The diffusion equation: Analytical and numerical solutions in one and two spatial dimensions applied to studying the temperature distribution of the lithosphere

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Abstract

1 Introduction

How things spread or diffuse is an ubiquitous phenomenon in nature. One example is when there is a temperature gradient between two points, heat diffuses through the material or medium from the hotter point to the colder point. Or when putting a drop of dye in a water container, the dye spreads out in the liquid in a diffusion process. Another example is from fluid dynamics when there is water between two parallel plates moving with different velocities, in which case the velocity of the water flow will diffuse from the faster plate towards the slower plate.

Diffusion processes can be described mathematically by the diffusion equation. Solving this equation enables us to see quantitatively how some quantity, e.g. temperature, diffuses through space in time. In this report the temperature distribution in the lithosphere on the western coast of Norway is studied. It is proposed that on the west coast there was an active subducting zone about 1 Gy ago [1] [2]. Due to this subducting zone the mantle is re-fertilised with radioactive elements and is expected to more enriched with these elements than normal mantle [3]. The temperature evolution of this mantle is studied in this report to simulate the changes in temperature expected due to these radioactive elements. Prior to that, this report solves the one dimensional and two dimensional diffusion equation numerical and analytically in order to test the accuracy of the simulations produced.

2 Theory

2.1 The diffusion equation

The diffusion equation is a partial differential equation which has the form

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

where D is a constant called the diffusion coefficient or diffusivity and $\nabla^2 \equiv \frac{\partial^2}{\partial x^2} + \frac{\partial^2}{\partial y^2} + \frac{\partial^2}{\partial z^2}$. D has dimensions time/length^2. This equation is quite general, and $u(\mathbf{x},t)$ is not restricted to one specific physical meaning. u can for example represent the temperature gradient at some point in space and time, or it can represent the velocity of the fluid flow between two infinite parallel plates that have a relative velocity between them in the parallel direction. Diffusion intuitively means that something 'spreads out'. So a solution $u(\mathbf{r},t)$ to the diffusion equation gives how u spreads out in time from its initial state at $t=0$, at any given point $\mathbf{x}$ in space.

We can get the diffusion equation to a simpler and dimensionless form. We can define new, dimensionless spatial variables $\hat{\mathbf{x}} \equiv (\hat{x},\hat{y},\hat{z})$ through $\alpha\hat{x} \equiv x$, $\alpha\hat{y} \equiv y$ and $\alpha\hat{z} \equiv z$ where α is some constant with dimension length, so $\alpha\hat{\mathbf{x}} \equiv \mathbf{x}$. Then the diffusion equation becomes

$$\frac{\partial^2 u}{\partial(\alpha\hat{x})^2} + \frac{\partial^2 u}{\partial(\alpha\hat{y})^2} + \frac{\partial^2 u}{\partial(\alpha\hat{z})^2} = \frac{1}{\alpha^2}\left(\frac{\partial^2 u}{\partial\hat{x}^2} + \frac{\partial^2 u}{\partial\hat{y}^2} + \frac{\partial^2 u}{\partial\hat{z}^2}\right) = D\frac{\partial u}{\partial t} \tag{2}$$

$$\Updownarrow \tag{3}$$

$$\frac{\partial^2 u}{\partial\hat{x}^2} + \frac{\partial^2 u}{\partial\hat{y}^2} + \frac{\partial^2 u}{\partial\hat{z}^2} \equiv \hat{\nabla}^2 u = \alpha^2 D\frac{\partial u}{\partial t} \equiv \frac{\partial u}{\partial\hat{t}}, \tag{4}$$

where $[\alpha^2 D] = \text{length}^2 \cdot (\text{time} \cdot \text{length}^{-2}) = \text{time}$ and we have defined the dimensionless variable $\hat{t} \equiv t/(\alpha D)$ and the dimensionless nabla operator $\hat{\nabla}^2 \equiv \frac{\partial^2}{\partial\hat{x}^2} + \frac{\partial^2}{\partial\hat{y}^2} + \frac{\partial^2}{\partial\hat{z}^2}$. So our dimensionless and simplified diffusion equation is

$$\hat{\nabla}^2 u(\hat{\mathbf{x}},\hat{t}) = \frac{\partial u(\hat{\mathbf{x}},\hat{t})}{\partial\hat{t}}. \tag{5}$$

In the subsequent parts of this report we will only use the dimensionless form of the diffusion equation, so for simplicity we will use the symbols x, y, z, t for the dimensionless variables instead of $\hat{x}, \hat{y}, \hat{z}, \hat{t}$.

2.2 Analytical solution to the diffusion equation in one dimension

The one-dimensional diffusion equation is the diffusion equation with only one spatial variable, so $\mathbf{x} \to x$. Then Eq. (5) becomes

$$\frac{\partial^2 u(x,t)}{\partial x^2} = \frac{\partial u(x,t)}{\partial t}. \tag{6}$$

For boundary conditions

$$u(0,t) = 0, \quad t \geq 0, \tag{7}$$

and

$$u(L,t) = 1, \quad t \geq 0, \tag{8}$$

and initial condition

$$u(x,0) = 0, \quad 0 < x < L, \tag{9}$$

the final result for the solution of $u(x,t)$ is

$$u(x,t) = \frac{2}{\pi}\sum_{n=1}^{\infty}(-1)^n \frac{\sin(n\pi x/L)}{n}\, e^{-n^2\pi^2 t/L^2} + \frac{x}{L}. \tag{10}$$

The derivation of the solution can be found in the appendix.

2.3 The algorithms for solving the diffusion equation in one dimension

Three slightly different algorithms will be implemented for solving the heat equation. These methods are the forward Euler method, the backward Euler method and the Crank-Nicolson method.

2.3.1 The forward Euler method

The dimensionless diffusion equation is given by

$$\frac{\partial^2 u(x,t)}{\partial x^2} = \frac{\partial u(x,t)}{\partial t}, \tag{11}$$

or

$$u_{xx} = u_t, \tag{12}$$

where the solution u has both spacial and temporal dependencies x and t, respectively. We can discretise this function and find the derivatives with the forward Euler method. The right hand side of Eq. goes to

$$u_t \approx \frac{u(x,t+\Delta t) - u(x,t)}{\Delta t} = \frac{u(x_i,t_j+\Delta t) - u(x_i,t_j)}{\Delta t}, \tag{13}$$

where Δt is the time step size, i and j are the spacial and time indices, respectively. The local approximation error goes like $O(\Delta t)$. The left hand side of Eq. 2.3.1 goes to

$$u_{xx} \approx \frac{u(x+\Delta x,t) - 2u(x,t) + u(x-\Delta x,t)}{\Delta x^2}, \tag{14}$$

or

$$u_{xx} \approx \frac{u(x_i+\Delta x,t_j) - 2u(x_i,t_j) + u(x_i-\Delta x,t_j)}{\Delta x^2}, \tag{15}$$

where Δx is the step size in the spacial dimension. The local approximation error goes like $O(\Delta x^2)$.

In a more simplified way where $u(x_i,t_j)$ is shortened to u_{ij} this can be written as

$$\frac{u_{i,j+1} - u_{i,j}}{\Delta t} = \frac{u_{i+1,j} - 2u_{i,j} + u_{i-1,j}}{\Delta x^2}, \tag{16}$$

or

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

where $\alpha = \Delta t/\Delta x^2$. It is written in this form, since $u_{i,j+1}$ is the only unknown in this equation. This results in a matrix vector multiplication given by

$$V_{j+1} = \hat{A}V_j = \hat{A}^2 V_{j-1} = ... = A^{\hat{j}+1}V_0, \tag{18}$$

where $\hat{A}$ is

$$\begin{vmatrix} \text{1-2}\alpha & \alpha & 0 & ... & 0 \\ \alpha & \text{1-2}\alpha & \alpha & ... & 0 \\ 0 & \alpha & ... & ... & ... \\ ... & ... & ... & ... & \alpha \\ 0 & 0 & ... & \alpha & \text{1-2}\alpha \end{vmatrix}$$

2.3.2 The backward Euler method

We can also use the backward method in the same way to find the numerical solution to the diffusion equation. The right hand side of Eq. 2.3.1 is given by

$$u_t \approx \frac{u_{i,j} - u_{i,j-1}}{\Delta t} \tag{19}$$

which again has a local approximation error which goes like $O(\Delta t)$. The spacial derivative is given by

$$u_{xx} = \frac{u_{i+1,j} - 2u_{i,j} + u_{i-1,j}}{\Delta x^2}, \tag{20}$$

which has a local approximation error which goes like $O(\Delta x^2)$. By equating these two equations and putting $u_{i,j-1}$ to the left hand side gives

$$u_{i,j-1} = -\alpha u_{i-1,j} + (1 + 2\alpha)u_{i,j} - \alpha u_{i+1,j}. \tag{21}$$

This can be written as a matrix vector multiplication given by

$$V_j = \hat{A}^{-1} V_{j-1} = \hat{A}^{-1}(\hat{A}^{-1} V_{j-2}) = \hat{A}^{-j} V_0, \tag{22}$$

where $\hat{A}$ is

$$\begin{vmatrix} 1+2\alpha & -\alpha & 0 & ... & 0 \\ -\alpha & 1+2\alpha & -\alpha & ... & 0 \\ 0 & -\alpha & ... & ... & ... \\ ... & ... & ... & ... & -\alpha \\ 0 & 0 & ... & -\alpha & 1+2\alpha \end{vmatrix}$$

Unlike the explicit scheme, this method does not have any stability critieria and is valid for all Δt and Δx. This can be proven since the specral radius of $\hat{A}$ must be less than one, i.e $(\hat{A}) < 1$. Numerically Eq. 22 can be solved using the Thomas algorithm for a tri-diagonal matrix, which is much faster than for example using Gaussian Elimination.

2.3.3 The Crank-Nicolson method

The Crank-Nicolson method is a combination of the two schemes given above. By writing them both is a more general way, the implicit and explicit schemes are given by

$$\frac{\theta}{\Delta x^2}(u_{i-1,j} - 2u_{i,j} + u_{i+1,j}) + \frac{1-\theta}{\Delta x^2}(u_{i+1,j-1} - 2u_{i,j-1} + u_{i-1,j-1}) = \frac{1}{\Delta t}(u_{i,j} - u_{i,j-1}) \tag{23}$$

where $\theta = 0$ yields the explicit scheme and $\theta = 1$ yields the implicit scheme. However, Crank and Nicolson created a new scheme using $\theta = 1/2$. This new scheme has a truncation error which goes like $O(\Delta t^2)$ and $O(\Delta x^2)$ which is a great improvement over the previous schemes. Imputting $\theta = 1/2$ into Eq. 23 gives

$$\alpha(u_{i-1,j} - 2u_{i,j} + u_{i+1,j} + u_{i+1,j-1} - 2u_{i,j-1} + u_{i-1,j-1}) = 2(u_{i,j} - u_{i,j-1}), \tag{24}$$

and by placing $j-1$ and j terms on either side gives

$$\alpha u_{i-1,j} - \alpha 2u_{i,j} - 2u_{i,j} + \alpha u_{i+1,j} = -\alpha u_{i+1,j-1} + \alpha 2u_{i,j-1} - 2u_{i,j-1} - \alpha u_{i-1,j-1}. \tag{25}$$

By multiplying both sides by -1 and writing this in matrix vector form gives

$$(2\hat{I} + \alpha\hat{B})V_j = (2\hat{I} - \alpha\hat{B})V_{j-1}, \tag{26}$$

where $\hat{I}$ is the identity matrix and $\hat{B}$ is a tri-diagonal matrix

$$\begin{vmatrix} 2 & -1 & 0 & ... & 0 \\ -1 & 2 & -1 & ... & 0 \\ 0 & -1 & ... & ... & ... \\ ... & ... & ... & ... & -1 \\ 0 & 0 & ... & -1 & 2 \end{vmatrix}$$

2.3.4 Truncation errors of the different algorithms

2.4 Solving the diffusion equation in two dimensions

The method for solving the two-dimensional diffusion equation is by using the Jacobi solver, which is an iterative method. The analytic solution is given in Appendices. B.

Starting with the two dimensional diffusion equation

$$\frac{\partial^2 u(x,y,t)}{\partial x^2} + \frac{\partial^2 u(x,y,t)}{\partial y^2} = \frac{\partial u(x,y,t)}{\partial t}, \tag{27}$$

or

$$u_{xx} + u_{yy} = u_t \tag{28}$$

and by discretising the spatial components and discretising the temporal component with the Backward Euler method gives three equations,

$$u_{xx} \approx \frac{u^l_{i+1,j} - 2u^l_{i,j} + u^l_{i-1,j}}{\Delta x^2}, \tag{29}$$

$$u_{yy} \approx \frac{u^l_{i,j+1} - 2u^l_{i,j} + u^l_{i,j-1}}{\Delta y^2}, \tag{30}$$

$$u_t \approx \frac{u^l_{i,j} - u^{l-1}_{i,j}}{\Delta t}. \tag{31}$$

When these are put together this gives the following equation

$$\alpha \left[u^l_{i+1,j} + u^l_{i-1,j} + u^l_{i,j+1} + u^l_{i,j-1} - 4u^l_{i,j} \right] = u^l_{i,j} - u^{l-1}_{i,j} \tag{32}$$

where $\alpha = \Delta t / \Delta x^2$ and we make the assumption that it is a square lattice, i.e $\Delta x = \Delta y$. This equation can be simplified a by renaming the following components as $\Delta^{i,j}_l$

$$\Delta^l_{i,j} = u^l_{i+1,j} + u^l_{i-1,j} + u^l_{i,j+1} + u^l_{i,j-1}, \tag{33}$$

which leads to

$$u^l_{i,j} = \frac{1}{(1+4\alpha)} \left[\alpha \Delta^l_{i,j} + u^{l-1}_{i,j} \right]. \tag{34}$$

Now on the left hand side is an unknown, but on the right hand side are both known variables and unknown variables. Hence, in order to solve this equation it is necessary to use an iterative solver like the Jacobi method which makes an initial guess for the unknown variables on the right hand side. After each iteration this guess becomes better and better. The method for the Jacobi algorithm is given in Algorithm. 1.

2.5 Simulating Heat diffusion in the Earth's Lithosphere in two dimensions

The two dimensional diffusion equation in the section above has the physical constants scaled away. Since in this report we study the temperature diffusion in the lithosphere, the dimensionless equation is no longer useful and we require some physical constant to be used. The equation becomes

Algorithm 1: THE JACOBI METHOD: with parallelisation package OpenMP

```
N = length of the lattice.
MaxIterations = 100,000
matrix Aprev = solution from previous time step.
matrix Aold = 1.0 for all i and j

/* Start the iterative solver */
for k = 0,1,2,..., MaxIterations do
    sum = 0.0
     pragma omp parallel default(shared) private(i,j) reduction(+:sum)
     pragma omp for
    for i = 1,... N-1 do
        for j =1,... N-1 do
            A(i,j) = (1/(1 + 4*alpha))*( Aprev(i,j) + alpha*( Aold(i+1,j)
            + Aold(i,j+1) + Aold(i-1,j) + Aold(i,j-1) ) )

    /* Sum the error at each location and make Aold = A for the next iteration.
       */
    for i = 1,2,... N-1 do
        for j = 1,2,... N-1 do
            sum += fabs( Aold(i,j) - A(i,j) )
            Aold(i,j) = A(i,j)

    /* End parallel task.  */

    /* Does the error reach the stopping criteria */

    if sum /= (N*N)) is less than abstol then
        return k

/* Jacobi solver reached the end of max iterations without convergence */
return MaxIterations
/* End of function */
```

$$k\left(\frac{\partial^2 u(x,y,t)}{\partial x^2}+\frac{\partial^2 u(x,y,t)}{\partial y^2}\right)+Q=c_p\rho\frac{\partial u(x,y,t)}{\partial t}, \tag{35}$$

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 from radioactive elements. The lithosphere is assumed to have constant density of 3.510 Kg/m^3, constant thermal conductivity of 2.5 $W/m/°C$ and constant specific heat capacity of 1000 $J/Kg/°C$. Inside the lithosphere the quantity of radioactive elements varies, hence it is separated into three regions. From 0 km to 20 km in depth (upper crust) the heat production is 1.40 $\mu W/m^3$, from 20 km to 40 km in depth (lower crust) the heat production is 0.35 $\mu W/m^3$ and between 40 km and 120 km (mantle) the heat production is 0.05 $\mu W/m^3$.

When radioactive enrichment occurs, the mantle become enriched with Uranium, Thorium and Potassium, which further contribute to the heat production in this region. These elements each have their own half lives. Therefore to compute the heat production as a function of time the following equation is used.

$$Q(t)=Q(t=0)\left[0.4\left(\frac{1}{2}\right)^{t/U_{1/2}}+0.4\left(\frac{1}{2}\right)^{t/Th_{1/2}}+0.2\left(\frac{1}{2}\right)^{t/K_{1/2}}\right], \tag{36}$$

where the heat production at time $t=0$, $Q(t=0)$, equal 0.5 $\mu W/m^3$, $U_{1/2}$ is the half life of Uranium equal to 4.47 Gy, $Th_{1/2}$ is the half life of Thorium equal to 14.0 Gy and $K_{1/2}$ is the half life of Potassium equal to 1.25 Gy. The values 0.4 and 0.2 in front of the half-life equations indicate the elements relative quantity in the mantle. The thermal boundary conditions of the lithosphere are 8 $°C$ at the top of the upper crust and 1300 $°C$ at the bottom of the mantle. Note that all quantities in this report have been scaled in the code script with units in Kilograms, Joules, Giga years, and Kilometres for consistency, although in the report text they are not. To accommodate these conditions and physical constants the two dimensional diffusion equation is altered as shown in below.

$$k(u_{xx}+u_{yy})+Q=c_p\rho u_t \tag{37}$$

These constant can be moved around giving

$$\frac{k}{c_p\rho}(u_{xx}+u_{yy})+\frac{Q}{c_p\rho}=u_t. \tag{38}$$

After discretising this equation and renaming $\beta=1/(c_p\rho)$ gives

$$u_{i,j}^l=\frac{1}{1+4k\alpha\beta}\left[k\alpha\beta\Delta_{i,j}^l+Q\Delta t\beta+u_{i,j}^{l-1}\right] \tag{39}$$

3 Method

The one dimensional diffusion solver was run with $dx = 0.01$ and $dt \approx 5 \times 10^{-5}$ to compare the numerical solution with the analytical solution. Another experimental run was with parameters $dx = 0.1$ and $dt \approx 6 \times 10^{-3}$.

The two dimensional diffusion solver was run in the dimensionless case to compare the numerical with the analytic solution. The test runs were $dt = 5 \times 10^{-5}$ and $dx = 0.01$ as shown in Fig. 6 and Fig. 5. Another test run was $dt = 1 \times 10^{-3}$ and $dx = 0.1$ as shown in the appendix B.

4 Results

4.1 Analytic and Numerical solutions to the one-dimensional diffusion equation

Figs. 1 and 2 show the solutions of the one-dimensional diffusion equation for $N_x = 10$ and $N_x = 100$ x values, respectively. They show the analytical solution as well as the numerical solutions obtained from the explicit, implicit and Crank-Nicolson schemes.

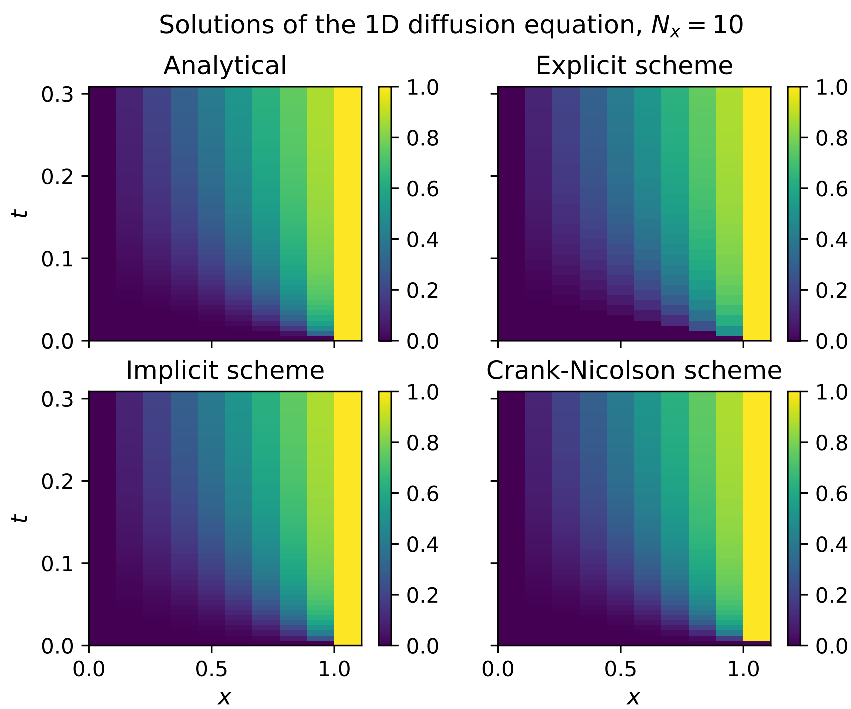

Figure 1: Color plots showing the solution of the one dimensional diffusion equation found with four different approaches: the analytical solution, the explicit scheme, the implicit scheme and the Crank-Nicolson scheme. The x axis shows the spatial component x between $x = 0$ and $x = 1$, and the y axis shows the time t. There are $N_x = 10$ evenly spaced points, which gives a step size of $\Delta x = 1/9 \approx 1/10$. The number of terms included in the sum of the analytical solution (see Eq. (10)) is 10 000. The timestep is $\Delta t = \frac{1}{2}\Delta x^2 \approx 6.17 \cdot 10^{-3}$.

Figs. 3 and 4 show the solutions of the one-dimensional diffusion equation at two distinct time points for $N_x = 10$ and $N_x = 100$ respectively.

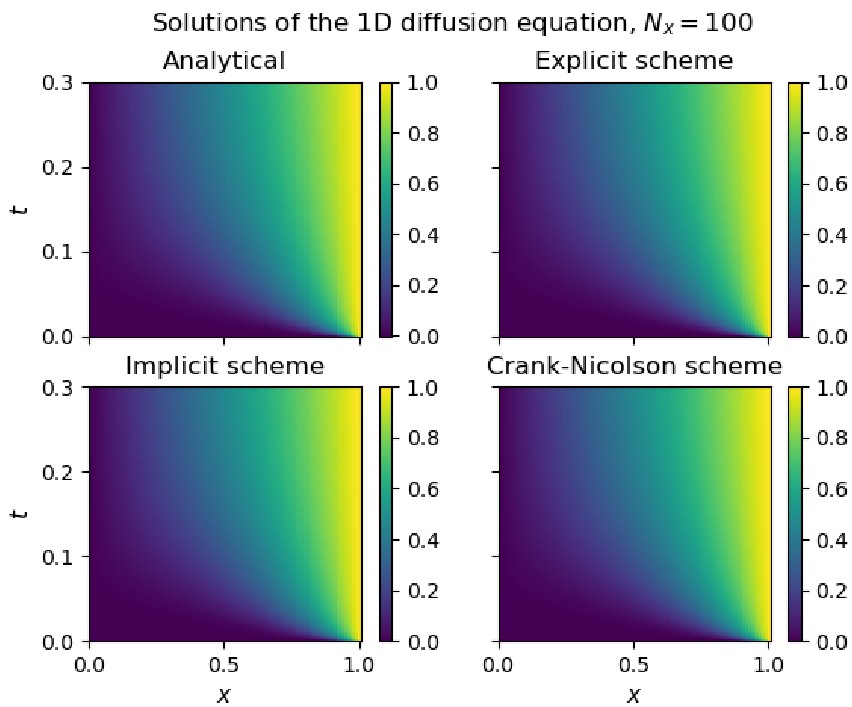

Figure 2: Color plots showing the solution of the one dimensional diffusion equation found with four different approaches: the analytical solution, the explicit scheme, the implicit scheme and the Crank-Nicolson scheme. The x axis shows the spatial component x between $x = 0$ and $x = 1$, and the y axis shows the time t. There are $N_x = 100$ evenly spaced points, which gives a step size of $\Delta x = 1/99 \approx 1/100$. The number of terms included in the sum of the analytical solution (see Eq. (10)) is 10 000. The timestep is $\Delta t = \frac{1}{2}\Delta x^2 \approx 5.10 \cdot 10^{-5}$.

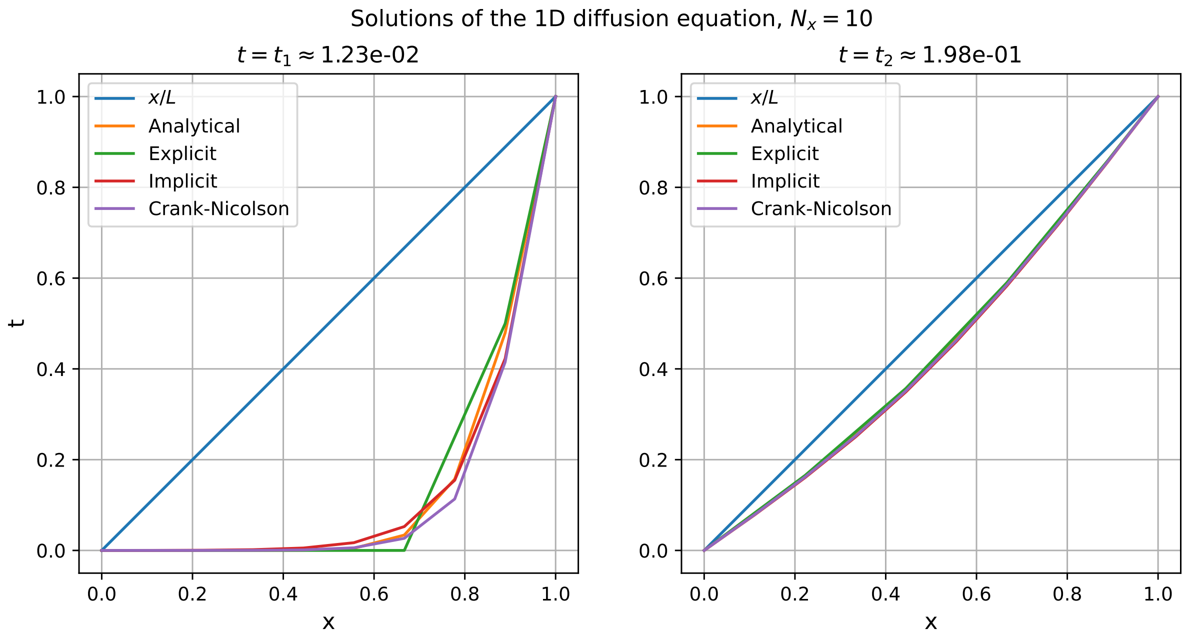

Figure 3: The solution to the one dimensional diffusion equation for all schemes with $\Delta x \approx 0.1$ at a time point t_1 when $u(x,t)$ is very curved (left plot) and at a time point t_2 when $u(x,t)$ is close to linear. The timestep is $\Delta t \approx 6.2 \times 10^{-3}$.

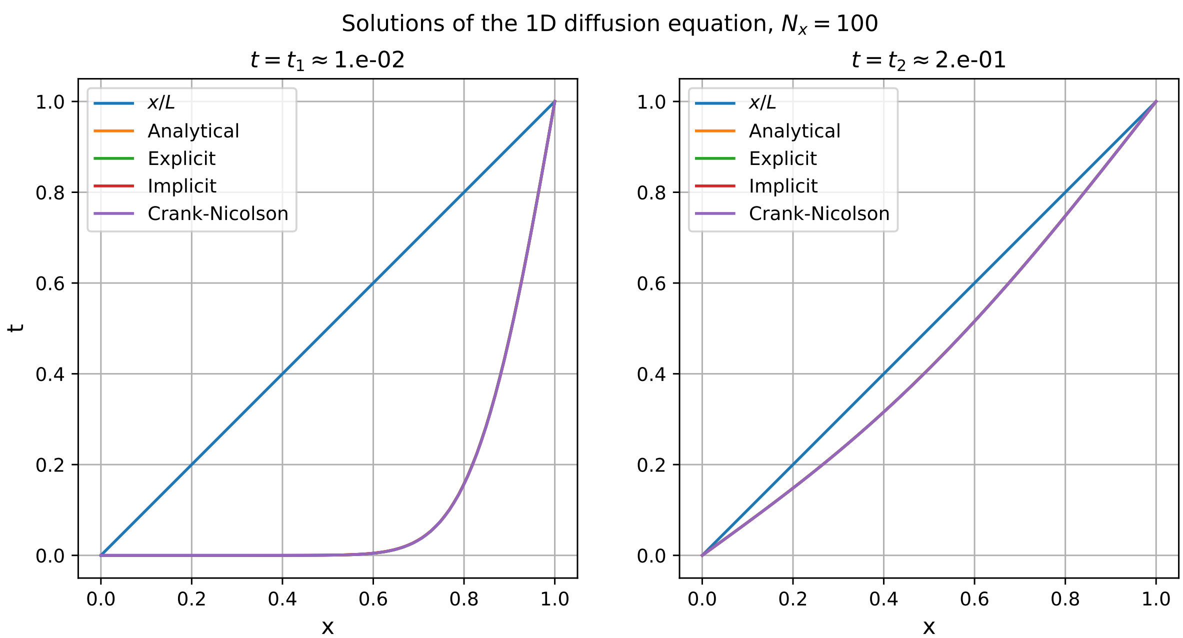

Figure 4: The solution to the one dimensional diffusion equation for all schemes with $\Delta x \approx 0.01$ at a time point t_1 when $u(x,t)$ is very curved (left plot) and at a time point t_2 when $u(x,t)$ is close to linear. The timestep is $\Delta t \approx 5.1 \times 10^{-5}$.

4.2 Analytic and Numerical solutions to the two-dimensional diffusion equation

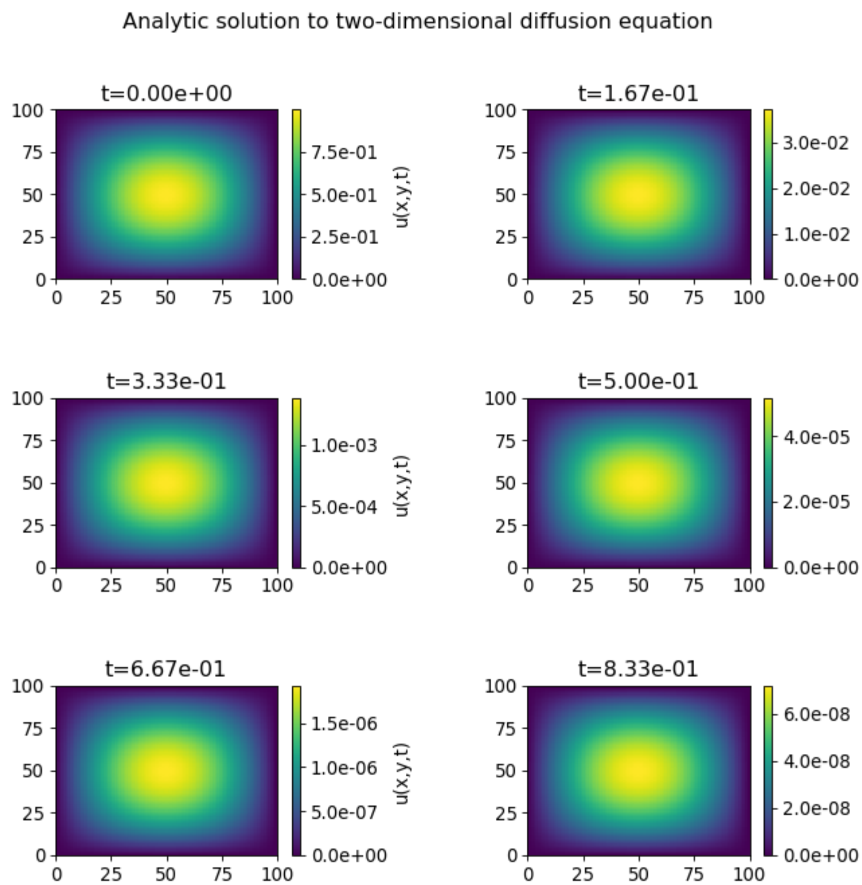

Figure 5: Analytic solution to the 2D diffusion equation with $dt = 5 \times 10^{-5}$ and $dx = 0.01$. The code script results a file with 20,000 time points, however only six of these are shown at the given time t.

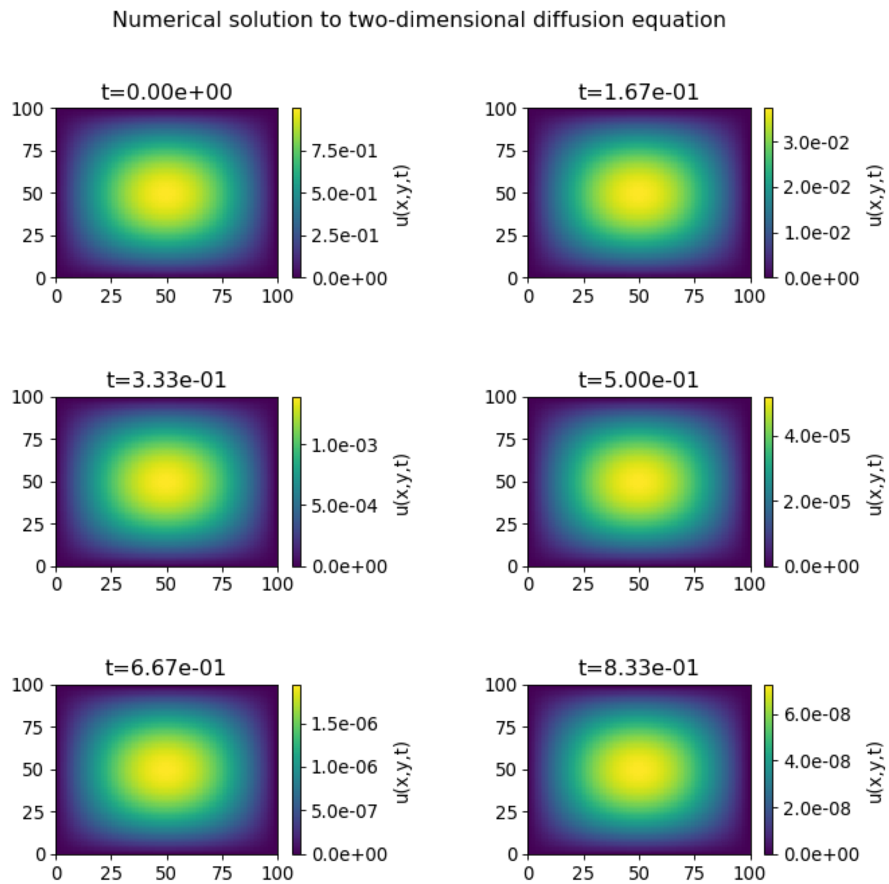

Figure 6: Numerical solution to the 2D diffusion equation with $dt = 5 \times 10^{-5}$ and $dx = 0.01$. The code script results a file with 20,000 time points, however only six of these are shown at the given time t.

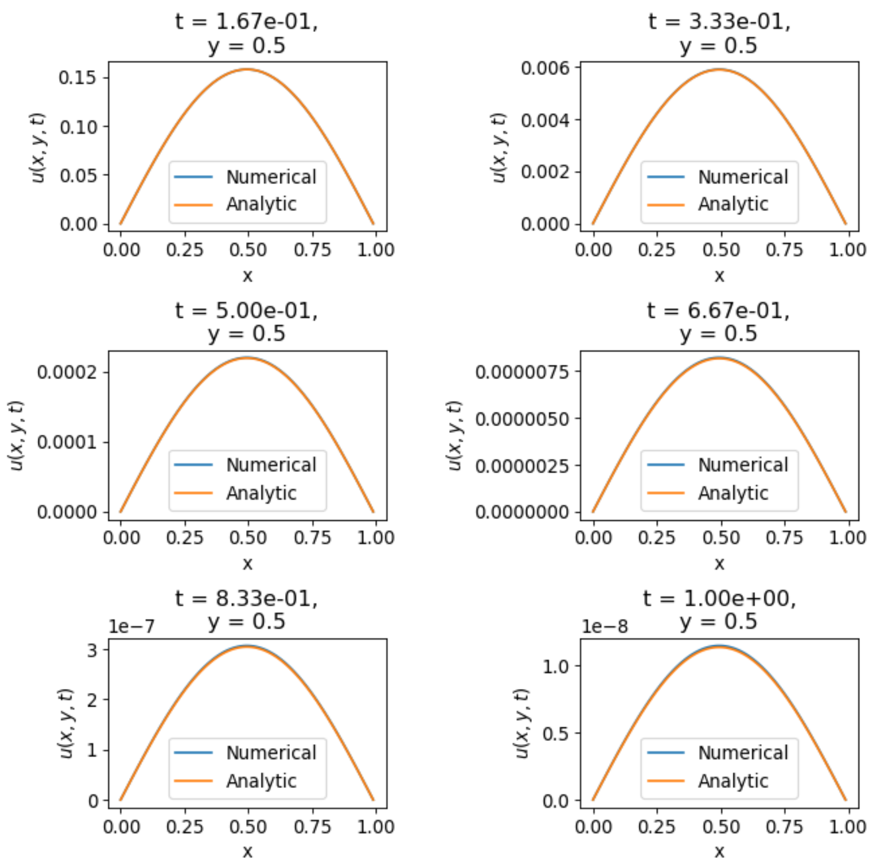

Figure 7: Comparison of the numerical and analytic solution to the 2D diffusion equation with $dt = 5 \times 10^{-5}$ and $dx = 0.01$. The subplots shows that for the dt and dx used that there is good agreement between the two.

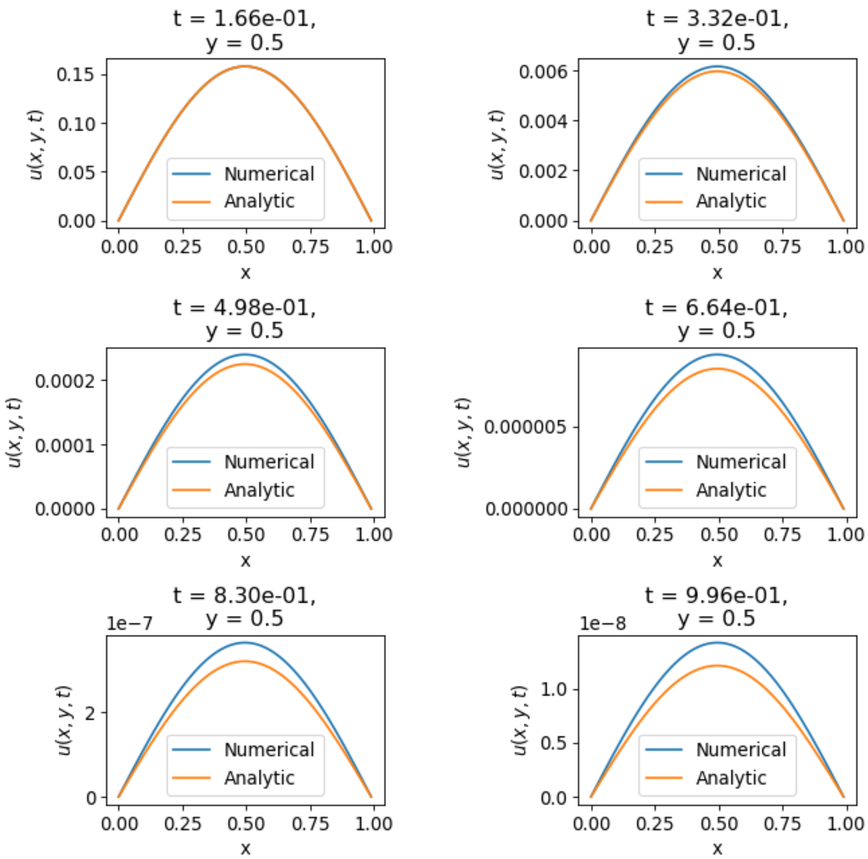

Figure 8: Comparison of the numerical and analytic solution to the 2D diffusion equation with $dt = 1 \times 10^{-3}$ and $dx = 0.01$. The subplots shows that for the dt and dx used that the convergence between the two is fairly good, but could be improved with smaller intervals.

4.3 Temperature in the Lithosphere before radioactive enrichment

Fig. 9 shows the temperature distribution before radioactive enrichment in the mantle. The heat production as a function of depth is, however, included. The heat production in the upper crust, lower crust and mantle is 1.4 $\mu W/m^3$, 0.35 $\mu W/m^3$ and 0.05 $\mu W/m^3$, respectively. The results show that the boundary conditions on the sides of the lithosphere are important. These boundary conditions were changed and the results show that they change the temperature distribution depending on their value. In the case of 9 the side boundary conditions are 281.15 K, the same as the top surface of the upper crust.

Discussion - Therefore it could be of great interest to compare these results with the one dimensional case which does not require boundary conditions for the width or sides of the lithosphere.

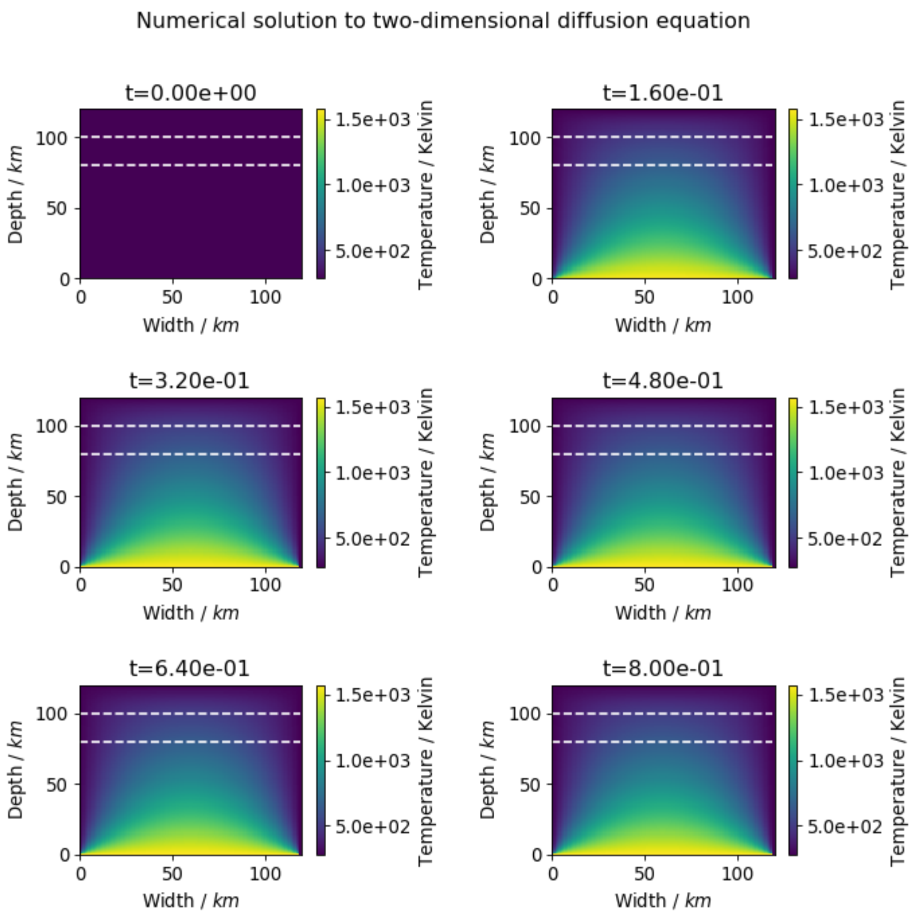

Figure 9: Temperature in the lithosphere beginning 1.0 Gy ago till the present. The figure shows six time steps in the range between 1.0 Gy ago to the present. The x and y axis of each subplot are 120 km in width and 120 km in height, respectively. The boundary conditions are 281.15 K at the surface and sides, and 1573.15 K at the bottom.

4.4 Temperature in the Lithosphere after radioactive enrichment

Fig. 10 shows the evolution of the lithosphere after being enriched 1 Gy ago with Uranium, Thorium and Potassium. The figure does shows some difference to Fig. 9 in the temperature distribution, though this is better visible in Fig. 11. Fig. 11 shows a cross-section of Figs. 9 and 10. The cross-section was chosen by taking the middle column, which is likely to be least influenced by the side boundary condition. However, for the sake of comparison any column is possible since both use the same boundary conditions.

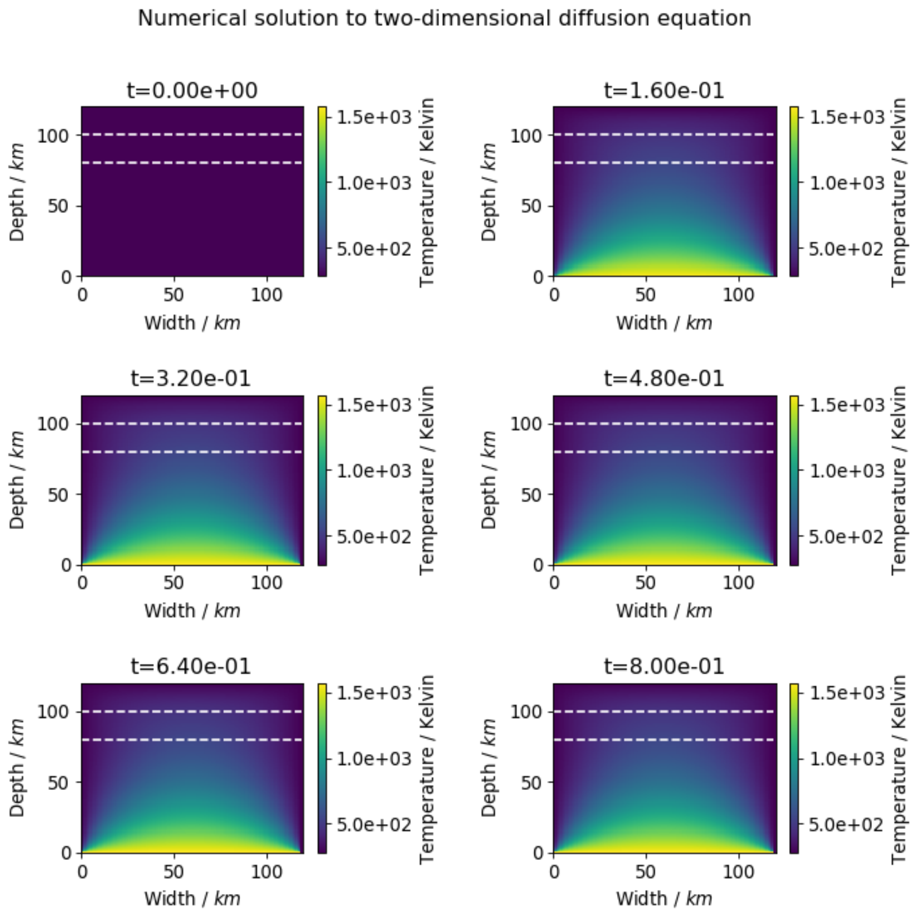

Figure 10: Temperature in the lithosphere after radioactive enrichment beginning 1.0 Gy ago till the present. The figure shows six time steps in the range between 1.0 Gy ago to the present. The x and y axis of each subplot are 120 km in width and 120 km in height, respectively. The boundary conditions are 281.15 K at the surface and sides, and 1573.15 K at the bottom.

Fig. 11 shows that after enrichment the temperature in the upper crust, lower crust and mantle are larger than before enrichment. The maximum difference in temperature between before and after enrichment is 169 K, which lies in the mantle. By averaging over depth, the mean temperature difference in the mantle between before and after enrichment is 127 K with standard deviation 45 K. This changes slightly as the lithosphere evolves over time as radioactivity and decreases. The figure shows that since radioactivity is decreasing the temperature in the lithosphere also decreases slightly over time. Again by averaging over depth, the difference in temperature directly after enrichment and 1 Gy later is on average 18 K with standard deviation of 7 K. This decrease in temperature is likely due to the decrease in radioactivity.

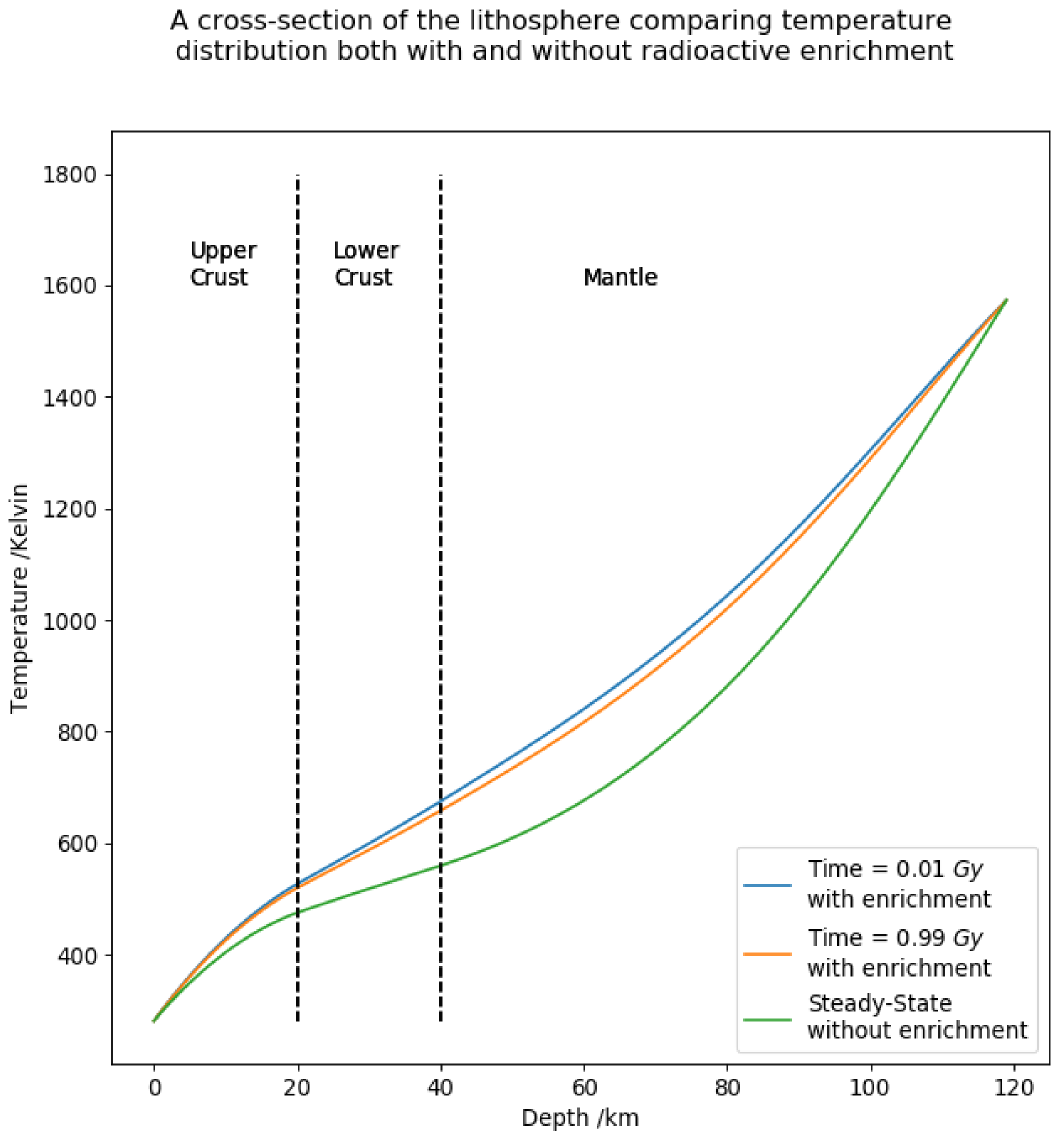

Figure 11: The temperature distribution in the lithosphere with and without radioactive enrichment in the mantle 1 Gy ago.

5 Discussion

6 Conclusion

7 Github address

Github address: `https://github.com/amundwf/comp-phys-project5.git`

References

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A Derivation of the analytical solution of the one-dimensional diffusion equation

Here, a detailed derivation of the analytical solution of the one-dimensional diffusion equation will be presented. As presented earlier, the diffusion equation is given by

$$\frac{\partial^2 u(x,t)}{\partial x^2} = \frac{\partial u(x,t)}{\partial t} \quad \Longleftrightarrow \quad \frac{\partial^2 u(x,t)}{\partial x^2} - \frac{\partial u(x,t)}{\partial t} = 0. \tag{40}$$

The domain in this problem is $0 \leq x \leq L$ and $t \geq 0$.

The boundary conditions of this problem are given by

$$u(0,t) = 0, \quad t \geq 0, \tag{41}$$

and

$$u(L,t) = 1, \quad t \geq 0, \tag{42}$$

and the initial condition is given by

$$u(x,0) = 0, \quad 0 < x < L. \tag{43}$$

To make it easier to calculate the solution, we want to modify $u(x,t)$ to a new function $v(x,t)$ which is zero at both boundaries, that is,

$$v(0,t) = v(L,t) = 0. \tag{44}$$

This can be achieved by defining v as

$$v(x,t) \equiv u(x,t) + f(x), \tag{45}$$

where $f(x)$ is an unknown function that only varies in space and not in time and makes $v(x,t)$ satisfy the boundary conditions in Eq. (44). The end point values of $f(x)$ can then be found:

$$\begin{aligned} v(0,t) = 0 = u(0,t) + f(0) &= 0 + f(0) \\ &\Updownarrow \\ f(0) &= 0 \end{aligned}$$

and

$$
\begin{gathered}
v(L,t) = 0 = u(L,t) + f(L) = 1 + f(L) \\
\Updownarrow \\
f(L) = -1.
\end{gathered}
$$

The initial condition for $v(x,t)$ is

$$v(x,0) = u(x,0) + f(x) = 0 + f(x) = f(x). \tag{46}$$

We will also assume that $v(x,t)$ is a solution of the diffusion equation, and we will now use this to find the expression for $f(x)$.

$$
\begin{align}
\partial_{xx}^2 v(x,t) &= \partial_t v(x,t) \tag{47}\\
\partial_{xx}^2 (u(x,t) + f(x)) &= \partial_t (u(x,t) + f(x)) \tag{48}\\
\partial_{xx}^2 u + \partial_{xx}^2 f(x) &= \partial_t u + 0 \tag{49}\\
(\partial_{xx}^2 u - \partial_t u) + \partial_{xx}^2 f(x) &= 0 \tag{50}\\
\partial_{xx}^2 f(x) &= 0. \tag{51}
\end{align}
$$

Eq. (51) is an ordinary differential equation that is easily solved by integrating twice:

$$
\begin{aligned}
f(x) &= \iint \partial^2 f(x)\,dx\,dx \\
&= \int \left(\int 0\,dx \right) dx \\
&= \int C\,dx \\
&= Cx + D
\end{aligned}
$$

for some undetermined constants C and D. These constants are found by using the boundary conditions:

$$
\begin{gathered}
f(0) = 0 = C \cdot 0 + D = D \\
\Updownarrow \\
D = 0 \\
\Updownarrow \\
f(x) = Cx,
\end{gathered}
$$

and

$$
\begin{gathered}
f(L) = -1 = C \cdot L \\
\Updownarrow \\
C = -\frac{1}{L}
\end{gathered}
$$

so we get

$$f(x) = \left(-\frac{1}{L} \right) x = -\frac{x}{L}. \tag{52}$$

In order to find the solution to the diffusion equation, we will use separation of variables. That is, we will assume that v is of the form $v(x,t) = X(x) \cdot T(t)$. Using this assumption, the diffusion equation becomes

$$\begin{aligned}
\partial^2_{xx}(X(x)T(t)) &= \partial_t(X(x)T(t)) \\
T(t)\partial^2_{xx}X(x) &= X(x)\partial_t T(t) \\
&\Updownarrow \\
\frac{X''(x)}{X(x)} &= \frac{T'(t)}{T(t)}.
\end{aligned}$$

Since the left hand side only depends on x it is constant in t, and since the right hand side only depends on t it is constant in x. Therefore the above equation has to be constant in both t and x, and we can denote this constant as $-\lambda^2$:

$$\frac{X''(x)}{X(x)} = \frac{T'(t)}{T(t)} \equiv -\lambda^2 = \text{constant}. \tag{53}$$

Then we have the following equations:

$$X''(x) = -\lambda^2 X(x) \tag{54}$$

and

$$T'(t) = -\lambda^2 T(t). \tag{55}$$

Eq. (54) is an ordinary differential equation with the general solution

$$X(x) = A\sin(\lambda x) + B\cos(\lambda x), \tag{56}$$

and Eq. (55) has the general solution

$$T(t) = Ce^{-\lambda^2 t}. \tag{57}$$

The solution of $v(x,t)$ will therefore have the form

$$v(x,t) = X(x)T(t) = (A\sin(\lambda x) + B\cos(\lambda x)) \cdot Ce^{-\lambda^2 t}. \tag{58}$$

The boundary conditions give:

$$\begin{aligned}
v(0,t) = X(0)T(t) &= 0 \\
&\downarrow \\
X(0) &= 0 \\
(A \cdot 0 + B \cdot 1) &= 0 \\
B &= 0 \\
&\Downarrow \\
X(x) &= A\sin(\lambda x)
\end{aligned}$$

and

$$
\begin{aligned}
v(L,t) = X(L)T(t) &= 0 \\
&\downarrow \\
X(L) &= 0 \\
A\sin(\lambda L) &= 0 \\
&\Updownarrow \\
&\lambda L = n\pi \\
&\Downarrow \\
&\lambda \equiv \lambda_n = \frac{n\pi}{L} \\
&\Downarrow \\
&X(x) = A\sin(n\pi x/L) \equiv A_n \sin(\lambda_n x).
\end{aligned}
$$

where $n = 1, 2, \ldots$ and we have chosen $X(0), X(L) = 0$ instead of the trivial solutions $T(t) = 0$. Then the solution of $v(x,t)$ is

$$v(x,t) = A_n \sin(\lambda_n x) \cdot Ce^{-\lambda_n^2 t} \equiv C_n \sin(\lambda_n x)e^{-\lambda_n^2 t} \tag{59}$$

Since the diffusion equation linear, any sum of solutions is also a solution to the diffusion equation. So the general solution is the sum of all the possible solutions, which would be a sum over all values of n:

$$v(x,t) = \sum_{n=1}^{\infty} C_n \sin(\lambda_n x)e^{-\lambda_n^2 t}. \tag{60}$$

The initial condition gives

$$v(x,0) = f(x) = \sum_{n=1}^{\infty} C_n \sin(n\pi x/L) \cdot 1, \tag{61}$$

which is a Fourier series. From the theory of Fourier series, the coefficients are found from the formula

$$C_n = \frac{2}{L}\int_0^L f(x)\sin(n\pi x/L)\,dx. \tag{62}$$

With $f(x) = -x/L$ this becomes

$$
\begin{aligned}
C_n &= \frac{2}{L}\int_0^L \left(-\frac{x}{L}\right)\sin\left(\frac{n\pi}{L}x\right)\,dx \\
&= -\frac{2}{L^2}\int_0^L x\sin\left(\frac{n\pi}{L}x\right)\,dx \\
&= -\frac{2}{L^2}\cdot\frac{L^2}{n^2\pi^2}\left(\sin(n\pi) - n\pi\cos(n\pi)\right) \\
&= -\frac{2}{n^2\pi^2}(0 - n\pi(-1)^n) \\
&= \frac{2}{n\pi}(-1)^n.
\end{aligned}
$$

where the integral has been looked up. Substituting this expression for C_n into Eq. (60) we get the general solution for v,

$$v(x,t) = \frac{2}{\pi}\sum_{n=1}^{\infty}(-1)^n \frac{\sin(n\pi x/L)}{n}\,e^{-n^2\pi^2 t/L^2}. \tag{63}$$

Then finally we find the general solution for $u(x,t)$ from Eq. (45):

$$u(x,t) = v(x,t) - f(x) + = \frac{2}{\pi}\sum_{n=1}^{\infty}(-1)^n \frac{\sin(n\pi x/L)}{n}\, e^{-n^2\pi^2 t/L^2} + \frac{x}{L}. \tag{64}$$

B Derivation of the analytical solution of the two-dimensional diffusion equation

In the two-dimensional case for the diffusion equation, again we assume the separation of variables, i.e,

$$u(x,y,t) = X(x)Y(y)T(t) \tag{65}$$

and therefore the diffusion equation goes to,

$$\frac{X_{xx}}{X} + \frac{Y_{yy}}{Y} = \frac{T_t}{T} \tag{66}$$

This leads to two equations

$$\frac{X_{xx}}{X} + \frac{Y_{yy}}{Y} = -\nu^2 \tag{67}$$

and

$$\frac{T_t}{T} = -\nu^2 \tag{68}$$

where ν is a constant. Eq. 67 can further be re-aranged so that each spatial component is separate. This is shown by the following

$$\frac{X_{xx}}{X} + \frac{Y_{yy}}{Y} + \nu^2 = -\kappa^2, \tag{69}$$

which leads to two equations

$$X_{xx} + \kappa^2 X = 0 \tag{70}$$

and

$$Y_{yy} + \rho^2 Y = 0, \tag{71}$$

where $\rho^2 = \nu^2 - \kappa^2$. This gives two general equation for the solution of X and Y.

$$X(x) = A\cos\kappa x + B\sin\kappa x \tag{72}$$

and

$$Y(y) = C\cos\rho y + D\sin\rho y. \tag{73}$$

By using the boundary conditions that $X(0) = X(L) = Y(0) = Y(L) = 0$ places restrictions on the two equations above. The initial conditions are given by $u(x,y,0) = \sin(\pi x/L)\sin(\pi y/L)$. Applying the boundary conditions leads to

$$\begin{aligned}
X(0) = A \quad &\longrightarrow \quad A = 0 \\
Y(0) = C \quad &\longrightarrow \quad C = 0 \\
X(L) = B\sin\kappa L \quad &\longrightarrow \quad \kappa = n\pi/L \\
Y(L) = D\sin\rho L \quad &\longrightarrow \quad \rho = m\pi/L
\end{aligned}$$

where n and m are equal to $\pm 1, \pm 2, \pm 3...$. The general solution to the temporal component $T(t)$ is the same as in the one dimensional case, $T(t) = \text{Constant} \exp -\nu^2 t$. This leads to the analytic equation for the two dimensional case.

$$u(x,y,t) = \sum_{n=1}^{\infty} \sum_{m=1}^{\infty} A_{nm} \sin\left(\frac{n\pi x}{L}\right) \sin\left(\frac{m\pi y}{L}\right) e^{\frac{-(n^2+m^2)\pi^2 t}{L^2}}, \tag{74}$$

The initial condition gives

$$u(x,y,0) = \sin\left(\frac{\pi x}{L}\right) \sin\left(\frac{\pi y}{L}\right) = \sum_{n=1}^{\infty} \sum_{m=1}^{\infty} A_{nm} \sin\left(\frac{n\pi x}{L}\right) \sin\left(\frac{m\pi y}{L}\right) \tag{75}$$

By using the theory of Fourier series, these coefficients A_{nm} are

$$A_{nm} = \left(\frac{2}{L}\right)^2 \int_0^L \int_0^L \sin\left(\frac{\pi x}{L}\right) \sin\left(\frac{\pi y}{L}\right) \sin\left(\frac{n\pi x}{L}\right) \sin\left(\frac{m\pi y}{L}\right) dx dy. \tag{76}$$

Using the definition of orthogonal polynomials

$$\int_0^L \sin\left(\frac{n\pi x}{L}\right) \sin\left(\frac{m\pi x}{L}\right) dx = \begin{cases} \frac{L}{2} & \text{if } n = m \\ 0 & \text{if } n \neq m \end{cases} \tag{77}$$

results in the solution to A_{nm} only when $n = m = 1$,

$$A_{nm} = \left(\frac{2}{L}\right)^2 \left(\frac{L}{2}\right)^2 = 1 \tag{78}$$

This gives the solution to the two dimensional diffusion equation

$$u(x,y,t) = \sin\left(\frac{\pi x}{L}\right) \sin\left(\frac{\pi y}{L}\right) e^{-2\pi^2 t/L^2} \tag{79}$$