Scientific Computing: Set I

Kasper Nicholas (10678859) & Steven Raaijmakers (10804242)

I. Introduction

The wave equation and the diffusion equation are two of the most important concepts numerous scientific disciplines[1]. Physical experiments incorporating the two respective mechanisms can be costly, time consuming and even dangerous. Hence, numerical simulations are a commonly used alternative for assessing the (time) evolution and subsequent characteristics of systems pertaining these equations.

In this report our main goal is the discretization of the wave equation and time-dependent and independent diffusion. Firstly, the translation of continuous PDE's into discrete approximations of both equation are scrutinised. In the subsequent section we discuss the numerical implementation of the discrete schemes. Thereafter, three improvements on the diffusive iteration scheme are implemented and compared in order to assess the respective efficiency of each method. Similarly we consider diffusion with two-dimensional objects and insulating materials. Finally, we present and discuss the results of all simulations and subsequent visualisations in order to compare the discrete approximations of the wave equation and diffusion to their continuous theoretical counterparts.

II. Theory

A. The discretized 1-D wave equation

In order to numerically implement the wave equation we wish to firstly discretize its differential form. We start with the one-dimensional wave equation, which is a continuous partial differential equation (PDE):

$$\frac{\partial^2 \psi}{\partial t^2} = c^2 \frac{\partial^2 \psi}{\partial x^2} \tag{1}$$

Here c is the wave number which governs the spatial frequency of the wave. For the discretization of the wave equation we require the following notation:

$$\psi(x,t) \equiv u(i,j)$$

Firstly, the spacial component is rewritten using this notation. We calculate the subsequent derivative by means of Taylor's theorem and the difference quotient. Taylor's theorem tells us that:

$$f(x+\Delta x) = f(x) + \Delta x f'(x) + \frac{\Delta x^2}{2!} f"(x) + \dots$$

and

$$f(x-\Delta x) = f(x) - \Delta x f'(x) + \frac{\Delta x^2}{2!} f"(x) - \dots$$

Moreover, the difference quotient approximates $f'(x)$ as Δx tends to zero:

$$f'(x) = \lim_{x \to 0} \frac{f(x+\Delta x) - f(x)}{\Delta x}$$

It is important to note that we deem higher order terms than the first derivative as negligible in our derivation because they converge to zero as Δx tends to zero. Therefore we obtain a solution with only the first order derivative of x in the following equation:

$$\begin{aligned}
\frac{\partial \psi}{\partial x} &= \frac{u(i+1,j) + u(i,j)}{\Delta x} \\
\frac{\partial \psi}{\partial x} &= \frac{u(i,j) + u(i-1,j)}{\Delta x} \\
\frac{\partial^2 \psi}{\partial x^2} &= \frac{u(i+1,j) + u(i-1,j) - 2u(i,j)}{\Delta x}
\end{aligned}$$

Secondly, we wish to discretize the time component as follows:

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

When we substitute the space and time components in (1) with their new discrete forms we end up with:

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

Now, we can rewrite this to obtain the solution for our wave equation at $t = j + 1$:

$$u(i, j+1) = (\frac{\Delta tc}{\Delta x})^2 \cdot (u(i+1, j) + u(i-1, j) \\ -2u(i, j)) - u(i, j-1) + 2u(i, j) \tag{2}$$

We observe that our wave equation at $t + 1$ is dependent on two previous moments t and $t - 1$. In conclusion, this rewritten form of the wave equation can be implemented numerically in the next section (III).

B. Time-dependent diffusion

The time-dependent diffusion equation is governed by the following PDE:

$$\frac{\partial c}{\partial t} = D\nabla^2 c \tag{3}$$

Similar to the wave equation we can again approximate this continuous PDE with finite difference approximations and Taylor expansions. We obtain the following discrete equation for time-dependent diffusion:

$$c_{i,j}^{k+1} = c_{i,j}^k + \frac{\partial tD}{\partial x^2} \cdot (c_{i+1,j}^k + c_{i-1,j}^k + c_{i,j+1}^k \\ +c_{i,j-1}^k - 4c_{i,j}^k) \tag{4}$$

It is important to note this discrete approximation only hold if:

$$\frac{4\partial tD}{\partial x^2} \leqslant 1 \tag{5}$$

This determines the maximum time step ∂t one can take for the above scheme to hold. This five point scheme only requires local information in order to update for the next time step and therefore allows for subsequent parallel numerical computation. In order to assess the accuracy of any numerical results we require a comparison with the analytic solution of (3). The solution is:

$$c(x, t) = \sum_{i=0}^{\infty} \text{erfc}\left(\frac{1 - x + 2i}{2\sqrt{Dt}}\right) \\ -\text{erfc}\left(\frac{1 + x + 2i}{2\sqrt{Dt}}\right) \tag{6}$$

where erfc(...) is the Gauss error function.

C. Time-independent diffusion

Lastly we wish to discretize the time-independent diffusion equation, which is governed by the following PDE:

$$\nabla^2 c = 0 \tag{7}$$

This is done in the same manner as for the time-dependent diffusion equation and results in:

$$\frac{1}{4}(c_{i+1,j} + c_{i-1,j} + c_{i,j+1} + c_{i,j-1}) = c_{i,j} \tag{8}$$

Note that the superscript k which indicates the current time step is absent in this equation.

III. Methods

In this section we merely focus on the numerical methodology without the use of algorithms due to the simplicity of the implemented code and its close resemblance to the equations and methods that are referred to. If deemed necessary, the code can be found in the attachments.

A. The wave equation

After the derivation of the discrete wave equation in section II we can now implement (2) numerically. The wave equation is subsequently calculated for $c = 1$ and $\Delta t = 0.001$. Furthermore, we consider three cases with different initial conditions (IC):

(i) $\Psi(x, t = 0) = \sin(2\pi x)$
(ii) $\Psi(x, t = 0) = \sin(5\pi x)$
(iii) $\Psi(x, t = 0) = \sin(5\pi x)$ if $1/5 < x < 2/5$, else $\Psi = 0$

For each set of IC we calculate Ψ for all t with respect to the displacement x. Moreover, Ψ is plotted for all three IC at various t in order to illustrate the difference in displacement and periodicity.

B. Time-dependent diffusion

After the implementation of the wave equation in one spatial dimension we consider time-independent diffusion in two dimensions as in (4). Here, the concentration $c(x, y, t)$ also dependent on the diffusion coefficient D, which is set to 1 throughout our simulations. Furthermore, we assume $x, y \leqslant 1$ and the following boundary conditions:

$$c(x, y = 1, t) = 1 \quad \text{and} \quad c(x, y = 0, t) = 0 \\ c(x = 0, y, t) = c(x = 1, y, t)$$

For the IC we take:

$$c(x, y, t = 0) = 0 \text{ for } 0 \leqslant x \leqslant 1 \ , 0 \leqslant y < 1$$

We observe that the subsequent diffusive system only depends on the y-coordinate and on time due to symmetry in x.

The resulting scheme, based on (8), is required to adhere the stability condition in (5). Violation of this

requirement halts the initiated simulation until the initial parameters are sufficiently altered.

In other words we are required to choose adequate values for the number of steps with respect to Δt. Thereafter the concentration $c(x, y, t)$ is compared to the analytic solution in (1) in order to assess the accuracy of our discretized diffusion scheme. Moreover we animate the time evolution of the diffusion scheme in order to analyse the progression of $c(x, y, t)$ Finally, for $t = \{0.001, 0.01, 0.1, 1\}$ the resulting c is visualised in a plot.

C. Time-independent diffusion

As opposed to time-dependent diffusion we are not interested in the evolution of the concentration c at time t, but rather in the steady state of the system. Three variations of the time-independent diffusion scheme, which is described in (8), are implemented in the following sections. Furthermore, we consider the same IC and boundary conditions to hold as for time-dependent diffusion. We also need to determine an updated stopping condition for our iterative process because it is no longer dependent on the time t.

1) The Jacobi Iteration: The Jacobi Iteration method is similar to the time-dependent scheme in (4) but takes the maximum allowed time step Δt. If we consider the following:

$$\frac{\partial tD}{\partial x^2} = \frac{1}{4}$$

Then the Jacobi Iteration method is easily derived from (4) as:

$$c_{i,j}^{k+1} = \frac{1}{4}(c_{i+1,j}^{k} + c_{i-1,j}^{k} + c_{i,j+1}^{k} + c_{i,j-1}^{k}) \tag{9}$$

Contrary to time-dependent diffusion our steady state is reached when the following convergence for all values of (i, j) occurs for a predetermined small enough ϵ:

$$\delta \equiv \max_{i,j} |c_{i,j}^{k+1} - c_{i,j}^{k}| < \epsilon \tag{10}$$

This is subsequently also our stopping condition when (9) is implemented numerically. The implementation of the Jacobi Iteration requires the calculation of $c_{i,j}^{k}$ and $c_{i,j}^{k+1}$ at each step, making it a relatively slow iterative process. An improvement would incorporate the updating of only one matrix. This can be accomplished with the Gauss-Seidel Iteration method and is discussed in the next section.

2) The Gauss-Seidel Iteration: The improvement in terms of computational complexity with respect to the Jacobi Iteration is the Gauss-Seidel Iteration method. During an iteration newly obtained values are immediately used, assuming the iteration proceeds along the rows (i.e. incrementing i for fixed j). The Gauss-Seidel iteration subsequently is dictated by:

$$c_{i,j}^{k+1} = \frac{1}{4}(c_{i+1,j}^{k} + c_{i-1,j}^{k+1} + c_{i,j+1}^{k} + c_{i,j-1}^{k+1}) \tag{11}$$

The improvement of this method compared to the Jacobi Iteration is that the update can be performed in place. The amount of iterations required for convergence is, however, not significantly improved. Hence we implement a third iterative scheme called the Successive Over Relaxation (SOR) in the next section.

3) Successive Over Relaxation: The SOR method is obtained from the Gauss-Seidel by an over-correction of the new iterate:

$$c_{i,j}^{k+1} = \frac{\omega}{4}(c_{i+1,j}^{k} + c_{i-1,j}^{k+1} + c_{i,j+1}^{k} + c_{i,j-1}^{k+1}) + (1-\omega)c_{i,j}^{k} \tag{12}$$

For $0 < \omega < 2$ the method converges. For $\omega < 1$ we refer to the process as under relaxation. The new value is now the weighted average of the Gauss-Seidel method and the previous value. For $\omega = 1$ we observe the same results as with the Gauss-Seidel in (11).

The optimal ω minimizes the amount of iterations needed for convergence and can typically be found in the interval $1.7 < \omega < 2$.

D. Diffusion with 2-D objects

Our last addition to the diffusive scheme is the inclusion of rectangular objects. These objects can either act as sinks where diffusion completely comes to a halt, or as insulating material.

For the implementation of the sinks we use the SOR with its corresponding optimal $omega$. However, for the insulating material we need to go back to the use of the time-dependent diffusion described in section . We set D to a small value for all points inside the objects. The use of the insulating material causes the diffusion to progress more, and subsequently the concentration c in the object is lower than in the space surrounding it.

IV. Results

A. Discretized wave equation

The result of the various (IC) with the mentioned values for $\Delta t = 0.001$ and $c = 1$ are shown in in Fig.

1, 2 and 3. An animated versions of these plots can be found in the attachments.

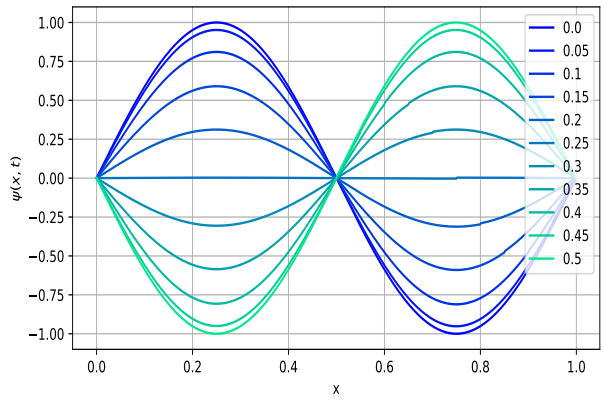

Fig. 1: The wave equation with IC: $\Psi(x, t = 0) = \sin(2\pi x)$ for t = 0, 0.05, ..., 0.5.

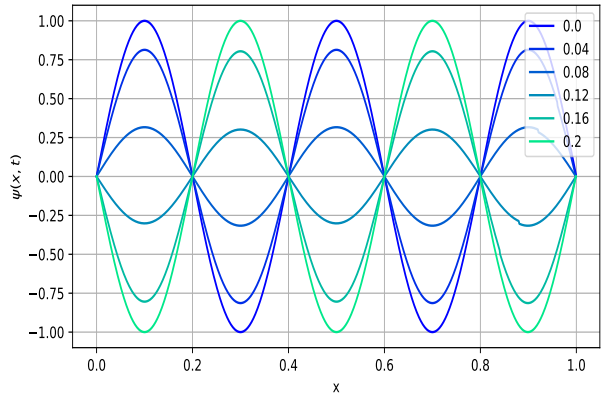

Fig. 2: The wave equation with IC: $\Psi(x, t = 0) = \sin(5\pi x)$ for t = 0, 0.04, ..., 0.2.

B. Time-dependent diffusion

For the time-dependent diffusion we have compared the analytic solution of (6) to the numerical solution (section III-D) of which we have plotted the result in Fig. 4. We observe a more angular plot for the numerical solution due to the discretized nature of the scheme.

The 2-D domain of the numerical solution is shown in Fig. 5, in which we see the domain changing over time. An animated version can be found in the attachments.

C. Time-independent diffusion

For $N = 50$, we have solved (3) using the Jacobi iteration, the Gauss-Seidel iteration and the SOR. The

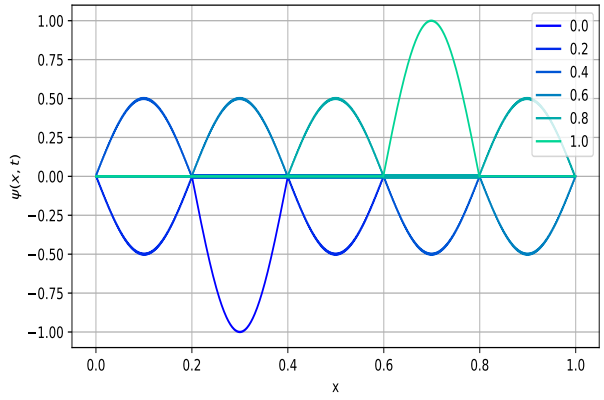

Fig. 3: The wave equation with IC: $\Psi(x, t = 0) = \sin(5\pi x)$ if $1/5 < x < 2/5$, else $\Psi = 0$. This function is plotted for t = 0, 0.2, ..., 1.

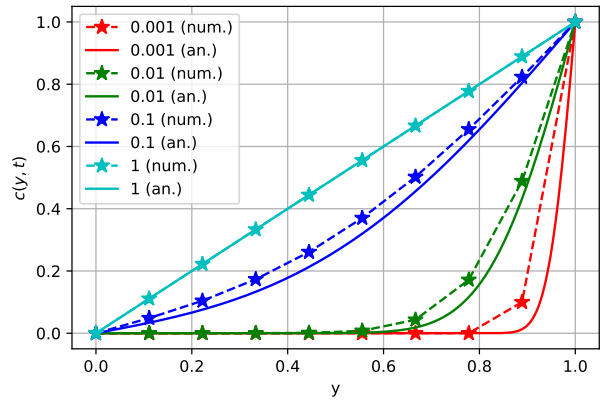

Fig. 4: Analytic and numerical solutions of time-dependent diffusion for t = 0.001, 0.01, 0.1 and 1.

comparison of these three methods to the analytic solution for the 1D domain is shown in Fig. 6. This figure shows use that the SOR has the most accurate approach, while the Jacobi and Gauss-Seidel iteration have a significantly worse approach. We note that the better performing methods have a more accurate approach of the analytic solution.

Not only are we interested in the accuracy of the approach but also of the performance of the different methods. Therefore we investigate how the convergence measure of (10) depends on the number of iterations k, which we illustrate in Fig. 7. This plot shows us the Jacobi iteration indeed needs the most iterations to converge, while we also can verify that the SOR needs the least amount of iterations. For the three different values of ω plotted in this figure, we see that $\omega = 1.9$ has the best performance.

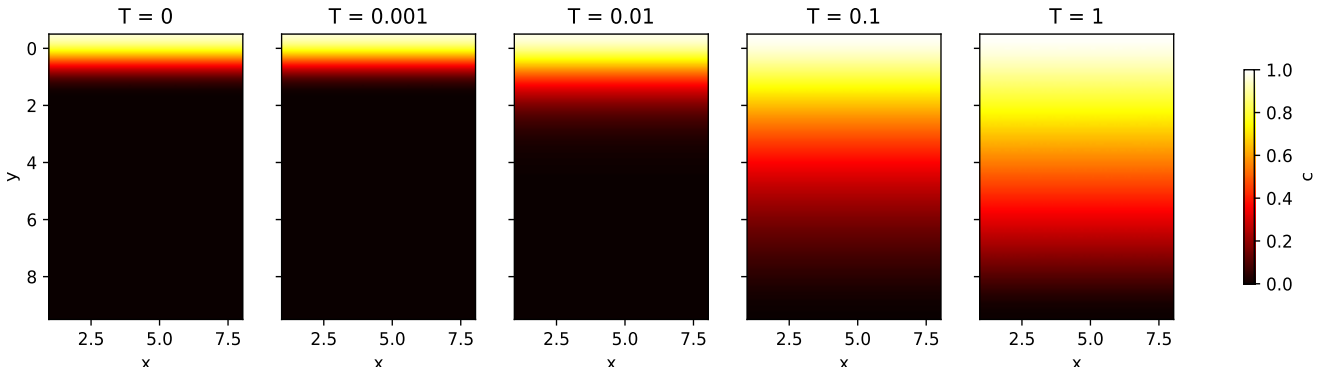

Fig. 5: Heatmaps of numerical solutions for time-dependent diffusion.

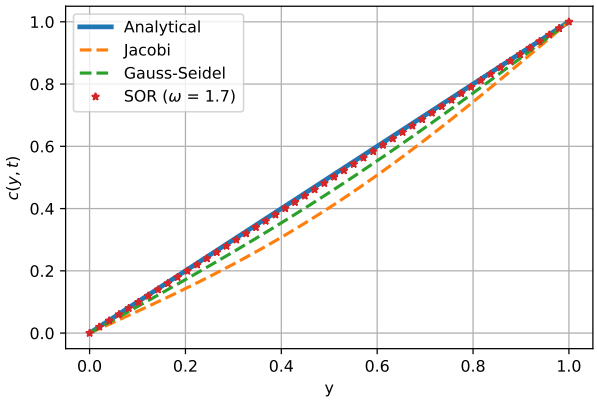

Fig. 6: Analytic and numerical solutions of time-independent diffusion at equilibrium ($T = 1, \epsilon = 10^{-5}$).

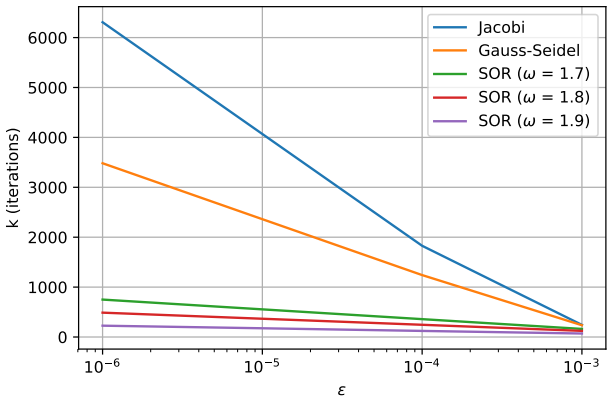

Fig. 7: Convergence for different solutions to diffusion equation ($N = 50$).

In order to expound this observation we need to determine the optimal ω for $N = 50$. This can be deduced from Fig. 8, in which the number of iterations k needed to converge for different ω and different N is plotted. The exact values can be found in table I. This table and plot show us that for $N = 50$ the optimal $\omega = 1.9214$, hence the better performance of the SOR with $\omega = 1.9$ over $\omega = 1.8$ and $\omega = 1.7$ in Fig. 7.

N	30	50	70	90
Optimal ω	1.8757	1.9214	1.9443	1.9557

TABLE I: Optimal ω for different N.

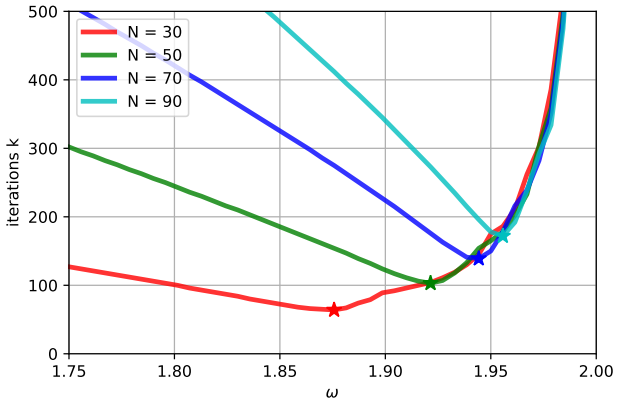

Fig. 8: Number of iterations required for equilibrium. $N = 30$, 50, 70 and 90. Optimal ω is indicated for each N with a star.)

In Fig. 8 we also observe that the optimal ω is increasing for a larger value of N.

D. Diffusion with 2D-objects

In a domain of $N = 50$ we added 2-D sink-like objects; they pertain a concentration of zero. The diffusion scheme used is the SOR with its corresponding optimal value of $\omega = 1.9214$. The result of the various setups are shown in Fig. 9.

We are interested in how the addition of objects influences the number of iterations for convergence and

the optimal ω. The answer to this can be found in table II. Firstly, this table shows us the amount of iterations is decreasing when objects are added into the domain. We also notice that the domain including three squares has better performance in comparison to the other two setups, while their total surface is equal. This is most likely due to the multiple squares having a higher total circumference and thus having more contact points. Lastly, this table shows us the optimal ω is decreasing by the addition of more objects.

1) Insulating material: Finally, we have added an object consisting of insulation material, which can be seen in Fig. 10. We see that over time the object blends into the background.

Objects	None	One square	Two squares	Three squares
Total Surface	-	400	400	400
Iterations k	122	100	98	82
Optimal ω	1.9214	1.8357	1.7557	1.7100

TABLE II: Iterations needed for convergence for various setups with $N = 50$.

V. Discussion

The results of the discretized wave equation that are presented in Fig. 1, 2 and 3 indicate three systems with varying frequencies and subsequent behaviour. The figures show a number of maxima and minima that is equal to the number within the sin in the respective initial conditions. Due to the extra spatial restriction in Fig. 3 we observe an increase in amplitude at $x = 0.3$ and $x = 0.7$ as one would expect with the boundary conditions and coinciding IC. The wave simulations indicate discrete implementation of this scheme is adequate and efficient. Variations in the wave and IC are easily implemented, and result in little numerical complexity and computational costs.

However when we consider the discrete diffusion simulations it is of importance to choose an efficient scheme. The result of time-dependent diffusion depicted in Fig. 4 indicate a lacking similarity of the numerical solution compared to the analytic solution. However, as the time is incremented the numerical solution approaches the analytic solution until they finally coincide for $t = 1$. In other words, time-evolution of the diffusive system is rather inaccurate, but at equilibrium it is a good approximation of the theoretical continuous solution. Due to this inaccuracy at intermediate times t we are more interested in the equilibrium state of our discrete diffusion scheme.

The final time-independent discrete scheme is implemented according the Jacobi, the Gauss-Seidel and the SOR. In Fig. 6 we observe the numerical solution of the SOR scheme with $\omega = 1.7$ is the most accurate of the three schemes as it overlaps almost completely with the analytic solution concentration values for increasing y. Moreover, Fig. 7 also illustrates the SOR requires the least number of iterations to converge to a steady state. This number decreases even further when sink-like objects are added to the 2-D scheme. Conversely, the number of iterations k until a steady state lead to an increase in the optimal ω, as is shown in 8. The inclusion of an insulating object results in different diffusive behaviour before the equilibrium is reached. However, as soon as the steady state is reached the diffusive system is no different than for SOR simulations without any objects in the system.

In conclusion, it is important to choose adequate discretization schemes for more complex partial differential equations. Where the wave equation was easily implemented and assessed for various IC we did notice a substantial increase in computation times for discrete diffusion simulations. Subsequent variations of time-independent diffusion methods illustrated the variation in computational costs and accuracy of subsequent results. Our results indicated the SOR scheme for $N = 50$ and $\omega = 1.9214$ led to a high accuracy in simulation results and short simulation times. Moreover, the inclusion of sink-like objects and insulating material allows for simulations of complex diffusive systems. The use of the SOR diffusion scheme is therefore deemed a useful discretization technique for the analysis of numerically implemented diffusive systems.

References

[1] M Heath. *Computing: An introductory survey*. McGraw-Hill, 1998.

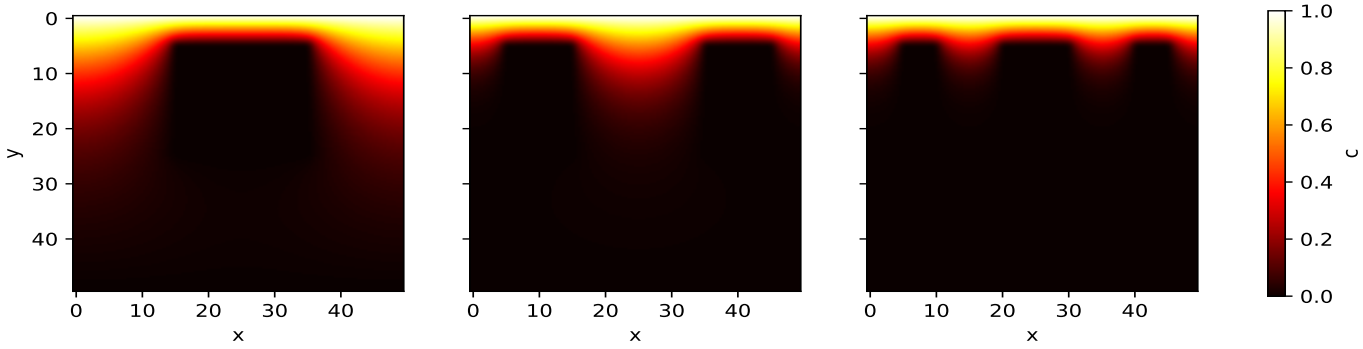

Fig. 9: Heat maps of numerical solutions for time-dependent diffusion. From left to right we add one, two and three square sinks respectively.

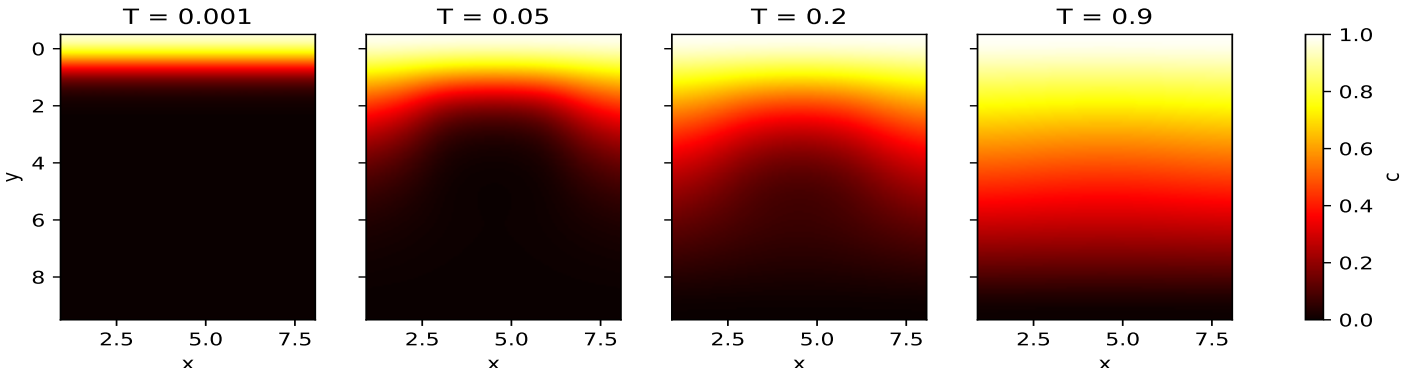

Fig. 10: Heat maps of time-independent diffusion for an insulating object