Diffusion

Sebastian Amundsen, Marcus Berget and Andreas Wetzel

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1 Introduction

2 Theory

2.1 Heat equation

The general heat equation can be written as,

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

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

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

or

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

2.2 Numerical methods for solving the heat equation

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

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

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

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

and

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

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

2.2.1 Explicit forward Euler method

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

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

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

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

By using the forward formula to approximate the derivatives we obtain

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

and

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

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

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

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

2.2.2 Implicit backward Euler method

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

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

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

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

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

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

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

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

We can reformulate the problem as a matrix vector multiplication:

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

We can then write the problem as:

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

2.2.3 Crank-Nicholson scheme

The Crank-Nicholson scheme is given by

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

and

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

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

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

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

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

We can rewrite equation 20 as:

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

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

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

2.3 Analytical solution for one dimensional diffusion equation

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

$$u(x,t) = \sum_{n=1}^{\infty} \frac{2}{L} \int_0^L g(x) \sin(n\pi x/L) dx \sin(n\pi x/L) \tag{22}$$

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

3 Method

4 Implementation

5 Results

6 Discussion

7 Concluding remarks

A Appendix

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B Appendix

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

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

The initial condition is $u(x,0) = g(x)$, when $0 < x < L$. We also have $u(0,t) = 0$ and $u(L,t) = 0$, when $t \leq 0$. We use separation of variables when solving 23:

$$u(x,t) = F(x)G(t) \tag{24}$$

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

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

and

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

We can now use the relation given equation 2:

$$\begin{aligned} F\frac{\partial G}{\partial t} &= G\frac{\partial^2 F}{\partial x^2} \\ \frac{1}{G}\frac{\partial G}{\partial t} &= \frac{1}{F}\frac{\partial^2 F}{\partial x^2} \end{aligned} \tag{25}$$

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

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

We can now use equation 24 to find the general solution u:

$$\begin{aligned} u = GF &= Ae^{-\lambda^2 t}[B\cos{(\lambda x)} + C\sin{(\lambda x)}] \\ &= e^{-\lambda^2 t}[C_1\cos{(\lambda x)} + C_2\sin{(\lambda x)}] \end{aligned} \tag{26}$$

The boundary conditions gives us the solution:

$$u(x,t) = A_n \sin{(n\pi x/L)} e^{-n^2\pi^2 t/L} \tag{27}$$

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

$$u(x,t) = \sum_{n=1}^{\infty} A_n \sin\left(n\pi x/L\right) \tag{28}$$

We decide the coefficient A_n by using the initial condition:

$$u(x,0) = g(x) = \sum_{n=1}^{\infty} A_n \sin\left(n\pi x/L\right) \tag{29}$$

Which gives us that:

$$A_n = \frac{2}{L}\int_0^L g(x)\sin\left(n\pi x/L\right)dx \tag{30}$$

We can insert this A_n in equation 28, which gives us the final expression [1].

References

References

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

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