# A NUMERICAL STUDY OF THE DIFFUSION/HEAT EQUATION IN ONE AND TWO DIMENSIONS.

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#### Abstract

#### I. Introduction

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

#### II. METHOD

In order to get an overview of which methods being used we take a closer look at the different types of methods in this section. Where we will look at three different types of methods for solving the diffusion equation [1]. There are three methods being implemented in this text - Forward Euler, Backward Euler and Crank-Nicolson. All in which is slightly different from one another.

#### i. Explicit Scheme: Forward Euler

To start of we look at the Forward Euler method for solving partial differential equation, such as the diffusion equation [1].

$$\frac{\partial^2 u(x,t)}{\partial x^2} = \frac{\partial u(x,t)}{\partial t}, t > 0, x \in [0,L]$$

This equation can be solved through a central difference approximation. If we look at the time-dependent derivative we get:

$$\frac{\partial u(x,t)}{\partial t} = u_t = \frac{u(x_i, t_j + \Delta t) - u(x_i, t_j)}{\Delta t} + O(\Delta t)$$
 (2)

This expression is only exact if it contains the local approximation error of  $O(\Delta t)$ . Where  $\Delta t$  is the time-step, and  $t_j$  is the total time after j time steps. The same goes for step-length:

$$t_j = j\Delta t$$
  $j > 0$   
 $x_i = i\Delta x$   $0 < i < n+1$ 

Where i & j is the iterations of steps and time respectively. The step-length  $\Delta x$  is defined as:

$$\Delta x = \frac{1}{n+1}$$

Further on, we need to approximate the second derivative which is dependent on the position.

$$\frac{\partial^2 u(x,t)}{\partial x^2} = u_{xx} = \frac{u(x_i + \Delta x, t_j) - 2u(x_i, t_j) + u(x_i - \Delta x, t_j)}{\Delta x^2} + O(\Delta x^2)$$
(3)

Where in this case we have an local approximation error of  $O(\Delta x^2)$ . Once we have the equations [2] [3], we can discretize these for simplifications. We can now write equation [1] in a discretized version:

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

Rearranging this equation so that we can find the solution of the next time j + 1:

$$u_{i,j+1} = \alpha u_{i+1,j} + (1 - 2\alpha)u_{i,j} + \alpha u_{i-1,j} \tag{4}$$

Where we now have define  $\alpha = \frac{\Delta t}{\Delta x^2}$ . Now we would like to investigate the boundary conditions which is applied to our system. At the time t = 0, we have the solution:

$$u(x,0) = u_{i,0} = 0$$
  $0 < x < L$ 

And for the boundary condition of the x-region, which stretches from  $0 \to L$ , where L = 1, we get:

$$u(0,t) = u_{0,j} = 0$$
  $t \ge 0$   
 $u(L,t) = u_{n+1,j} = 1$   $t \ge 0$ 

Where n + 1 indicates the last iteration in space, yielding  $L = x_{n+1} = (n+1)\Delta x = 1$ , since  $\Delta x = 1/(n+1)$ . Once we have the boundary conditions of the diffusion equation we are able to rewrite it as a vector  $\mathbf{V}_i$ , which is dependent of time.

$$\mathbf{V}_{j} = \begin{bmatrix} u_{1,j} \\ u_{2,j} \\ \cdots \\ \vdots \\ u_{n,j} \end{bmatrix}$$

If we take a closer look at equation 9 we can see that we can create a matrix consisting of  $\alpha$  and  $-2\alpha$ :

By this we may write the discretized version of the diffusion equation in matrix form.

$$\begin{bmatrix} u_{1,j+1} \\ u_{2,j+1} \\ \vdots \\ u_{n,j+1} \end{bmatrix} = \begin{bmatrix} 1-2\alpha & \alpha & 0 & \dots & \dots & 0 \\ \alpha & 1-2\alpha & \alpha & 0 & \dots & \dots \\ 0 & \alpha & 1-2\alpha & \alpha & 0 & \dots \\ \vdots \\ 0 & \dots & \dots & \dots & \dots & \dots & \dots \\ \vdots \\ 0 & \dots & \dots & \dots & \alpha & 1-2\alpha & \alpha \\ 0 & \dots & \dots & 0 & \alpha & 1-2\alpha \end{bmatrix} \begin{bmatrix} u_{1,j} \\ u_{2,j} \\ \vdots \\ u_{n,j} \\ u_{n,j} \end{bmatrix}$$

In closed matrix form it reads:

$$\mathbf{V}_{j+1} = \mathbf{A}\mathbf{V}_j \tag{5}$$

Further on we may rewrite  $\bf A$  as an identity matrix and a tridiagonal Toeplitz matrix  $\bf B$ , where  $\bf B$  is:

$$\therefore \quad \mathbf{V}_{i+1} = (\hat{I} - \alpha \mathbf{B}) \mathbf{V}_i \tag{6}$$

This is the Forward Euler method, the basic idea is that by knowing the previously calculated  $V_j$ , it is possible to calculate the next  $V_{j+1}$ . This is called the explicit scheme, since the next function  $u_{i,j+1}$  is explicitly given by equation [9].

#### ii. Implicit Scheme: Backward Euler

Backward Euler exhibits very much the same approach as Forward Euler. We start by approximating the the diffusion equation at hand.

$$\frac{\partial^2 u(x,t)}{\partial x^2} = \frac{\partial u(x,t)}{\partial t}, t > 0, x \in [0,L]$$

Dividing up into a time-dependent derivative part and a space-dependent derivative part. The difference, however, is that this methods exploits the backwards formula. The time-dependent derivative is then formulated as such:

$$\frac{\partial u(x,t)}{\partial t} = u_t = \frac{u(x_i, t_j) - u(x_i, t_j - \Delta t)}{\Delta t} + O(\Delta t)$$
(7)

Where the truncation error  $O(\Delta t)$ , just as for the Forward Euler method. Step-length  $\Delta x$  and time-step  $\Delta t$  has the same definition as defined by Forward Euler method. The space-dependent derivative is written in the same way as the Forward Euler method.

$$\frac{\partial^2 u(x,t)}{\partial x^2} = u_{xx} = \frac{u(x_i + \Delta x, t_j) - 2u(x_i, t_j) + u(x_i - \Delta x, t_j)}{\Delta x^2} + O(\Delta x^2)$$
(8)

The same truncation error is added just as for the Forward Euler method. Once these equation is written out we discretize just as earlier.

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

Rearranging this equation so that we can find the solution of previous time j-1 - hence Backward Euler.

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

Where we have defined  $\alpha$  as previously, namely as  $\frac{\Delta t}{\Delta x^2}$ . Just as last section we can define a matrix  $\mathbf{A}_{BE}$ , subscript BE for Backward Euler.

We are using the same boundary conditions as last section. We can then also define the same vector  $\mathbf{V}_i$ , and compactly write the diffusion equation in matrix form.

$$\mathbf{V}_{j} = \begin{bmatrix} u_{1,j} \\ u_{2,j} \\ \dots \\ \dots \\ u_{n,j} \end{bmatrix}$$

In compact matrix form we get a slighlty different answere than the Forward Euler method, since we know are looking the previous solution of time  $u_{i,j-1}$ :

$$\mathbf{V}_{i-1} = \mathbf{A}_{BE} \mathbf{V}_i \tag{10}$$

Where the  $\mathbf{A}_{BE}$  may be rewritten as a tridagonal Toeplitz matrix  $\mathbf{B}$ . Little matrix algebra means we can rewrite the equation.

$$\mathbf{V}_{j-1} = (\hat{I} + \alpha \mathbf{B}) \mathbf{V}_j \tag{11}$$

where  $\mathbf{B}$  is defined as:

$$\therefore \quad \mathbf{V}_{i} = (\hat{I} + \alpha \mathbf{B})^{-1} \mathbf{V}_{i-1} \tag{12}$$

We can see that this method is different than the Forward Euler method, since this method relies on determining the vector  $u_{i,j-1}$ , instead of  $u_{i,j+1}$ , therefore it is called an implicit scheme.

#### iii. Crank-Nicolson scheme

The third and final method is the Crank-Nicolson scheme. The basic idea here is to combine the Forward Euler and Backward Euler in some sense. So for a more general approach than derived previously we can find a way to express the diffusion equation as a combination of explicit and implicit schemes. This gives us the so-called Crank-Nicolson Scheme, after Crank and Nicolson.

We begin with by introducing a parameter  $\theta$  ( $\theta - rule$ ), and and using  $\theta$  to express both the explicit and implicit scheme, depending on the choice of  $\theta$ :

Explicit scheme- Forward Euler

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

Implicit scheme- Backward Euler

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

These equations was derived in the previous subsection, now, by combining these and applying the  $\theta - rule$  we get:

$$\frac{u_{i,j} - u_{i,j-1}}{\Delta t} = \frac{\theta}{\Delta x^2} (u_{i+1,j} - 2u_{i,j} + u_{i-1,j}) + \frac{1 - \theta}{\Delta x^2} (u_{i+1,j-1} - 2u_{i,j-1} + u_{i-1,j-1})$$
(13)

We can see by equation 13, that by setting  $\theta = 0$ , we simply end up with the Forward Euler - explicit scheme. The time-part indexed by j is moved one step earlier for the Forward Euler method in order to match it with the Backward Euler expression. Further on we see the we get the Backward Euler- Implicit scheme if  $\theta$  is chosen to be 1. This is all fine, as we are able to reproduce the different schemes with a specific choice of  $\theta$ . The last choice of  $\theta$  that we will present is however the most interesting one,  $\theta = 1/2$ . For this choice of  $\theta$  we end up with the Crank-Nicolson scheme. For the previous schemes we saw that the truncation error of the time derivative was  $O(\Delta t)$ , the Crank-Nicolson Scheme on the other hand has a truncation error which goes like  $O(\Delta t^2)$ .

The way we proceed from here is to rearrange equation 13 when  $\theta = 1/2$  is implemented.

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

Defining  $\alpha = \Delta t/\Delta x^2$  as before:

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

Further on by rearranging the equation so that we have the "Forward Euler" on one side and "Backward Euler" on the other side we get:

$$-\alpha u_{i+1,j} + (2+2\alpha)u_{i,j} - \alpha u_{i-1,j} = \alpha u_{i+1,j-1} + (2-2\alpha)u_{i,j-1} + \alpha u_{i-1,j-1}$$
(14)

Where we can identify the left-hand side to be:

And the right-hand side:

These matrices -  $\mathbf{A}_{CN_1}$  &  $\mathbf{A}_{CN_2}$  are simply tridiagonal matrices, we can then construct a matrix  $\mathbf{B}$ , which will be the tridiagonal matrix:

We may rewrite equation 14 in a matrix- form:

$$(2\hat{I} + \alpha \mathbf{B})\mathbf{V}_j = (2\hat{I} - \alpha \mathbf{B})\mathbf{V}_{j-1}$$

$$\therefore \quad \mathbf{V}_j = (2\hat{I} + \alpha \mathbf{B})^{-1} (2\hat{I} - \alpha \mathbf{B}) \mathbf{V}_{j-1}$$
 (15)

Where  $V_j$  and  $V_{j-1}$  is as defined previously, simply vectors containing  $(u_{i,j})$  for  $i \in (1,n)$ . Table 1 gives an overview over the truncation error for the three methods introduced as well as the stability requirements.

#### iv. Stability requirements

Table 1: Overview of Schemes truncation error and stability requirements

Scheme	Truncation Error	Stability requirements
Forward Euler	$O(\Delta x^2) \& O(\Delta t)$	$\Delta t \le \frac{1}{2} \Delta x^2$
Backward Euler	$O(\Delta x^2) \& O(\Delta t)$	$\mathbb{N} \in \Delta x$ and $\Delta t$
Crank-Nicolson	$O(\Delta x^2) \ \& \ O(\Delta t^2)$	$\mathbb{N} \in \Delta x$ and $\Delta t$

#### III. IMPLEMENTATION

#### IV. NUMERICAL RESULTS

V. DISCUSSION

VI. CONCLUSION

## Appendices

#### A. ANALYTICAL SOLUTION TO THE ONE DIMENSIONAL HEAT EQUATION.

In one dimension, the heat equation have the following form:

$$\frac{\partial^2 u(x,t)}{\partial x^2} = \frac{\partial u(x,t)}{\partial t}, \quad t > 0, \quad x \in [0,L]$$

We have a Dirichlet boundary problem, where one end is fixed at zero and the other at one at all times, u(0,t)=0 & u(L,t)=1 for  $t\geq 1$ . A physical interpretation of this problem can be a rod fixed at both ends to two different heat sources that keeps the temperature at each side fixed. Heat will then flow from the hot end to the cold end until steady-state temperature distribution is achieved. The initial condition  $\left(u(x,0)=0 \quad 0 < x < L\right)$  states that the rod is at zero for every position except for the end points which are defined from the boundary condition. For all  $t\geq t_{ss}$ , where  $t_{ss}$  is the time where steady-state is achieved in the system, the solution is expected to be a linear function  $u_0(x)=ax+b$ , which satisfies the 1D-Laplace equation  $\left(\frac{d^2u_0(x)}{dx^2}=0\right)$ . From the boundary condition at x=0, the constant b=0 and a=1/L. An ansatz on the solution to be a product of a space dependent part and a time dependent part in addition to the linear term will be used to try to solve the partial differential problem at hand  $\left(u(x,t)=\frac{x}{L}+F(x)G(t)\right)$ . The notation used in these calculations will be (') for space derivatives and (·) over the function for time derivatives.

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

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

$$\frac{1}{F(x)}F''(x) = \frac{1}{G(t)}\dot{G}(t) = -k^2$$

The last equation states that the spacial part on the left hand side (L.H.S) and the time part on the right hand side (R.H.S) must be equal to some constant. This constant is chosen to be squared for reasons shown later in the calculations, while the minus sign is there to make it so that the solutions will not "blow up" when time goes on. First we will solve the time-dependent part:

$$\frac{1}{G(t)}\dot{G}(t) = -k^2$$

$$\frac{1}{G(t)} \cdot \frac{dG(t)}{dt} = -k^2$$

$$\int \frac{dG(t)}{G(t)} = \int -k^2 dt$$

$$\ln G(t) = -k^2 t$$

$$G(t) = e^{-k^2 t}$$

No constant is included in the above expression, since all constants will be baked into the spacial part constant. From the solution, the choice of negative constant now makes sense, as the time dependent part will fall exponentially to zero for large values of t. Next we solve for the spacial part, this is a well known equation called the Helmholtz equation  $(d^2F(x)/dx^2 + k^2F(x) = 0)$ . This equation generalizes to more dimensions as  $\nabla^2 F(x_1, x_2, ..., x_n) + k^2 F(x_1, x_2, ..., x_n) = 0$ , which must be further separated, which will be done in the other section of the appendix, the solution to the 2D problem. Helmholtz equation will be solved using the complex conjugate roots of the auxiliary equation.

$$\frac{d^2F(x)}{dx^2} + k^2F(x) = 0$$

$$\lambda^2 + k^2 = 0 \implies \lambda_{\pm} = \pm ik$$

$$\implies F(x) = A\sin(kx) + B\cos(kx)$$

The  $\cos(kx)$  term from the solution of Helmholtz, will be disregarded because of the boundary condition stating that u(0,t)=0. The other boundary condition for x=L can be achieved when  $\sin(kL)=0$  which gives us the quantization  $k=\frac{n\pi}{L}$ .

$$u_n(x,t) = A_n \sin(\frac{n\pi}{L}x)e^{-\frac{n^2\pi^2}{L^2}t}$$
 (16)

Equation 16 gives us a basis of eigenfunctions that can be spanned to give the whole solution.

$$u(x,t) = u_0(x) + \sum_{n=1}^{\infty} u_n(x,t) = \frac{x}{L} + \sum_{n=1}^{\infty} A_n \sin\left(\frac{n\pi}{L}x\right) e^{-\frac{n^2\pi^2}{L^2}t}$$

The next step is to find the coefficients  $A_n$ , by finding the Fourier sine series that can describe the initial temperature distribution in the rod. This function can be modeled with a Heaviside step function, H(x-L), i.e. 0 for x < L and 1 for  $x \ge L$ , but for this problem we have  $x \in [0, L]$ , so we are not interested in points beyond L.

$$u(x,0) = H(x-L) = \frac{x}{L} + \sum_{n=1}^{\infty} A_n \sin\left(\frac{n\pi}{L}x\right)$$

$$H(x-L) - \frac{x}{L} = \sum_{n=1}^{\infty} A_n \sin\left(\frac{n\pi}{L}x\right)$$

$$\implies A_n = \frac{2}{L} \int_0^L \left( H(x - L) - \frac{x}{L} \right) \sin\left(\frac{n\pi}{L}x\right) dx$$

$$=H(x-L)\left(\frac{2\cos\left(n\pi\right)}{n\pi}-\frac{2\cos\left(\frac{n\pi}{L}x\right)}{n\pi}\right)-\frac{2\sin\left(\frac{n\pi}{L}x\right)}{n^2\pi^2}+\frac{2x\cos\left(\frac{n\pi}{L}x\right)}{n\pi L}\bigg|_{0}^{L}$$

$$A_n = \frac{2 \cdot (-1)^n}{n\pi}$$

The solution for this integral was found through the use of WolframAlpha.<sup>1</sup> The integral could have been split up into two integrals, one with the Heaviside, and one with the linear term. Solving this would have given 0 for the first integral, meaning the only contribution comes from the linear term integral. This means that an initial approximation of u(x,0) = 0 could have been made and would end with the same result. Inserting the limits 0 and L in the equation terminates all terms except the last cosine term for x = L. This cosine term will change between (-1) and 1 for odd and even n respectively, so that  $A_n = \frac{2 \cdot (-1)^n}{n\pi}$ . From this we now have an analytical solution to the 1D heat equation for the given boundary conditions.

$$u(x,t) = \frac{x}{L} + \sum_{n=1}^{\infty} 2 \frac{(-1)^n}{n\pi} \sin\left(\frac{n\pi}{L}x\right) e^{-\frac{n^2\pi^2}{L^2}t}$$
(17)

#### B. Analytical solution to the two dimensional heat equation

In two dimensions the heat equation looks fairly equal to the one dimensional. Using the nabla operator for Cartesian coordinates in two dimensions give the following partial derivative equation.

$$\left(\frac{\partial^2}{\partial x^2} + \frac{\partial^2}{\partial y^2}\right)u(x, y, t) = \nabla^2 u(x, y, t) = \frac{\partial u(x, y, t)}{\partial t}$$
(18)

The boundaries will be fixed to zero, giving the boundary conditions u(0,y,t)=u(L,y,t)=u(x,0,t)=u(x,L,t)=0. Initial condition for the surface at t=0 is given by the function  $f(x,y)=\sin(\frac{\pi}{L}x)\sin(\frac{\pi}{L}y)$ . By variable separation, such as in the 1 dimensional case, an analytical solution can be made for the given conditions. Ansatz:

u(x, y, t) = X(x)Y(y)T(t)

$$X(x)Y(y)\frac{\partial T(t)}{\partial t} = Y(y)T(t)\frac{\partial^2 X(x)}{\partial x^2} + X(x)T(t)\frac{\partial^2 Y(y)}{\partial y^2}$$

$$\frac{1}{T(t)}\frac{\partial T(t)}{\partial t} = \frac{1}{X(x)}\frac{\partial^2 X(x)}{\partial x^2} + \frac{1}{Y(y)}\frac{\partial^2 Y(y)}{\partial y^2} = -k^2$$

So far this looks like the calculation for the one dimensional case, and the temporal part actually has the same solution:  $T(t) = e^{-k^2 t}$ . Next is to calculate the space parts.

$$-k^{2} = \frac{1}{X(x)} \frac{\partial^{2} X(x)}{\partial x^{2}} + \frac{1}{Y(y)} \frac{\partial^{2} Y(y)}{\partial y^{2}}$$

$$-\bigg(\frac{1}{Y(y)}\frac{\partial^2 Y(y)}{\partial y^2} + k^2\bigg) = \frac{1}{X(x)}\frac{\partial^2 X(x)}{\partial x^2} = -p^2$$

X(x):

$$\nabla^2 X(x) + p^2 X(x) = 0$$

$$\implies X(x) = \sin(px) + \cos(px)$$

<sup>&</sup>lt;sup>1</sup>https://bit.ly/2PjawmT - Wolfram Alpha link for solution

Y(y):

$$\nabla^2 Y(y) + Y(y)(k^2 - p^2) = \nabla^2 Y(y) + Y(y)q^2 = 0$$

$$\implies Y(y) = \sin(qy) + \cos(qy)$$

Both the x-term and y-term have the form of Helmholtz equation, solved as explained for one dimension. Due to the boundary conditions, the cosine terms from both must be disregarded and the constants p and q will be quantified as  $\frac{n\pi}{L}$  and  $\frac{m\pi}{L}$  respectively. This implies the constant  $k^2 = (n^2 + m^2)\pi^2/L^2$ , and we can write a general solution as a superposition as in the one dimensional case

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

$$A_{nm} = \left(\frac{2}{L}\right)^2 \int_0^L \int_0^L \sin\left(\frac{\pi}{L}x\right) \sin\left(\frac{\pi}{L}y\right) \sin\left(\frac{n\pi}{L}x\right) \sin\left(\frac{m\pi}{L}y\right) dx dy = 1$$

When calculating the coefficient  $A_{nm}$ , the orthogonality properties of sine functions are used:  $\int_0^L \sin\left(\frac{n\pi}{L}x\right) \sin\left(\frac{m\pi}{L}x\right) dx = \frac{L}{2}\delta_{nm}.$  This property made sure that the only contribution to the sum comes when n=m=1 giving the analytical solution as follows:

$$u(x,y,t) = \sin\left(\frac{\pi x}{L}\right) \sin\left(\frac{\pi y}{L}\right) e^{-\frac{2\pi^2}{L^2}t} \tag{19}$$