Eötvös Loránd University

Modern Numerical Methods in Physics

CPNUMMETHF17EM

Energy Levels of the Hydrogen Molecule Ion (H_2^+)

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Contents

1 Introduction

The study of the heat diffusion is important to understand how the heat evolves through time in different materials with different boundary conditions. Sometimes, it is quite difficult or impossible to solve the problem analytically; therefore, simulations using the heat equations is important, for example, to model a new product, it is possible to test dimensions, geometry and materials to choose the best parameters in a simulated environment.

In this project it will be a rectangular metal sheet, with specific boundary conditions, such as, opposite sides with constant temperature, another side with heat flux and the last side have perfect insulation. For that the Crank-Nicolson method will be used.

2 Physical Principles

The heat flows from hot to cold, enunciating it mathematically we can say that the heat flow ($\boldsymbol{H}$) is proportional to the gradient of the temperature ($T(\boldsymbol{x}, t)$) across the material,

$$\boldsymbol{H} = -k \nabla T(\boldsymbol{x}, t), \tag{1}$$

where k is the thermal conductivity. To quantize the total amount of heat ($Q(t)$) in a specific time we can calculate by integrating the temperature over the volume multiplied by a constant of proportionality, so it is written as

$$Q(t) = \int d\boldsymbol{x} C_p \rho(\boldsymbol{x}) T(\boldsymbol{x}, t), \tag{2}$$

where C_p is the specific heat and $\rho(\boldsymbol{x})$ is the density. If we consider that the energy is conserved in the system, the rate that Q decreases over time is equal to the heat that flows from the material; therefore, the equation is

$$\frac{\partial T(\boldsymbol{x}, t)}{\partial t} = \frac{k}{c_p \rho} \nabla^2 T(\boldsymbol{x}, t), \tag{3}$$

to simplify we can compress the constants, using the definition of the thermal diffusivity (α), which is

$$\alpha = \frac{k}{c_p \rho}, \tag{4}$$

when we considered that the energy is conserved, it implies that the material is isolated from the exterior. In other words, the heat does not flow outside the system. For our case, we used Cartesian coordinates in 2 dimensions, so the final partial differential equation is

$$\frac{\partial T(x, y, t)}{\partial t} = \alpha \left(\frac{\partial^2}{\partial x^2} + \frac{\partial^2}{\partial y^2} \right) T(x, y, t). \tag{5}$$

However, in our case we have a constant heat flux coming in from one of the sides, so we have that

$$\frac{\partial T(x,y,t)}{\partial t} = hf(x,y), \tag{6}$$

where h is just a positive constant that is the rate of the heat being transfer trough the system, and $f(x,y)$ is a function to define the boundary conditions of this source of heat. Adding this condition, we get a modified heat equation as [2] [1]

$$\frac{\partial T(x,y,t)}{\partial t} = \alpha\left(\frac{\partial^2}{\partial x^2} + \frac{\partial^2}{\partial y^2}\right)T(x,y,t) + hT(x,y,t)f(x,y). \tag{7}$$

3 Numerical Method

To solve Partial Differential Equations (PDE) a good method is the Crank-Nicolson, it is more precise and stable than the Time-stepping method [1].

3.1 Crank-Nicolson

To understand the Crank-Nicolson method in 2D, it is better to derive first the one-dimensional case, because after all the two-dimensional one is similar to solve the one-dimensional problem twice. The computational part of the problem is to calculate a tridiagonal matrix equation, which is explained in the last subsection.

3.1.1 Crank-Nicolson 1D

The heat equation (3) in one dimension can be written as a time derivative in the left-hand side. For this, we use a central-difference approximation with a split time step ($t \to t + \Delta t/2$). Moreover, for the space derivative in the right-hand side, we also perform a central-difference approximation, but now it is a double derivative and the time is $t = t + \Delta t$; therefore, the expression can be approximated by

$$\frac{T_i^{\tau+1} - T_i^{\tau}}{\Delta t} = \frac{\alpha}{2(\Delta x)^2}[(T_{i+1}^{\tau+1} - 2T_i^{\tau+1} + T_{i-1}^{\tau+1}) + (T_{i+1}^{\tau} - 2T_i^{\tau} + T_{i-1}^{\tau})], \tag{8}$$

to simplify we can define

$$\eta = \frac{\alpha \Delta t}{2(\Delta x)^2}, \tag{9}$$

so it leads to

$$T_i^{\tau+1} - T_i^{\tau} = \eta[(T_{i+1}^{\tau+1} - 2T_i^{\tau+1} + T_{i-1}^{\tau+1}) + (T_{i+1}^{\tau} - 2T_i^{\tau} + T_{i-1}^{\tau})], \tag{10}$$

reordering the equation such that the future values of temperature are in the left and present values in the right, we have

$$-\eta T_{i+1}^{\tau+1} + (1+2\eta)T_i^{\tau+1} - \eta T_{i-1}^{\tau+1} = \eta T_{i+1}^{\tau} + (1-2\eta)T_i^{\tau} + \eta T_{i-1}^{\tau}. \tag{11}$$

We can rewrite this expression in matrix form like

$$\begin{pmatrix} (1+2\eta) & -\eta & 0 & 0 & \dots & 0 \\ -\eta & (1+2\eta) & -\eta & 0 & \dots & 0 \\ 0 & -\eta & (1+2\eta) & -\eta & \dots & 0 \\ \vdots & \vdots & \vdots & \vdots & \vdots & \vdots \\ 0 & 0 & \dots & -\eta & (1+2\eta) & -\eta \\ 0 & 0 & \dots & 0 & -\eta & (1+2\eta) \end{pmatrix} \begin{pmatrix} T_1^{\tau+1} \\ T_2^{\tau+1} \\ T_3^{\tau+1} \\ \vdots \\ T_{i-1}^{\tau+1} \\ T_i^{\tau+1} \end{pmatrix} = \begin{pmatrix} T_1^{\tau} \\ T_2^{\tau} \\ T_3^{\tau} \\ \vdots \\ T_{i-1}^{\tau} \\ T_i^{\tau} \end{pmatrix}, \tag{12}$$

note that the first matrix is tridiagonal, the second is the temperature values of the future time and the third is the values in the present time [1].

3.1.2 Crank-Nicolson 2D

However, the project is a two-dimensional room, so we actually need to solve equation 5. As same as before, we use central-difference with $t = t + \Delta t$, then we have that

$$\begin{aligned} \frac{T_{i,j}^{\tau+1} - T_{i,j}^{\tau}}{\Delta t} =& \frac{\alpha}{2(\Delta x)^2}[(T_{i+1,j}^{\tau+1} - 2T_{i,j}^{\tau+1} + T_{i-1,j}^{\tau+1}) + (T_{i+1,j}^{\tau} - 2T_{i,j}^{\tau} + T_{i-1,j}^{\tau})] \\ &+ \frac{\alpha}{2(\Delta y)^2}[(T_{i,j+1}^{\tau+1} - 2T_{i,j}^{\tau+1} + T_{i,j-1}^{\tau+1}) + (T_{i,j+1}^{\tau} - 2T_{i,j}^{\tau} + T_{i,j-1}^{\tau})], \end{aligned} \tag{13}$$

we can make the approximation that $\Delta x = \Delta y$, but the geometry of the system is not a square; therefore, the number of steps are different for each direction. Similarly to the one dimensional case, we can simplify the equation using 9, then we have

$$\begin{aligned} T_{i,j}^{\tau+1} - T_{i,j}^{\tau} = \eta[&(T_{i+1,j}^{\tau+1} - 2T_{i,j}^{\tau+1} + T_{i-1,j}^{\tau+1}) + (T_{i+1,j}^{\tau} - 2T_{i,j}^{\tau} + T_{i-1,j}^{\tau}) \\ &+ (T_{i,j+1}^{\tau+1} - 2T_{i,j}^{\tau+1} + T_{i,j-1}^{\tau+1}) + (T_{i,j+1}^{\tau} - 2T_{i,j}^{\tau} + T_{i,j-1}^{\tau})], \end{aligned} \tag{14}$$

defining the operators

$$\delta_x^2 f_{i,j} = f_{i+1,j} - 2f_{i,j} + f_{i-1,j} \qquad \delta_y^2 f_{i,j} = f_{i,j+1} - 2f_{i,j} + f_{i,j+1}, \tag{15}$$

we can rewrite as

$$T_{i,j}^{\tau+1} - T_{i,j}^{\tau} = \eta[\delta_x^2 T_{i,j}^{\tau+1} + \delta_x^2 T_{i,j}^{\tau} + \delta_y^2 T_{i,j}^{\tau+1} + \delta_y^2 T_{i,j}^{\tau}], \tag{16}$$

reordering the equation

$$(1 - \eta\delta_x^2 - \eta\delta_y^2)T_{i,j}^{\tau+1} = (1 + \eta\delta_x^2 + \eta\delta_y^2)T_{i,j}^{\tau}, \tag{17}$$

or

$$(1-\eta\delta_x^2)(1-\eta\delta_y^2)T_{i,j}^{\tau+1} = (1+\eta\delta_x^2)(1+\eta\delta_y^2)T_{i,j}^{\tau}, \tag{18}$$

if we consider $\eta^2\delta_x^2\delta_y^2 = \eta^2\delta_y^2\delta_x^2 \cong 0$, since η is a small number.

Now we separate into two equations using an intermediate matrix $T^*_{i,j}$ as follows

$$\begin{aligned}(1-\eta\delta_x^2)T_{i,j}^{*} &= (1+\eta\delta_y^2)T_{i,j}^{\tau}\\ (1-\eta\delta_y^2)T_{i,j}^{\tau+1} &= (1+\eta\delta_x^2)T_{i,j}^{*},\end{aligned} \tag{19}$$

to check if the separation works, we substitute the second equation in 19 in the left-hand side of 18, then change the order of the multiplication so we can substitute the first equation of 19 to get the right-hand side of 18, as seen below

$$\begin{aligned}(1-\eta\delta_x^2)(1-\eta\delta_y^2)T_{i,j}^{\tau+1} &= (1-\eta\delta_x^2)(1+\eta\delta_x^2)T_{i,j}^{*}\\ = (1+\eta\delta_x^2)(1-\eta\delta_x^2)T_{i,j}^{*} &= (1+\eta\delta_x^2)(1+\eta\delta_y^2)T_{i,j}^{\tau}.\end{aligned} \tag{20}$$

Now letting 19 more explicit

$$\begin{aligned}-\eta T^*_{i+1,j} + (1+2\eta)T^*_{i,j} - \eta T^*_{i-1,j} &= \eta T^{\tau}_{i,j+1} + (1-2\eta)T^{\tau}_{i,j} + \eta T^{\tau}_{i,j-1}\\ -\eta T^{\tau+1}_{i,j+1} + (1+2\eta)T^{\tau+1}_{i,j} - \eta T^{\tau+1}_{i,j-1} &= \eta T^*_{i+1,j} + (1-2\eta)T^*_{i,j} + \eta T^*_{i-1,j},\end{aligned} \tag{21}$$

which is similar to 11, we have just to remember that the number of steps is different in each direction [3].

All of this was for the case where the system is isolated from the external environment. Nonetheless, it is easy to implement the heat source, we have to add the constant h in the main diagonal of the matrix, then the uncoupled form is [1]

$$\begin{aligned}-\eta T^*_{i+1,j} + (1+2\eta-h)T^*_{i,j} - \eta T^*_{i-1,j} &= \eta T^{\tau}_{i,j+1} + (1-2\eta+h)T^{\tau}_{i,j} + \eta T^{\tau}_{i,j-1}\\ -\eta T^{\tau+1}_{i,j+1} + (1+2\eta-h)T^{\tau+1}_{i,j} - \eta T^{\tau+1}_{i,j-1} &= \eta T^*_{i+1,j} + (1-2\eta+h)T^*_{i,j} + \eta T^*_{i-1,j}.\end{aligned} \tag{22}$$

The $f(x,y)$, the boundary conditions of the heat source is added as a factor just for certain positions, the equation is the same, but inside the code, it is checked if the calculation is being done on the bottom, so then we can add the this effect, and it consider as zero for all other positions. There are probably better ways to do it, but this was the simplest solution found.

3.1.3 Solving a Tridiagonal Matrix

Let's first consider the following matrix equation

$$\begin{pmatrix} b_1 & c_1 & 0 & 0 & \dots & 0\\ a_2 & b_2 & c_2 & 0 & \dots & 0\\ 0 & a_3 & b_3 & c_3 & \dots & 0\\ \vdots & \vdots & \vdots & \vdots & \vdots & \vdots\\ 0 & 0 & \dots & a_{n-1} & b_{n-1} & c_{n-1}\\ 0 & 0 & \dots & 0 & a_n & b_n \end{pmatrix} \begin{pmatrix} x_1\\ x_2\\ x_3\\ \vdots\\ x_{n-1}\\ x_n\end{pmatrix} = \begin{pmatrix} d_1\\ d_2\\ d_3\\ \vdots\\ d_{n-1}\\ d_n\end{pmatrix}, \tag{23}$$

to simplify this equation we can make the all the elements in the main diagonal equal to 1, and the elements of the lower diagonal equal to zero. To accomplish that, we need to divide the first row by the first element (b_1) and subtract from second row the first row times the element a_2, such that

$$\begin{pmatrix} 1 & \frac{c_1}{b_1} & 0 & 0 & \dots & 0 \\ a_2 - a_2 & b_2 - \frac{a_2 c_1}{b_1} & c_2 & 0 & \dots & 0 \\ 0 & a_3 & b_3 & c_3 & \dots & 0 \\ \vdots & \vdots & \vdots & \vdots & \vdots & \vdots \\ 0 & 0 & \dots & a_{n-1} & b_{n-1} & c_{n-1} \\ 0 & 0 & \dots & 0 & a_n & b_n \end{pmatrix} \begin{pmatrix} x_1 \\ x_2 \\ x_3 \\ \vdots \\ x_{n-1} \\ x_n \end{pmatrix} = \begin{pmatrix} \frac{d_1}{b_1} \\ d_2 \\ d_3 \\ \vdots \\ d_{n-1} \\ d_n \end{pmatrix}, \tag{24}$$

doing the same for the next rows, we get

$$\begin{pmatrix} 1 & h_1 & 0 & 0 & \dots & 0 \\ 0 & 1 & h_2 & 0 & \dots & 0 \\ 0 & 0 & 1 & h_3 & \dots & 0 \\ \vdots & \vdots & \vdots & \vdots & \vdots & \vdots \\ 0 & 0 & \dots & 0 & 1 & h_{n-1} \\ 0 & 0 & \dots & 0 & 0 & 1 \end{pmatrix} \begin{pmatrix} x_1 \\ x_2 \\ x_3 \\ \vdots \\ x_{n-1} \\ x_n \end{pmatrix} = \begin{pmatrix} p_1 \\ p_2 \\ p_3 \\ \vdots \\ p_{n-1} \\ p_n \end{pmatrix}, \tag{25}$$

where

$$h_1 = \frac{c_1}{b_1} \qquad p_1 = \frac{b_1}{b_1}, \tag{26}$$

and

$$h_i = \frac{c_i}{b_i - a_i h_{i-1}} \qquad p_i = \frac{d_i - a_i p_{n-1}}{b_i - a_i h_{i-1}}, \tag{27}$$

then

$$x_n = p_n \qquad x_i = p_i - h_i x_{i+1}, \tag{28}$$

it is important to notice that the vector x needs to be computed backward [1].

4 Results and Discussion

The program is able to simulate any rectangular shape, the sides are defined as parameters. It is also possible to set the precision both in time and space, in other words, the size of the steps. From the Von Neumann stability if we make the spatial stepping smaller it gets lets stable, and if we make the time stepping smaller it gets more stable, the thermal diffusivity is also an important factor, but it is assumed to be a constant. Therefore, to achieve a good resolution we need to find good values for the time and spatial stepping [1].

The thermal diffusivity chosen was from copper, and used as a constant value of $\alpha = 1.11 \times 10^{-4}$. In reality, it is not a constant, it varies over the temperature, but it doesn't vary too much. It is possible to add this effect by recalculating the diffusivity at each time and position based on the current temperature, but this was not include, because it is a small effect.

It is also possible to set as a parameter the strength of the heat source in the bottom, as same as the initial temperature of the copper sheet and the temperatures of the boundary conditions on the left and right border. These conditions are a linear increase of temperature on the right and decrease on the left. This is interesting because it shows a symmetric distribution with no heat source on the bottom, the image is symmetric along the main diagonal. However, the system actually has a heat source, so we can see the symmetry breaking on the bottom, and clearly see the effects of the heat source.

For all the simulation shown here, the time step was 0.5 s to compensate the resolution of 1 cm, even though 0.5 s doesn't show much effect between each step, it is necessary to keep the stability to have a precision of 1 cm. For testing, the spatial resolution were decreased so the time step could increase and the simulation took less computer time.

The initial temperature is also the same for all simulation, it is 27 $^\circ C$, and for most of simulations the boundary conditions on the left and right side goes from 0 $^\circ C$ to 100 $^\circ C$, just one of them was from 0 $^\circ C$ to 200 $^\circ C$ because it was simulated for a longer period of time, so we could see for longer the heat source effect and don't change the temperature scale during the whole process.

4.1 No Heat Source

Like mention before, to better see the effect of the heat source, we can look at a simulation without it, to look at the symmetry of the system. The dimensions of the rectangular is $3m \times 2m$. In Figure 1 , we can see the initial state, in Figure 2 is $t = 1\ min$, in Figure 3 is $t = 5\ min$, in Figure 4 is $t = 10\ min$, and finally in Figure 5 is $t = 30\ min$.

It is clear to see that the images look symmetric in relation to the main diagonal. There is also a gif that shows the evolution in every 30 s.

4.2 With Heat Source

It was simulated four different cases. The first is a rectangle of $3m \times 2m$ and $h = 7.0 \times 10^{-4}$. Again we have simulation at different times. At $t = 10\ min$, $t = 20\ min$, and $t = 30\ min$ in Figure 6,7 and 8 respectively. There is also a gif for better visualization.

The second case the source of the heat was increase to $h = 9.0 \times 10^{-4}$. Once more, we have simulation at different times. At $t = 10\ min$, $t = 20\ min$, and $t = 30\ min$ in Figure 9, 10 and 11 respectively.The gif is also available.

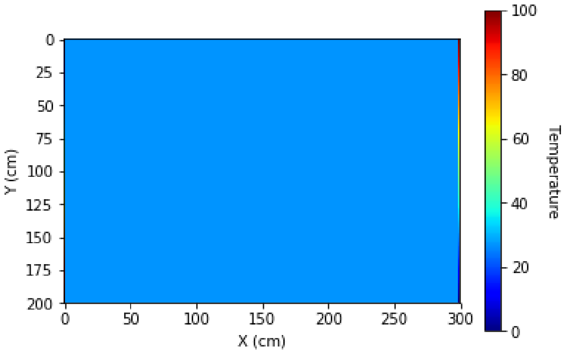

Figure 1: No heat source, at $t = 0 \ min$

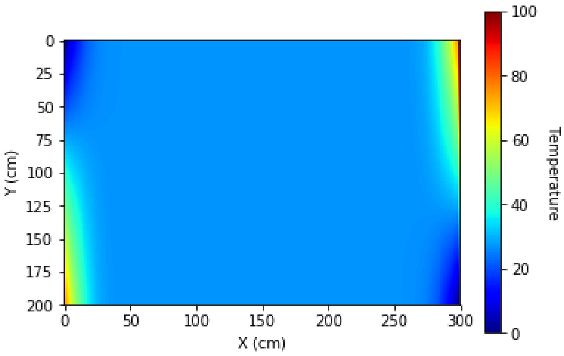

Figure 2: No heat source, at $t = 1 \ min$

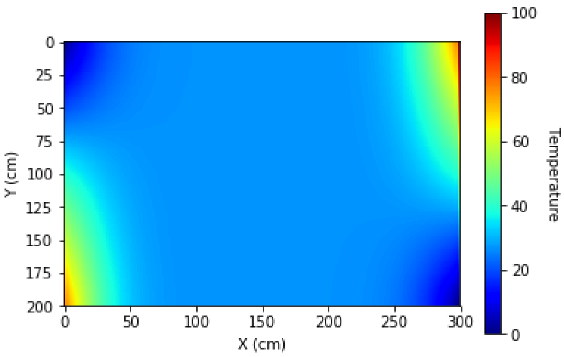

Figure 3: No heat source, at $t = 5 \ min$

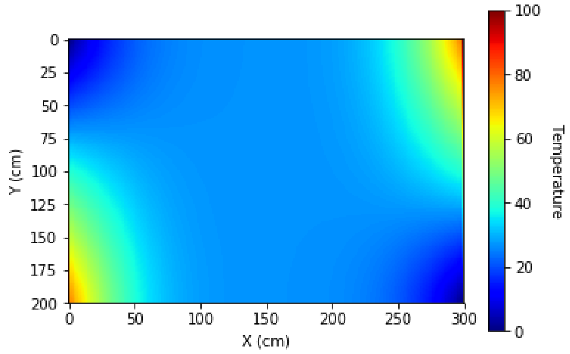

Figure 4: No heat source, at $t = 10\ min$

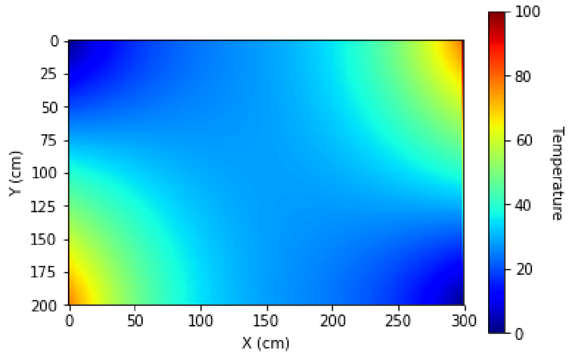

Figure 5: No heat source, at $t = 30\ min$

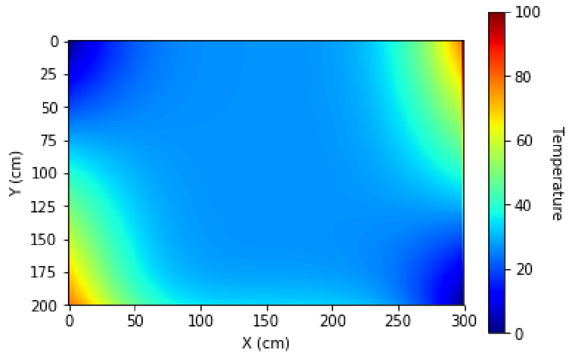

Figure 6: First case with heat source, at $t = 10\ min$

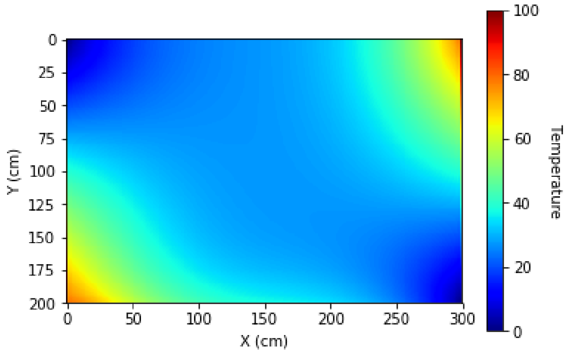

Figure 7: First case with heat source, at $t = 20\ min$

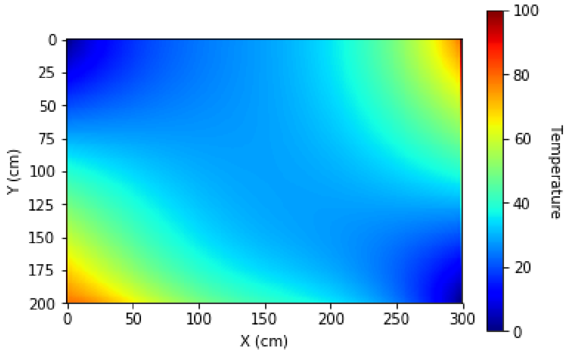

Figure 8: First case with heat source, at $t = 30\ min$

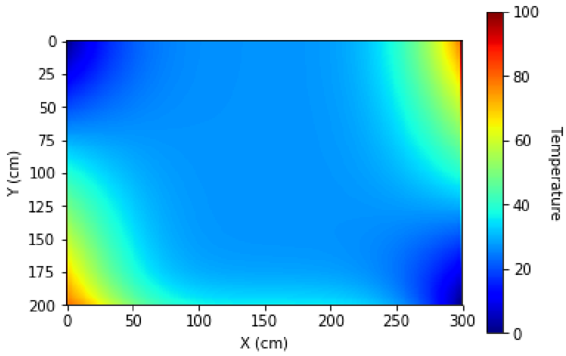

Figure 9: Second case with heat source, at $t = 10\ min$

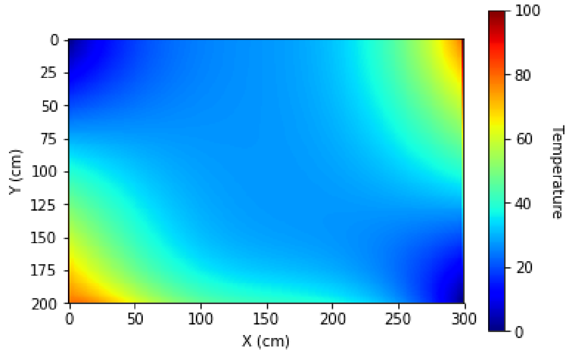

Figure 10: Second case with heat source, at $t = 20\ min$

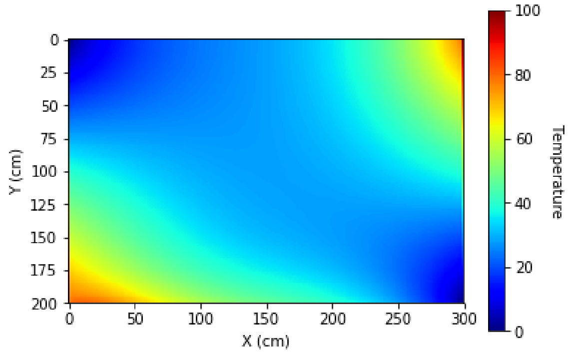

Figure 11: Second case with heat source, at $t = 30\ min$

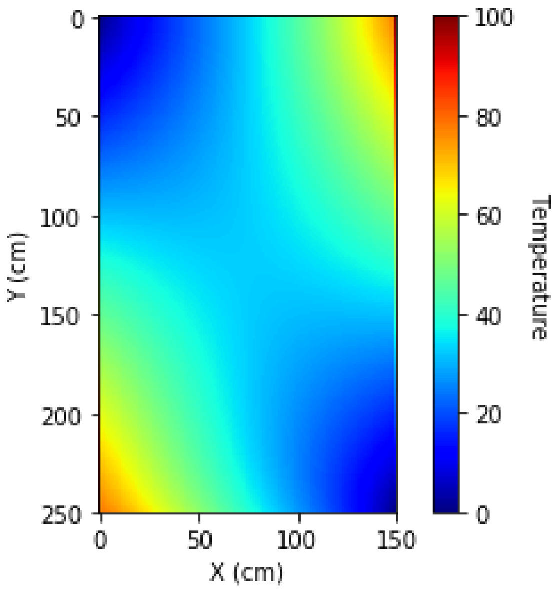

Figure 12: Third case with heat source, at $t = 20\ min$

The third case, the rectangle is $1.5m \times 2.5m$ and $h = 5.0 \times 10^{-4}$. The same heat distribution goes further in time, now we have the results from $t = 20\ min$, $t = 40\ min$, and $t = 60\ min$ in Figure 12, 13, and 14 respectively, the animation was also made.

For the fouth and final case, this is the simulation that went even further in time and also a smaller rectangle of $1m \times 1.5m$. The times rendered were $t = 15\ min$, $t = 30\ min$, $t = 45\ min$, $t = 60\ min$, $t = 75\ min$, $t = 90\ min$, $t = 105\ min$, and $t = 120\ min$ all in Figure 15, 16, 17, 18, 19, 20, 21, and 22. It was also created a gif with frames representing each minute.

From all the cases, it is possible to see a tail on the heat distribution on the bottom, and this is due to the heat source. It is breaking the symmetry.

5 Conclusion

The heat equation can be easily visualized with heat maps, and the animation also makes it even more clear to see the phenomenon. It was already mention in the report parts where the code could be improved, but there is another feature that could be added is real time simulation or an automatic creation of the gif.

It was initially a challenge to insert the heat source, because it is easier if the whole system is under this source not just the bottom. The solution was just add this effect when the routine was going over the lowest layer in the mash.

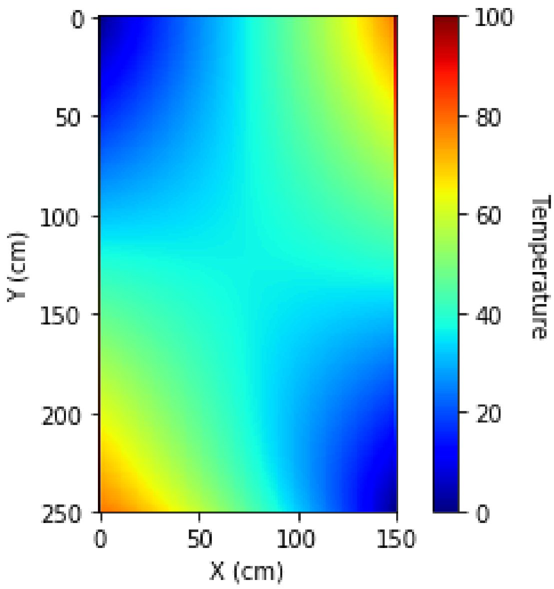

Figure 13: Third case with heat source, at $t = 40\ min$

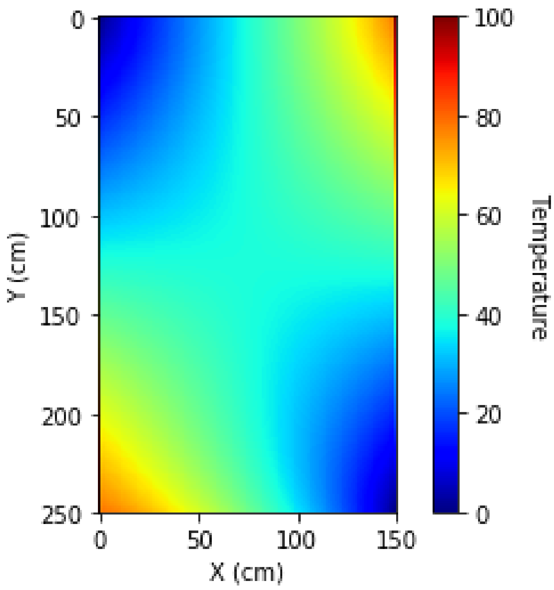

Figure 14: Third case with heat source, at $t = 60\ min$

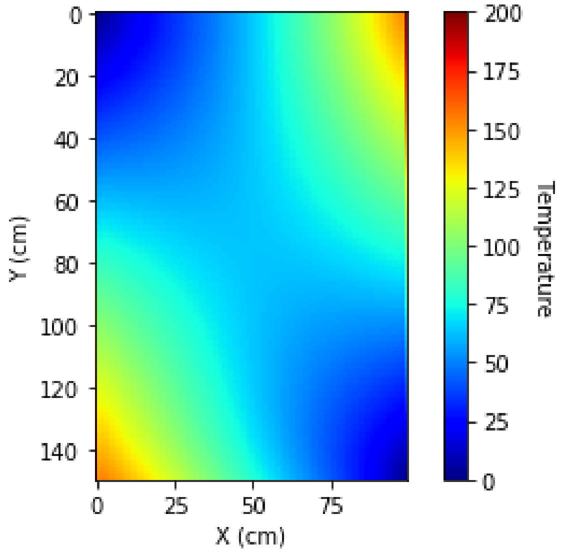

Figure 15: Fourth case with heat source, at $t = 15\ min$

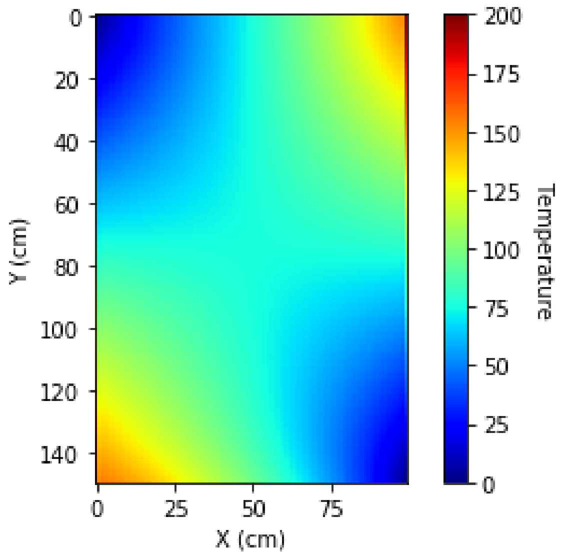

Figure 16: Fourth case with heat source, at $t = 30\ min$

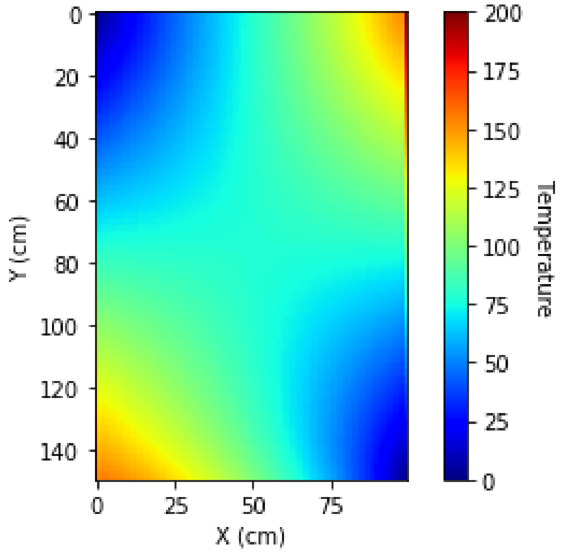

Figure 17: Fourth case with heat source, at $t = 45\ min$

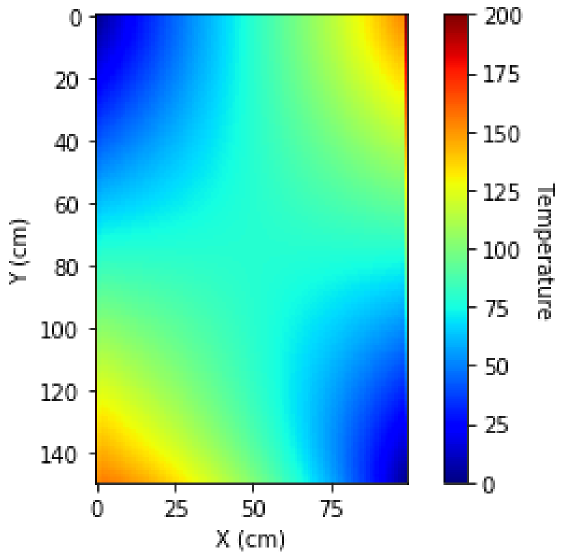

Figure 18: Fourth case with heat source, at $t = 60\ min$

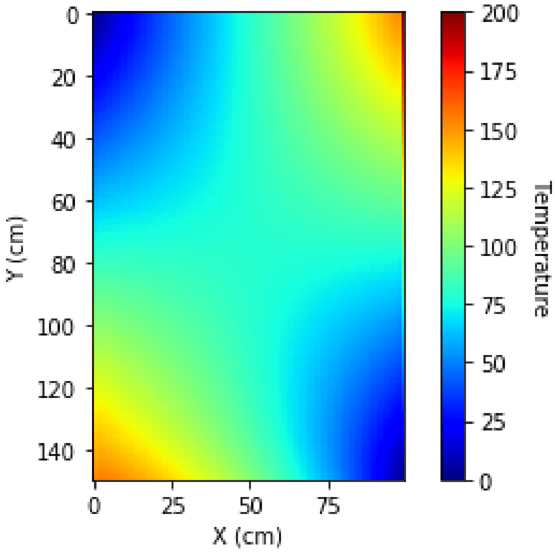

Figure 19: Fourth case with heat source, at $t = 75\ min$

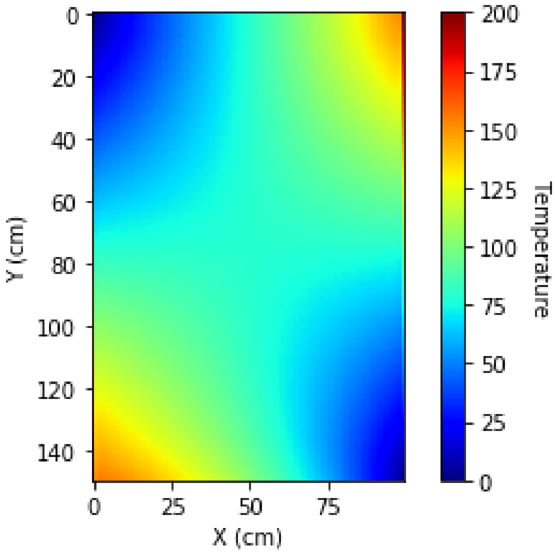

Figure 20: Fourth case with heat source, at $t = 90\ min$

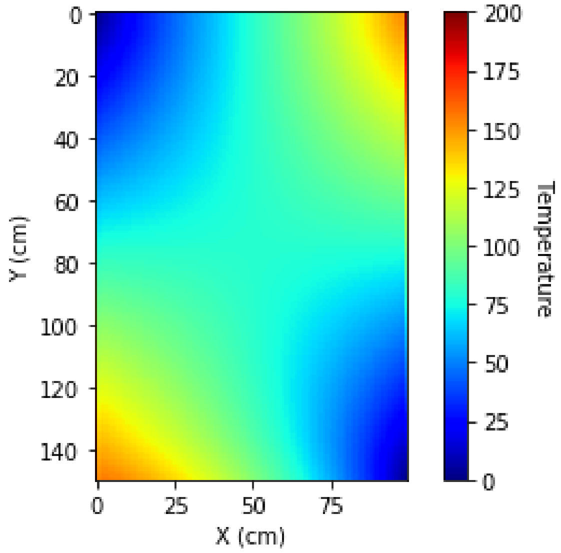

Figure 21: Fourth case with heat source, at $t = 105\ min$

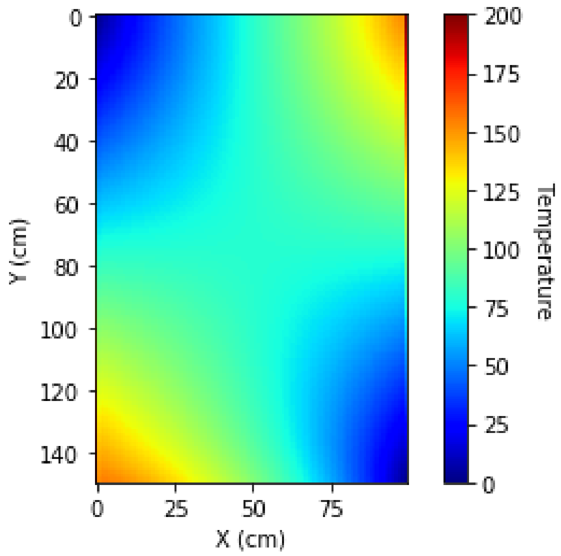

Figure 22: Fourth case with heat source, at $t = 120\ min$

There were a few other problems with the boundary conditions, in how to properly define it and how to compute the derivatives in this region. However, it was solved, just by trying over again with more caution.

In general, the simulation worked properly, and it showed interring results . It was possible to learn more about the modern numerical methods. The language used was Python, because I am more used to it, for coding, including data structure, and visualization.

References

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