U_j = \begin{bmatrix} u_{1,j} \\ u_{2,j} \\ \dots \\ u_{n,j} \end{bmatrix}$$

For a computation of the system over j time steps, then the matrix $\boldsymbol{A}$ is applied j times, then we can rewrite the problem as

$$U_j = \boldsymbol{A}U_{j-1} = \boldsymbol{A}\big(\boldsymbol{A}U_{j-2}\big) = \dots = \boldsymbol{A}^j U_0 \tag{5}$$

2.1.2 Backward Euler - Implicit Scheme

Another well known method of solving PDE's is the famous implicit scheme known as backward Euler. Here we start off with the so-called backward going Euler formula for the first derivative with respect to time, and discretize it.

$$u_t \approx \frac{u(x,t) - u(x,t-\Delta t)}{\Delta t} = \frac{u(x_i,t_j) - u(x_i,t_j-\Delta t)}{\Delta t}$$

still with a truncation error which goes like $O(\Delta t)$.

Then we use the approximated version for the second derivative with respect to position and discretize that as well

$$u_{xx} \approx \frac{u(x+\Delta x,t) - 2u(x,t) + u(x-\Delta x,t)}{\Delta x^2} = \frac{u(x_i+\Delta x,t_j) - 2u(x_i,t_j) + u(x_i-\Delta x,t_j)}{\Delta x^2}.$$

We now obtain

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

where $u_{i,j-1}$ is the only unknown quantity. By defining a matrix $\boldsymbol{A}$

$$\boldsymbol{A} = \begin{bmatrix} 1+2\alpha & -\alpha & 0 & 0 & \dots & 0 \\ -\alpha & 1+2\alpha & -\alpha & 0 & \dots & 0 \\ 0 & -\alpha & 1+2\alpha & -\alpha & 0 & 0 \\ \dots & \dots & \dots & \dots & \dots & \dots \\ 0 & \dots & \dots & -\alpha & 1+2\alpha & -\alpha \\ 0 & \dots & \dots & \dots & -\alpha & 1+2\alpha \end{bmatrix}$$

we can reformulate the problem as a matrix-vector multiplication

$$\boldsymbol{A}V_j = V_{j-1} \tag{6}$$

It means that we can rewrite the problem as

$$V_j = \boldsymbol{A}^{-1}V_{j-1} = \boldsymbol{A}^{-1}\big(\boldsymbol{A}^{-1}V_{j-2}\big) = \dots = A^{-j}V_0 \tag{7}$$

where the vector V_j is

$$V_j = \begin{bmatrix} u_{1,j} \\ u_{2,j} \\ \dots \\ u_{n,j} \end{bmatrix}$$

and V_0 is the initial vector at time $t=0$ defined by the initial value $u(x,0)$.

This is an implicit scheme since it relies on determining the vector $u_{i,j-1}$ instead of $u_{i,j+1}$. If α does not depend on time t, we then only need to invert the matrix once. Alternatively we can solve this system of equations using methods from linear algebra. These are however very cumbersome ways of solving since they involve $\sim O(N^3)$ operations for a $N \times N$. It is much faster to solve these linear equations using methods for tridiagonal matrices, since these involve only $\sim O(N)$ operations.

2.1.3 Crank-Nicolson - Implicit Scheme

It is possible to combine the implicit and explicit methods in a slightly more general approach. Introducing a parameter θ (the so-called θ-rule) we can set up an equation

$$\frac{\theta}{\Delta x^2}\big(u_{i-1,j}-2u_{i,j}+u_{i+1,j}\big)+\frac{1-\theta}{\Delta x^2}\big(u_{i+1,j-1}-2u_{i,j-1}+u_{i-1,j-1}\big)=\frac{1}{\Delta t}\big(u_{i,j}-u_{i,j-1}\big) \tag{8}$$

which for $\theta = 0$ yields the forward formula for the first derivative and the explicit scheme, while $\theta = 1$ yields the backward formula and the implicit scheme. These two schemes are called the backward and forward Euler schemes, respectively. For $\theta = 1/2$ we obtain a new scheme after its inventors, Crank and Nicolson. This scheme yields a truncation in time which goes like $O(\Delta t^2)$ and it is stable for all possible combinations of Δt and Δx.

To derive the Crank-Nicolson equation, one starts with the forward Euler scheme and Taylor expand $u(x, t + \Delta t)$, $u(x + \Delta x, t)$ and $u(x - \Delta x, t)$. However, for the Crank-Nicolson scheme one requires an additional Taylor expansion of $u(x, t + \Delta t)$, $u(x + \Delta x, t)$ and $u(x\Delta x, t)$ around $(x, t + \Delta t/2)$.

Omitting all the long and exciting derivation, which can be found here [1], we end up with the following equations

$$u_t \approx \frac{u(x, t + \Delta t) - u(x, t)}{\Delta t} = \frac{u(x_i, t_j + \Delta t) - u(x_i, t_j)}{\Delta t}.$$

The corresponding spatial second-order derivative reads

$$\begin{aligned} u_{xx} \approx & \frac{1}{2}\left(\frac{u(x_i + \Delta x, t_j) - 2u(x_i, t_j) + u(x_i - \Delta x, t_j)}{\Delta x^2} + \right. \\ & \left. \frac{u(x_i + \Delta x, t_j + \Delta t) - 2u(x_i, t_j + \Delta t) + u(x_i - \Delta x, t_j + \Delta t)}{\Delta x^2}\right). \end{aligned}$$

Note well that we are using a time-centered scheme wih $t + \Delta t/2$ as center. Using our previous definition of $\alpha = \frac{\Delta t}{\Delta x}$ we can rewrite Eq. 8 as

$$-\alpha u_{i-1,j} + (2 + 2\alpha)u_{i,j} - \alpha u_{i+1,j} = \alpha u_{i-1,j-1} + (2 - 2\alpha)u_{i,j-1} + \alpha u_{i+1,j-1} \tag{9}$$

or in matrix-vector form as

$$\Big(2\boldsymbol{I} + \alpha\boldsymbol{B}\Big)\boldsymbol{V}_j = \Big(2\boldsymbol{I} - \alpha\boldsymbol{B}\Big)\boldsymbol{V}_{j-1} \tag{10}$$

where the vector $\boldsymbol{V}_j$ is the same as defined in the implicit case (backward Euler) while the matrix $\boldsymbol{B}$ is

$$\boldsymbol{B} = \begin{bmatrix} 2 & -1 & 0 & 0 & \dots & 0 \\ -1 & 2 & -1 & 0 & \dots & 0 \\ 0 & -1 & 2 & -1 & 0 & 0 \\ \dots & \dots & \dots & \dots & \dots & \dots \\ 0 & \dots & \dots & -1 & 2 & -1 \\ 0 & \dots & \dots & \dots & -1 & 2 \end{bmatrix}$$

And we can rewrite the Crank-Nicholson scheme as follows

$$\boldsymbol{V}_j = \Big(2\boldsymbol{I} + \alpha\boldsymbol{B}\Big)^{-1}\Big(2\boldsymbol{I} - \alpha\boldsymbol{B}\Big)\boldsymbol{V}_{j-1} \tag{11}$$

$$\boldsymbol{V}_j = \Big(2\boldsymbol{I} + \alpha\boldsymbol{B}\Big)^{-1}\tilde{\boldsymbol{V}}_{j-1} \tag{12}$$

where $\tilde{\boldsymbol{V}}_{j-1} = \Big(2\boldsymbol{I} - \alpha\boldsymbol{B}\Big)\boldsymbol{V}_{j-1}$.

2.2 Truncation errors and stability properties

The truncation errors of all the different methods is given in table 1 and the derivation for them can be found here [1], where it is meticulously shown.

The stability criteria depends on the spectral radius, ρ_{max} of the matrix $\boldsymbol{A}$ in all the methods. The spectral radius of the matrix is defined as the largest absolute eigenvalue of the matrix

$$\rho(\boldsymbol{A}) = max\big\{|\lambda| : det\big(\boldsymbol{A} - \lambda\boldsymbol{I}\big) = 0\big\} \tag{13}$$

And the methods are stabile when they fulfil the condition of $\rho(\boldsymbol{A}) < 1$. The explicit scheme only satisfies the spectral radius for $\Delta t \leq \frac{1}{2}\Delta x^2$. However, the implicit schemes are always stable since their spectral radius always satisfies $\rho(\boldsymbol{A}) < 1$. This has been visualized in table 1. The proof for this can be found here [1].

Table 1: Truncation errors and stability

Scheme	**Truncation Error**	**Stability Requirements**
Crank-Nicolson	$O(\Delta x^2)$ & $O(\Delta t^2)$	Stable for all Δt & Δx
Backward Euler	$O(\Delta x^2)$ & $O(\Delta t)$	Stable for all Δt & Δx
Forward Euler	$O(\Delta x^2)$ & $O(\Delta t)$	$\Delta t \leq \frac{1}{2}\Delta x^2$

2.3 Diffusion Equation in Two Dimensions

In 2-dimensions the diffusion equation transforms into

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

And in this project we will be looking into the model with a square lattice for x and y. In addition, we will use the simple boundary conditions of

$$u(0,y,t) = u(L,y,t) = 0 \quad y \in (0,L) \quad t \geq 0,$$

and

$$u(x,0,t) = u(x,L,t) = 0 \quad x \in (0,L) \quad t \geq 0,$$

with initial conditions, i.e., the conditions at $t = 0$,

$$u(x,y,0) = \sin(\pi x)\sin(\pi y) \quad 0 < x,y < L$$

with $L = 1$ the length of the x,y-region of interest.

In this case as well, it also exists analytical solutions.

$$u(x,y,t) = \sin(\pi x)\sin(\pi y)e^{-2\pi^2 t} \tag{14}$$

where the derivation can be found in Appendix B.

2.3.1 Forward Euler - Explicit

$$\frac{\partial^2 u(x,y,t)}{\partial x^2} + \frac{\partial^2 u(x,y,t)}{\partial y^2} = \frac{\partial u(x,y,t)}{\partial t}, t > 0, x,y \in [0,1] \tag{15}$$

Forward Euler discretization for the time-derivative (compact notation):

$$u_t = \frac{u_{i,j}^{n+1} - u_{i,j}^n}{\Delta t} \tag{16}$$

Centered difference for the space derivatives:

$$u_{xx} = \frac{u_{i+1,j}^n - 2u_{i,j}^n + u_{i-1,j}^n}{\Delta x^2} \tag{17}$$

$$u_{yy} = \frac{u_{i,j+1}^n - 2u_{i,j}^n + u_{i,j-1}^n}{\Delta y^2} \tag{18}$$

This leads to

$$u_{i,j}^{n+1} = u_{i,j}^n + \alpha_x(u_{i+1,j}^n - 2u_{i,j}^n + u_{i-1,j}^n) + \alpha_y(u_{i,j+1}^n - 2u_{i,j}^n + u_{i,j-1}^n) \tag{19}$$

where

$$\alpha_x = \frac{\Delta t}{\Delta x^2} \tag{20}$$
$$\alpha_y = \frac{\Delta t}{\Delta y^2} \tag{21}$$

In this case, we will be using a uniform mesh, meaning $\Delta x = \Delta y$, resulting in $\alpha_x = \alpha_y = \alpha$. The scheme then looks like

$$u_{i,j}^{n+1} = u_{i,j}^n + \alpha(u_{i+1,j}^n + u_{i-1,j}^n + u_{i,j+1}^n + u_{i,j-1}^n - 4u_{i,j}^n) \tag{22}$$

2.3.2 Jacobi's Method - Implicit

$$\frac{\partial^2 u(x,y,t)}{\partial x^2} + \frac{\partial^2 u(x,y,t)}{\partial y^2} = \frac{\partial u(x,y,t)}{\partial t}, t > 0, x, y \in [0,1] \tag{23}$$

We discretize again position and time, and use the following approximation for the second derivatives for x and y

$$u_{xx} \approx \frac{u_{i+1,j}^n - 2u_{i,j}^n + u_{i-1,j}^n}{\Delta x^2} \tag{24}$$
$$u_{yy} \approx \frac{u_{i,j+1}^n - 2u_{i,j}^n + u_{i,j-1}^n}{\Delta y^2} \tag{25}$$

where

$$\alpha_x = \frac{\Delta t}{\Delta x^2} \tag{26}$$
$$\alpha_y = \frac{\Delta t}{\Delta y^2} \tag{27}$$

In this case, we will be using a uniform mesh, meaning $\Delta x = \Delta y$, resulting in $\alpha_x = \alpha_y = \alpha$.

We use now the so-called backward going Euler formula for the first derivative in time. In its discretized form we have

$$u_t \approx \frac{u_{i,j}^n - u_{i,j}^{n-1}}{\Delta t} \tag{28}$$

and this leads to

$$u_{i,j}^{n-1} = u_{i,j}^n + 4\alpha u_{i,j}^n - \alpha(u_{i+1,j}^n + u_{i-1,j}^n + u_{i,j+1}^n + u_{i,j-1}^n) \tag{29}$$
$$u_{i,j}^n = \frac{1}{1+4\alpha}\Big[\alpha(u_{i+1,j}^n + u_{i-1,j}^n + u_{i,j+1}^n + u_{i,j-1}^n) + u_{i,j}^{n-1}\Big] \tag{30}$$

or in a more compact form as

$$u_{i,j}^n = \frac{1}{1+4\alpha}\Big[\alpha\Delta_{i,j}^n + u_{i,j}^{n-1}\Big] \tag{31}$$

where $\Delta^n_{i,j} = u^n_{i+1,j} + u^n_{i-1,j} + u^n_{i,j+1} + u^n_{i,j-1}$.

It is possible to show that this equation can be transformed into a linear algebra problem of the type $\boldsymbol{Ax} = \boldsymbol{w}$, with $\boldsymbol{A}$ a matrix, $\boldsymbol{x}$ an unknown and $\boldsymbol{w}$ a known vector. An illustration of this can be found here [1].

To solve such a problem one can utilize iterative solvers, such as Jacobi's method. When setting up Jacobi's method, it is useful to rewrite the matrix $\boldsymbol{A}$ as

$$\boldsymbol{A} = \boldsymbol{D} + \boldsymbol{U} + \boldsymbol{L} \tag{32}$$

where $\boldsymbol{D}$ is a diagonal matrix, $\boldsymbol{U}$ is an upper triangular matrix and $\boldsymbol{L}$ is a lower triangular matrix. One can then rewrite the equation $\boldsymbol{Ax} = \boldsymbol{w}$ in terms of the matrices $\boldsymbol{D}, \boldsymbol{U}$ and $\boldsymbol{L}$.

$$\begin{align}
\boldsymbol{Ax} &= \boldsymbol{w} \tag{33}\\
(\boldsymbol{D} + \boldsymbol{U} + \boldsymbol{L})\boldsymbol{x} &= \boldsymbol{w} \tag{34}\\
\boldsymbol{x} &= \boldsymbol{D}^{-1}\big(\boldsymbol{w} - (\boldsymbol{U} + \boldsymbol{L})\boldsymbol{x}\big) \tag{35}\\
\boldsymbol{x}_{i+1} &= \boldsymbol{D}^{-1}\big(\boldsymbol{w} - (\boldsymbol{U} + \boldsymbol{L})\boldsymbol{x}_i\big) \quad i = 0, 1, 2, \ldots \tag{36}
\end{align}$$

However, Jacobi's method has some conditions that must be met, in order for it to converge. This method requires that the matrix $\boldsymbol{A}$ must be a positive/semi-positive definite matrix and be a diagonally dominant matrix.

2.4 Temperature distribution in the lithosphere

The purpose of this part is to calculate the thermal evolution of the lithosphere up to present following the emplacement of radioactive elements in the mantle wedge 1 Gy ago.

The equation to compute is the time evolution of the temperature distribution is the heat equation, which will be used only in 2D here, namely

$$\vec{\nabla}(k\vec{\nabla}T) + Q = \rho c_p \frac{\partial T}{\partial t} \tag{37}$$

where T is the temperature, ρ is the density, k is the thermal conductivity, c_p is the specific heat capacity and Q is the heat production.

To simplify the system, we will separate the lithosphere in 3 units: the upper crust, the lower crust and the mantle, all with different depth into the litosphere. The heat productions of the areas are illustrated below.

Table 2: The heat production (Q) of the different depth systems.

System	**Heat production** Q [$\mu W/m^3$]	**Depth** [km]
Upper Crust	1.4	0-20
Lower Crust	0.35	20-40
Mantle	0.05	40-120

Equation 37 has analytical solutions when studying at a steady state situation, and the full derivation for steady state case is shown in Appendix C. These solutions can be used as benchmark results to the numerical ones.

2.4.1 Heat production

As mentioned earlier, we will also study this system when it is affected by the heat production of the radioactive elements Uranium (U), Thorium (Th) and Potassium (K). We will look at the system in two situations. The first is when the heat production of the radioactive elements will remain constant over geological time and when the radioactivity will decrease with time.

The first situation is really straight forward, but to study the system where radioactivity will decrease with time, we need to include the half-lives of the radioactive elements. To implement this, the radioactive half-life formula is utilized

$$m_t = m_0 e^{-kt} \tag{38}$$

where m_t is the materials mass at time t, m_0 is the initial mass at time $t = 0$, k is the material's characteristic decay constant and t is the time.
The half-lives, concentrations, heat productions and decay constant of each material is presented in table 3.

Table 3: The distribution and heat production contributions of the radioactive elements U, Th, K in the mantle.

Radioactive Elements	**Concentration** [%]	**Halflife** [1Ga]	Q [$\mu W/m^3$]	**Decay constant** k [Gy^{-1}]
Uranium U	40	4.47	0.2	0.155
Thorium Th	40	14.0	0.2	0.0495
Potassium K	20	1.25	0.1	0.555

By utilizing equation 38 and the data in table 3, we can set up an equation that describes the heat production of the materials as a function of time.

$$Q_U(t) = Q_U e^{-kt} = 0.2e^{-0.155t}, \quad Q_{Th}(t) = Q_{Th} e^{-kt} = 0.2e^{-0.0495t} \quad \& \quad Q_K(t) = Q_K e^{-kt} = 0.1e^{-0.555t} \tag{39}$$

$$Q_{tot}(t) = Q_U(t) + Q_{Th}(t) + Q_K(t) = 0.2e^{-0.155t} + 0.2e^{-0.0495t} + 0.1e^{-0.555t} \tag{40}$$

$Q_{tot}(t)$ is the expression for the additional heat production caused by the radioactive elements.

2.4.2 Discretization & Scaling of Equations

To solve our partial differential equation we need to discretize. We do this in the following way:

$$T(x, y, t) = T(x_i, y_i, t_i) = T^n_{i,j}$$

And then we use the same approximations for the derivatives as for the implicit case in 2D.

$$\begin{aligned}
\frac{\partial^2 T}{\partial x^2} &= T^{xx} \approx \frac{T(x_i + \Delta x, y_j, t_n) - 2T(x_i, y_j, t_n) + T(x_i - \Delta x, y_j, t_n)}{\Delta x^2} \\
\frac{\partial^2 T}{\partial y^2} &= T^{yy} \approx \frac{T(x_i, y_j + \Delta y_j, t_n) - 2T(x_i, y_j, t_n) + T(x_i, y_j - \Delta y, t_n)}{\Delta y^2} \\
\frac{\partial T}{\partial t} &= T^t \approx \frac{T(x_i, y_j, t_n) - T(x_i, y_j, t_n - \Delta t)}{\Delta t}
\end{aligned}$$

$$\begin{aligned}
\vec{\nabla}(k\vec{\nabla}T) + Q &= \rho c_p \frac{\partial T}{\partial t} \\
k\Big(\frac{\partial^2 T}{\partial x^2} + \frac{\partial^2 T}{\partial y^2}\Big) + Q &= \rho c_p \frac{\partial T}{\partial t} \\
k\big(T^{n(xx)}_{i,j} + T^{n(yy)}_{i,j}\big) + Q &= \rho c_p T^{n(t)}_{i,j}
\end{aligned}$$

Using $\Delta x = \Delta y$, the equation now reads

$$\begin{aligned}
\frac{k}{\Delta x^2}\big(T^n_{i+1,j} + T^n_{i-1,j} + T^n_{i,j+1} + T^n_{i,j-1} - 4T^n_{i,j}\big) + Q &= \rho c_p \Big(\frac{T^n_{i,j} - T^{n-1}_{i,j}}{\Delta t}\Big) \\
\frac{k}{\rho c_p}\frac{\Delta t}{\Delta x^2}\big(\Delta^n_{i,j} - 4T^n_{i,j}\big) + \frac{\Delta t}{\rho c_p} Q &= T^n_{i,j} - T^{n-1}_{i,j}
\end{aligned}$$

where $\Delta^n_{i,j} = u^n_{i+1,j} + u^n_{i-1,j} + u^n_{i,j+1} + u^n_{i,j-1}$.

Rewriting the expression above to isolate $T^n_{i,j}$ one side, gives

$$T^n_{i,j} = \frac{1}{1 + 4\frac{k\Delta t}{\rho c_p \Delta x^2}} \left[\frac{k\Delta t}{\rho c_p \Delta x^2} \Delta^n_{i,j} + \frac{\Delta t}{\rho c_p} Q + T^{n-1}_{i,j} \right] \tag{41}$$

By introducing the parameter T_s that scales $T \in [0, 1]$ and the parameters x_s, t_s that scales the step sizes Δx and Δt gives

$$T^n_{i,j} = \frac{1}{1 + 4\frac{k t_s \Delta t}{\rho c_p x_s^2 \Delta x^2}} \left[\frac{k t_s \Delta t}{\rho c_p x_s^2 \Delta x^2} \Delta^n_{i,j} + \frac{t_s \Delta t}{T_c \rho c_p} Q + T^{n-1}_{i,j} \right] \tag{42}$$

and defining the parameters

$$\alpha = \frac{\Delta t}{\Delta x^2}, \quad \beta = \frac{k t_s}{x_s^2 \rho c_p} \quad \& \quad Q_c = \frac{t_s \Delta t}{\rho c_p T_c} \tag{43}$$

returns the following expression

$$T^n_{i,j} = \frac{1}{1 + 4\alpha\beta} \left[\alpha\beta\Delta^n_{i,j} + Q_c Q + T^{n-1}_{i,j} \right]. \tag{44}$$

And from the implicit scheme in 2D, we know that this kind of equation can be solved by transforming it into a linear algebra problem and utilize an iterative solver.

3 Implementation

Programs used in this project can be found on `https://github.com/jensbd/FYS4150/tree/master/Project5` and the Readme on the github repository explains how to run the scripts. All calculations are done in C++, while the plotting is done in Python.
The C++ programs are mainly based on the program codes found in the course's github repository `https://github.com/CompPhysics/ComputationalPhysics` [1]. We have also utilized the C++ library Armadillo [2] [3].

4 Results and Discussion

4.1 1D

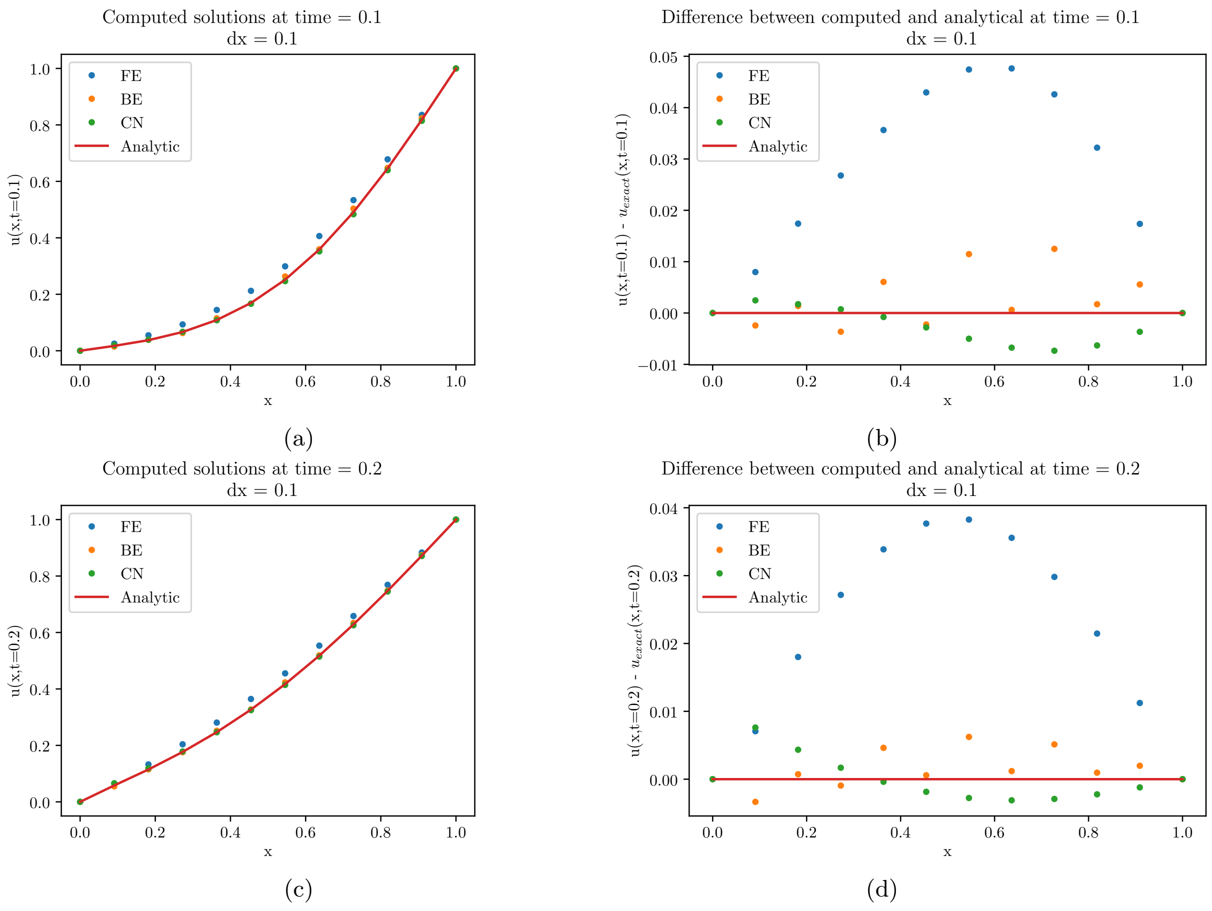


Figure 1: Comparison of the three schemes and analytic solution at time $t_1 = 0.1$ and $t_2 = 0.2$ with a step length of $\Delta x = 0.1$ and $\Delta t = 0.5\Delta x^2$.

From figure 1, we clearly see that the explicit Forward Euler scheme is the worst performer compared to the implicit schemes. Backward Euler and Crank-Nicolson are more closely matched, with a very slightly better performance from Crank-Nicolson. These results match the truncation errors listed in table 1, where Crank-Nicolson has the lowest truncation error with respect to time, where $\Delta t = \frac{1}{2}\Delta x^2$. Since Δt is so small compared to Δx the error will probably be dominated by Δx, which is confirmed by figure 1, where both implicit schemes give similar results.

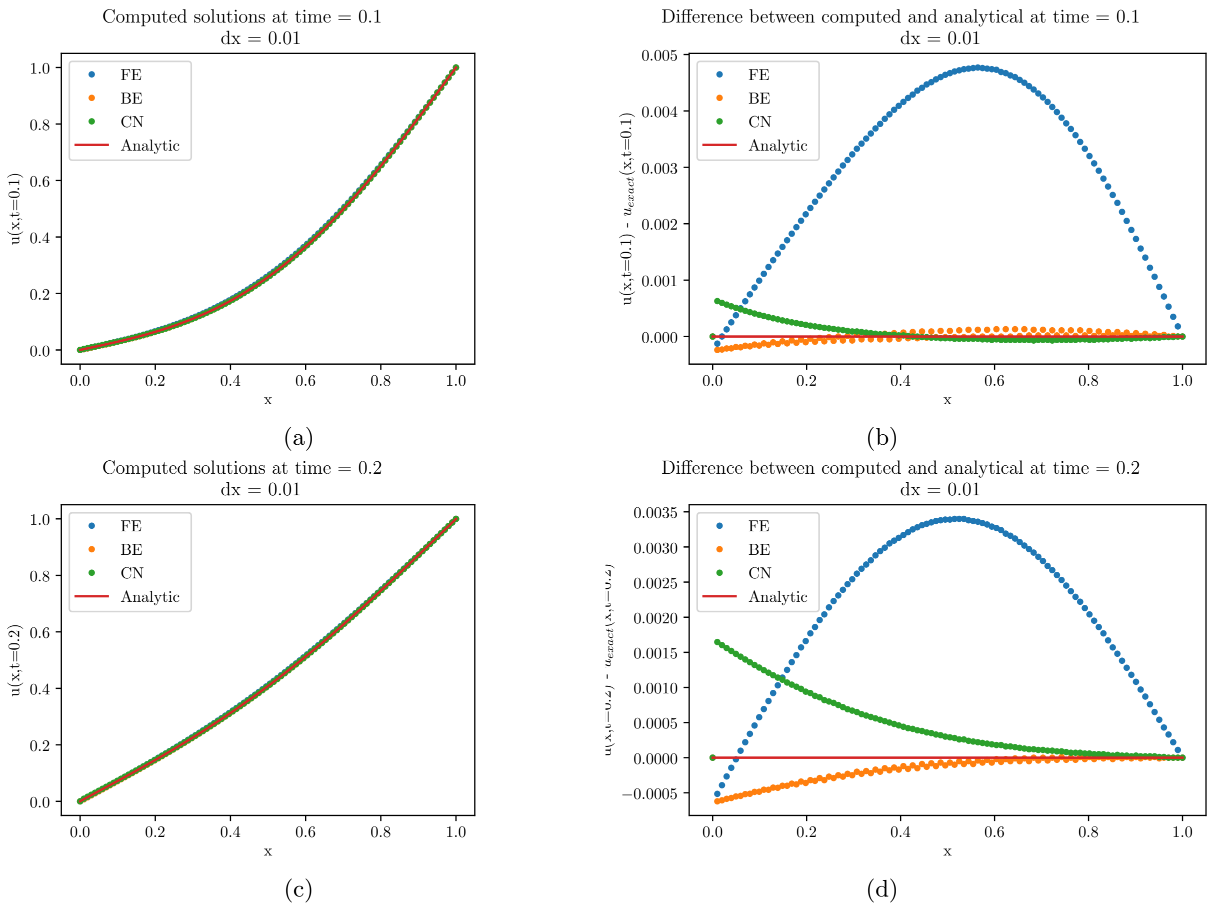


Figure 2: Comparison of the three schemes and analytic solution at time $t_1 = 0.1$ and $t_2 = 0.2$ with a step length of $\Delta x = 0.01$ and $\Delta t = 0.5\Delta x^2$.

In figure 2, where $\Delta x = 0.01$, we see the same trend as for $\Delta x = 0.1$, where forward Euler is still significantly worse than the implicit schemes. We also observe that the errors for all schemes have been reduced by a factor 10, as expected from the change of Δx. However in this scenario, Backward Euler seems to be the best performer, with an absolute maximum difference of ≈ 0.0005.

From these results, it is easy to see that the implicit schemes have much better performance than the explicit, therefore we chose an implicit scheme when going forward in this project.

4.2 2D

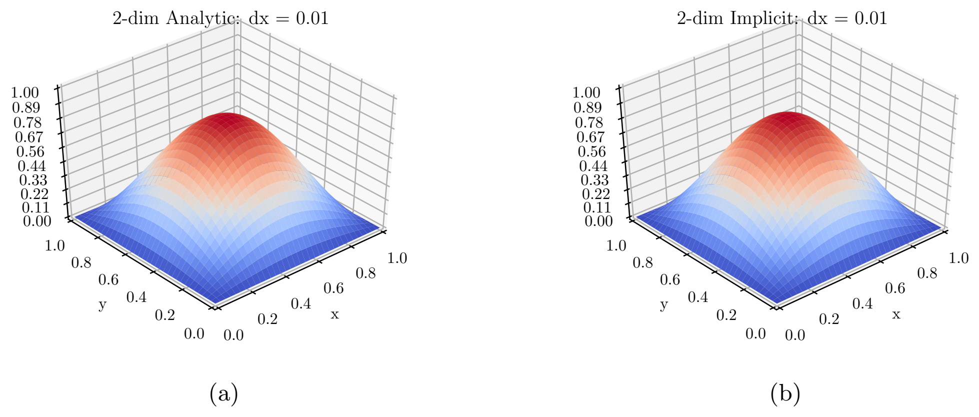


Figure 3: Comparison of analytical and numerical solution from the implicit scheme in 2 dimensions. We observe a very close match between the two figures.

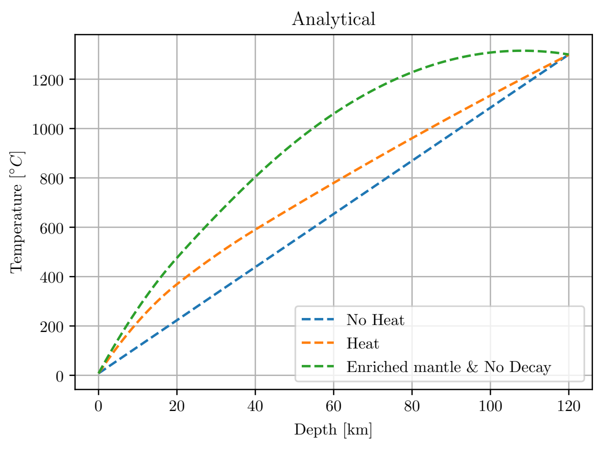
Table 4: Mean absolute differences between the 2-dimensional analytical solution and implicit scheme for different combinations of Δx and Δt, evaluated at one point in time.

Errors

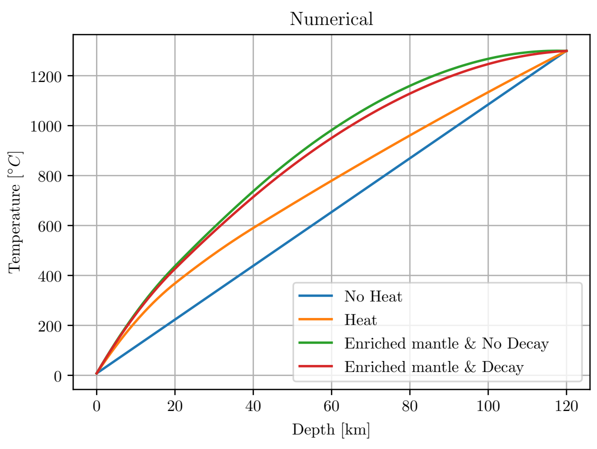
Δt	$\Delta x = 10^{-1}$	$\Delta x = 10^{-2}$
Δx	$7.87 \cdot 10^{-2}$	$6.51 \cdot 10^{-3}$
$\Delta x/10$	$5.11 \cdot 10^{-2}$	$5.05 \cdot 10^{-3}$
$\Delta x/100$	$4.83 \cdot 10^{-2}$	$5.07 \cdot 10^{-3}$

From table 4, we see that the error, as expected, is lower for the lower values of Δx and Δt. Interestingly however, this does not seem to hold for when $\Delta t = \Delta x/100$. Here, the error is more or less unchanged compared to the larger step-size above. We seem to have reached a limit for how small we can make Δt compared to Δx, and there may be very little to gain by decreasing Δt any further. Reducing the error from here will probably require a reduction in Δx, which will lead to a significant increase in runtime.

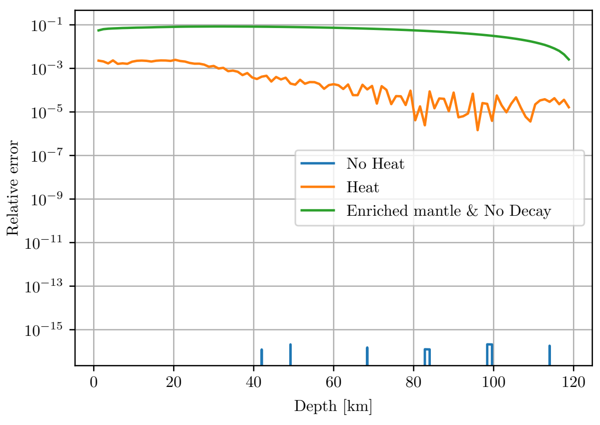
4.3 Lithosphere



(a)



(b)



(c)

Figure 4: Comparison of the analytical solution and numerical simulation of heat in the lithosphere with four different cases. Case 1 shows the situation for no heat production, case 2 shows the situation for heat production in each lithosphere layer, case 3 is the steady state situation for heat production and a constant enrichment of radioactive materials without decay, and lastly, case 4 shows the situation with an enriched mantle with radioactive decay. The last figure shows the relative error between the numerical simulations and analytical solutions for case 1-3.

From figure 4c, we see that the first case is almost perfectly approximated by the numerical simulation, and as expected, the error increases with the higher complexities of case 2 and 3. Since our simulations for case 1-3 seem reasonable and quite accurate, we can assume that our result for case 4 is valid and representative to some extent. In that case, we see that when the radioactive materials are decaying, the heat production decreases over time.

5 Conclusion

Appendices

A Analytical solution (1 dim)

We start of with the PDE

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

with initial conditions, i.e., the conditions at $t = 0$,

$$u(x,0) = 0 \qquad 0 < x < L$$

with $L = 1$ the length of the x-region of interest. The boundary conditions are

$$u(0,t) = 0 \qquad t \geq 0,$$

and

$$u(L,t) = 1 \qquad t \geq 0.$$

Then we make an assumption that the function $u(x,t)$ can be written in the form

$$u(x,t) = v(x,t) + ax$$

where $v(x,t)$ is the solution with boundary conditions $v(0,t) = 0$ and $v(1,t) = 0$, and where a is just a constant.

Then we make an ansatz, where we assume that the function $v(x,t)$ can be seperated in terms of it's variables.

$$v(x,t) = F(x)G(t)$$

If we plug this into the equation above, we get

$$F(x)\frac{\partial G(t)}{\partial t} = G(t)\frac{\partial^2 F(x)}{\partial x^2}$$

Then we define the derivatives of the functions $F(x)$ and $G(t)$ as

$$\frac{\partial G(t)}{\partial t} = G'(t) \quad \& \quad \frac{\partial^2 F(x)}{\partial x^2} = F''(x)$$

Then, the equations can be rewritten as

$$F(x)G'(t) = G(t)F''(x)$$
$$\frac{G'(t)}{G(t)} = \frac{F''(x)}{F(x)}$$

where the derivative is with respect to x on the left hand side (lhs) and with respect to t on the right hand side (rhs). This equation should hold for all x and t . We must then, require the rhs and lhs to be equal to a constant. We call this constant $-\omega^2$. This gives us the two differential equations,

$$\begin{aligned}\frac{G'(t)}{G(t)} &= -\omega^2 \quad \& \quad \frac{F''(x)}{F(x)} = -\omega^2 \\ G'(t) &= -\omega^2 G(t) \quad \& \quad F''(x) + \omega^2 F(x) = 0\end{aligned}$$

The general solutions to these differential equations are trivial and are equal to

$$G(t) = Ce^{-\omega^2 t} \quad \& \quad F(x) = A\sin(\omega x) + B\cos(\omega x)$$

By applying the boundary conditions of $v(x,t)$, we get

$$\begin{aligned}v(x,t) &= F(x)G(t) \\ v(0,t) &= F(0)G(t) = 0 \quad \rightarrow \quad \big(A\sin(\omega \times 0) + B\cos(\omega \times 0)\big)G(t) = 0 \quad \rightarrow \quad B = 0 \\ v(L,t) &= F(L)G(t) = 0 \quad \rightarrow \quad A\sin(\omega \times L)G(t) = 0 \quad \rightarrow \quad \sin(\omega \times L) = 0 \quad \rightarrow \quad \omega = \frac{n\pi}{L}\end{aligned}$$

To satisfy the boundary conditions we require $B = 0$ and $\omega = \frac{n\pi}{L}$. One solution is therefore found to be

$$v(x,t) = F(x)G(t) = A\sin(wx)Ce^{-\omega^2 t} = A\sin\big(\frac{n\pi}{L}x\big)Ce^{-\frac{n^2\pi^2}{L^2}t} = A_n\sin\big(\frac{n\pi}{L}x\big)e^{-\frac{n^2\pi^2}{L^2}t}$$

where we define the constant $A_n = A \cdot C$.

But there are infinitely many possible n values (infinite number of solutions). Moreover, the diffusion equation is linear and because of this we know that a superposition of solutions will also be a solution of the equation. We may therefore write

$$v(x,t) = \sum_{n=1}^{\infty} A_n \sin\big(\frac{n\pi}{L}x\big)e^{-\frac{n^2\pi^2}{L^2}t}$$

Now if we use this in the definition of $u(x,t)$ and apply it's boundary conditions, we end up with

$$\begin{aligned}u(x,t) &= ax + v(x,t) \\ u(0,t) &= a \times 0 + v(0,t) = 0 \\ u(L,t) &= a \times L + v(L,t) = 1 \quad \rightarrow \quad a = \frac{1}{L} \\ u(x,t) &= ax + v(x,t) = \frac{x}{L} + \sum_{n=1}^{\infty} A_n \sin\big(\frac{n\pi}{L}x\big)e^{-\frac{n^2\pi^2}{L^2}t}\end{aligned}$$

The coefficient A_n is in turn determined from the initial condition, which in this case is $u(x,0) = 0$.

$$\begin{aligned}u(x,0) &= \frac{x}{L} + \sum_{n=1}^{\infty} A_n \sin\big(\frac{n\pi}{L}x\big)e^{-\frac{n^2\pi^2}{L^2}\times 0} \\ 0 &= \frac{x}{L} + \sum_{n=1}^{\infty} A_n \sin\big(\frac{n\pi}{L}x\big) \quad \rightarrow \quad \sum_{n=1}^{\infty} A_n \sin\big(\frac{n\pi}{L}x\big) = -\frac{x}{L}\end{aligned}$$

The coefficient A_n is the Fourier coefficients for the function $g(x)$, which in this case is the expression $-\frac{x}{L}$. Because of this, A_n is given by (from the theory on Fourier series)

$$
\begin{aligned}
A_n &= \frac{2}{L}\int_0^L g(x)\sin\big(\frac{n\pi x}{L}\big)dx \\
A_n &= -\frac{2}{L}\int_0^L \frac{x}{L}\sin\big(\frac{n\pi x}{L}\big)dx, \quad u = \frac{n\pi}{L}x, \quad x = \frac{L}{n\pi}u \quad u(0)=0, \quad u(L)=n\pi, \quad du = \frac{n\pi}{L}dx \quad \to \quad dx = \frac{L}{n\pi}du \\
A_n &= -\frac{2}{L}\int_0^L \frac{x}{L}\sin\big(\frac{n\pi x}{L}\big)dx = -\frac{2}{L}\int_0^{n\pi}\frac{u}{n\pi}\sin u\frac{L}{n\pi}du = -\frac{2}{(n\pi)^2}\int_0^{n\pi} u\sin u du \\
A_n &= -\frac{2}{(n\pi)^2}\Big(\sin(n\pi) - n\pi\cos(n\pi)\Big) = \frac{2}{(n\pi)^2}\Big(n\pi\cos(n\pi) - \sin(n\pi)\Big) \\
A_n &= (-1)^n\frac{2}{n\pi}
\end{aligned}
$$

Then at last we have found the analytical solution to the PDE of $u(x,t)$ which is

$$u(x,t) = ax + v(x,t) = \frac{x}{L} + \sum_{n=1}^{\infty}\frac{(-1)^n 2}{n\pi}\sin\big(\frac{n\pi}{L}x\big)e^{-\frac{n^2\pi^2}{L^2}t}$$

B Analytical solution (2 dim)

In 2-dimensions the diffusion equation transforms into

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

And in this project we will be looking into the model with a square lattice for x and y.
In addition, we will use the simple boundary conditions of

$$u(0,y,t) = u(L,y,t) = 0 \qquad y \in (0,L) \qquad t \geq 0,$$

and

$$u(x,0,t) = u(x,L,t) = 0 \qquad x \in (0,L) \qquad t \geq 0,$$

with initial conditions, i.e., the conditions at $t = 0$,

$$u(x,y,0) = \sin(\pi x)\sin(\pi y) \qquad 0 < x, y < L$$

with $L = 1$ the length of the x, y-region of interest.

Just as we did in the 1-dimensional case, we make an ansatz, where we assume that the function $u(x,y,t)$ can be seperated in terms of it's variables.

$$u(x,y,t) = F(x)G(y)H(t)$$

If we plug this into the equation above, we get

$$F(x)G(y)\frac{\partial H(t)}{\partial t} = G(y)H(y)\frac{\partial^2 F(x)}{\partial x^2} + F(x)H(t)\frac{\partial^2 G(y)}{\partial y^2}$$

Then we define the derivatives of the functions $F(x)G(t)$ and $H(t)$ as

$$\frac{\partial H(t)}{\partial t} = H'(t) \quad \& \quad \frac{\partial^2 F(x)}{\partial x^2} = F''(x) \quad \& \quad \frac{\partial^2 G(y)}{\partial y^2} = G''(y)$$

Then, the equations can be rewritten as

$$F(x)G(y)H'(t) = G(y)H(t)F''(x) + F(x)H(t)G''(y)$$
$$\frac{H'(t)}{H(t)} = \frac{F''(x)}{F(x)} + \frac{G''(y)}{G(y)}$$

where the derivative is with respect to t on the left hand side (lhs) and with respect to x and y on the right hand side (rhs). This equation should hold for all x, y and t. We must then, require the rhs and lhs to be equal to a constant. We call this constant $-a^2$. This gives us the two differential equations,

$$\frac{H'(t)}{H(t)} = -a^2 \quad \& \quad \frac{F''(x)}{F(x)} + \frac{G''(y)}{G(y)} = -a^2 = -b^2 - c^2$$

We further assume that $\frac{F''(x)}{F(x)}$ is equal to a constant b and $\frac{G''(y)}{G(y)}$ is equal to a constant c, so that $a^2 = b^2 + c^2 \quad \to \quad a = \sqrt{b^2+c^2}$.

$$H'(t) = -a^2 H(t) \quad \& \quad F''(x) + bF(x) = 0 \quad \& \quad G''(y) + cG(y) = 0$$

The general solutions to these differential equations are trivial and are equal to

$$H(t) = Ae^{-a^2 t} \quad \& \quad F(x) = B\sin(bx) + C\cos(bx) \quad \& \quad G(y) = D\sin(cy) + E\cos(cy)$$

To satisfy the boundary conditions we require $C = E = 0$, $b = \frac{n\pi}{L}$ and $c = \frac{m\pi}{L}$. One solution is therefore found to be

$$\begin{aligned} u(x,y,t) &= F(x)G(y)H(t) = B\sin(bx)D\sin(cy)Ae^{-a^2 t} = B\sin\left(\frac{n\pi}{L}x\right)D\sin\left(\frac{m\pi}{L}y\right)Ae^{-\frac{(n^2+m^2)\pi^2}{L^2}t} \\ &= A_n \sin\left(\frac{n\pi}{L}x\right)\sin\left(\frac{n\pi}{L}y\right)e^{-\frac{2n^2\pi^2}{L^2}t} \end{aligned}$$

and since we are working with a square lattice, then $n = m$, and that simplifies the expression as shown above. In addition, we define the constant $A_n = A \cdot B \cdot D$.

The coefficient A_n is in turn determined from the initial condition. We require

$$u(x,y,0) = \sin(\pi x)\sin(\pi y) = A_n \sin\left(\frac{n\pi}{L}x\right)\sin\left(\frac{n\pi}{L}y\right)e^0$$

By utilizing $L = 1$, we see that $n = 1$ and $A_n = 1$ to satisfy the initial conditions. Then that means the function $u(x,y,t)$ can be read as

$$u(x,y,t) = A_n \sin\left(\frac{n\pi}{L}x\right)\sin\left(\frac{n\pi}{L}y\right)e^{-\frac{2n^2\pi^2}{L^2}t} = \sin(\pi x)\sin(\pi y)e^{-2\pi^2 t}$$

C Analytical steady state solutions to temperature distribution in the Lithosphere

Before radioactive enrichment, the temperature is steady-state $\frac{\partial T}{\partial t} = 0$ and depends only on the depth.

In this case, there exists analytical solutions.

$$\begin{aligned}
k\frac{\partial^2 T}{\partial x^2} + Q &= \frac{\partial T}{\partial t} = 0 \\
\frac{\partial^2 T}{\partial x^2} &= -\frac{Q}{k} \\
\frac{\partial T}{\partial x} &= -\frac{Q}{k}x + b \\
T(x) &= -\frac{Q}{2k}x^2 + bx + c = ax^2 + bx + c
\end{aligned}$$

where $a = -\frac{Q}{2k}$, b and c are integration constants, and x is the depth in km. But since we are looking at three different systems with the upper crust, $T_1(x)$, defined from 0 to 20 km depth, the lower crust ,$T_2(x)$, from 20 to 40 km depth and the mantle, $T_3(x)$, from 40 to 120 km depth. Then they will all have distinct functions with distinct integration constants regarding b and c.

By requiring continuous temperatures and derivatives in the transition between different systems.

$$\begin{aligned}
T_1(x=-20) = T_2(x=-20) \quad &\& \quad \frac{\partial}{\partial x}T_1(x=-20) = \frac{\partial}{\partial x}T_2(x=-20) \\
T_2(x=-40) = T_3(x=-40) \quad &\& \quad \frac{\partial}{\partial x}T_2(x=-40) = \frac{\partial}{\partial x}T_3(x=-40)
\end{aligned}$$

and applying the boundary conditions of the system, mainly

$$\begin{aligned}
T_1(0) &= c_1 = 8 \\
T_3(120) &= a_3 \cdot (120)^2 + b_3 \cdot (120) + c_3 = 1300
\end{aligned}$$

we end up with the following expressions for $T_1(x), T_2(x)$ and $T_3(x)$.

$$\begin{aligned}
T_1(x) &= -0.28x^2 - 23.66x + 8 \\
T_2(x) &= -0.07x^2 - 15.26x + 92 \\
T_1(x) &= -0.01x^2 - 10.46x + 188
\end{aligned}$$

With the addition of the radioactive elements Uranium (U), Thorium (Th) and Potassium (K) that provides an additional total heat production of $Q_{tot} = 0.5\mu W/m^3$ leads to different coefficients of a, b and c in the analytic solutions of T_1, T_2 and T_3. When including the extra heat production of the radioactive elements, the functions T_1, T_2 and T_3 now reads

$$\begin{aligned}
T_1(x) &= -0.28x^2 - 29x + 8 \\
T_2(x) &= -0.07x^2 - 20.6x + 92 \\
T_1(x) &= -0.11x^2 - 23.8x + 28
\end{aligned}$$

References

[1] Morten Hjorth-Jensen, Github Repository,
http://compphysics.github.io/ComputationalPhysics/doc/web/course

[2] Conrad Sanderson and Ryan Curtin. Armadillo: a template-based C++ library for linear algebra. Journal of Open Source Software, Vol. 1, pp. 26, 2016.

[3] Conrad Sanderson and Ryan Curtin. A User-Friendly Hybrid Sparse Matrix Class in C++. Lecture Notes in Computer Science (LNCS), Vol. 10931, pp. 422-430, 2018.