

Numerical Exploration of Classical Partial Differential Equations

TFY4235 - Assignment 1

ID -

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Abstract—Diffusion was modeled for an initial Dirac delta density and the numerical results are consistent with the exact solutions. Modeling unbounded systems with bounded systems was found to be precise as long as the diffusion process does not touch the boundaries. Reflective boundaries conserved the total mass of the system, while absorbent boundaries saw a decrease in mass. Furthermore, examination of space-dependent diffusivity profiles demonstrates that higher diffusivity accelerates the diffusion process. The study of waves gave a numerical stability criterion twice the expected amount, and modeling a wave in water suggests the absence of dispersion, which is crucial for a physically correct model. Finally, experiments with wave transportation using both the advection equation and Hopf's equation demonstrate the emergence of shock in the latter due to faster transport of higher points within the wave over time.

1. Introduction

Partial Differential Equations (PDEs) are a fundamental tool in physics and most other sciences. They provide a mathematical framework to model and understand the evolution and stationary states of various systems, from quantum physics to the dynamics of galaxies. Solving such equations are thus extremely important but can in many cases be complex. This paper aims to explore numerical solutions of several classical PDEs that describe the time evolution of a system.

The paper will focus on three specific equations that encapsulates the essence of many phenomena: the diffusion equation, the wave equation and Hopf's equation, also known as the inviscid Burger's equation. These equations offers intriguing insights into the nature of the systems they describe, but also create many considerations when solving them numerically. Particularly, the paper seeks to investigate solution regularity. How do solutions behave when presented with non-differentiable initial conditions or even non-continuous profiles? Do the equations fully capture the physical behaviour of systems? Lastly, we will also see how the shock phenomena can be better understood by analyzing Hopf's equation.

A numerical implementation of a solver is required to solve the time evolution of these equations. This paper implements several different methods such as Crank-Nicolson scheme and Law-Wendroff scheme which are finite difference methods. The numerical stability of these methods are important to extract the correct solutions and it will be investigated in this paper. [1]

2. Methodology

2.1. Diffusion

The diffusion equation is a partial differential equation that describes how quantities such as heat, mass or particles spread over time due to random motion. The equation can take many forms depending on the complexity of the problem

2.1.1. The diffusion equation. We'll study pure diffusion for a drop of ink in water where $u(x, t)$ is the density of ink in water, and has the evolution equation

$$\frac{\partial u}{\partial t} = \frac{\partial}{\partial x} \left(D \frac{\partial u}{\partial x} \right). \quad (1)$$

In Eq. (1) D is the diffusion constant, and we will consider both constant and position dependent cases of D . For constant diffusivity Eq. (1) reduces to

$$\frac{\partial u}{\partial t} = D \frac{\partial^2 u}{\partial x^2}. \quad (2)$$

To model a drop of ink we use the Diracs delta equation such that the ink is concentrated at one spot at time $t = 0$. The initial condition reads

$$u(x, t = 0) = \tilde{u}_0 \delta(x - x_0) \quad (3)$$

where \tilde{u}_0 can be treated as the mass which is concentrated at the infinitely small volume at $x = x_0$. [1] The dimensions are in a one-dimensional system L/T for D , uL for \tilde{u}_0 and $1/L$ for the delta function $\delta(x - x_0)$.

2.1.2. Boundary conditions and conservation of mass. The density of ink can be discretized with N intervals on a grid, where u_0 and u_N is the boundary points. If we model a drop of ink in a lake, the boundary conditions would read $\lim_{x \rightarrow \infty} u(x) = 0$, which means the concentration infinitely far away is zero. We can use this approximation because the drop of ink has such small volume compared to the lake, and we thus assume that the concentration becomes zero eventually. On the other hand, if we have a bounded system $x \in [a, b]$ with reflective boundaries the boundary conditions in the discretized system reads $u_{-1} = u_1$ and $u_{N-1} = u_{N+1}$. This means that the rate of change is zero on the boundary, $u_x(a, t) = u_x(b, t) = 0$ (where u_x is the partial derivative of u wrt. to x). In the case where the boundaries, instead of being reflective, are perfectly absorbent, the boundary conditions are $u_a = u_b = 0$. Conservation of mass is an important EGENSKAP of the physical system. In the case where the only source was the one at time $t = 0$, the equation which translates the conservation of the total mass \tilde{u}_0 is

$$\int_a^b u(x, t) dx = \tilde{u}_0 \quad (4)$$

Analytical solutions are in many cases not accessible and one has to lean on the results from the numerical calculations. However, it is good to use systems with analytical solutions to verify that the model works correctly. The unbounded problem has the analytical solution presented in Appendix A Eq. (23). This solution should also work well for a bounded problem as long as the density u goes to zero at the boundary and thus it should not be effected by any boundary effects. Since D has

the dimensions $[D] = L/T$, the characteristic time τ for the diffusion to reach all the area is $\tau = L/D$. This means that as long the time t follows

$$t < \tau = \frac{L}{D}, \quad (5)$$

the solution should not be affected by the boundaries and thus be valid.

An analytical solution for the bounded problem on the domain $[0, L]$ also exists and is presented in Appendix A Eq. (24).

2.1.3. Numerical solution. To solve the diffusion equation we have to discretize the equation. This can be done in many ways, but we'll use the Crank-Nicolson scheme to solve the bounded problem with both reflective and absorbing boundaries. The Crank-Nicolson scheme uses centered differences in space and time, combined with an average in time. The scheme is defined as

$$\begin{aligned} -\frac{\alpha}{2}u_{i-1}^{n+1} + (1 + \alpha)u_i^{n+1} - \frac{\alpha}{2}u_{i+1}^{n+1} \\ = \frac{\alpha}{2}u_{i-1}^n + (1 - \alpha)u_i^n + \frac{\alpha}{2}u_{i+1}^n, i = 1, \dots, N-1, \end{aligned} \quad (6)$$

where $\alpha = D\Delta t/(\Delta x)^2$ [2]. In Eq. (6) the superscript refers to the time point and the subscript to the discretized position. This creates a coupled system of equations which can be written as the matrix equation $\mathbf{A}\mathbf{U}^{n+1} = \mathbf{B}\mathbf{U}^n$, where \mathbf{A} and \mathbf{B} are tridiagonal matrices, and \mathbf{A} has $1 + \alpha$ on the diagonal and \mathbf{B} has $1 - \alpha$ on the diagonal. For absorbent boundaries the upper and lower diagonal is $-\alpha/2$ and $\alpha/2$ for \mathbf{A} and \mathbf{B} respectively. In the case where the boundaries are reflective, the first and last points are not divided by two for both \mathbf{A} and \mathbf{B} .

The Dirac's delta function is implemented in the discretized system as $1/\Delta x$, which approximates the value in a discretized system where Δx is the step length for the position.

2.1.4. Space dependent diffusivity. As stated, the diffusivity D can be position dependent, $D = D(x)$, and we must thus solve the original Eq. (1). For a step profile of diffusivity

$$D(x) = \begin{cases} D_+, & \text{if } x \geq 0 \\ D_-, & \text{if } x < 0 \end{cases}, \quad (7)$$

the numerical scheme must be treated with care around the discontinuity. A physical interpretation of such a position dependent diffusivity one can imagine the diffusion of temperature in a bar composed of two different metals joined together at the step. Since the diffusivity is no longer constant Eq. (1) is used. Using the finite difference central approximation with half-steps, the forward Euler (explicit) scheme becomes

$$\frac{u_i^{n+1} - u_i^n}{\Delta t} = \frac{1}{\Delta x^2} \left(D_{i+\frac{1}{2}}u_{i+1}^n - \Delta D_i u_i^n + D_{i-\frac{1}{2}}u_{i-1}^n \right), \quad (8)$$

where

$$D_{i+\frac{1}{2}} = \frac{D_i + D_{i+1}}{2} \quad \text{and} \quad \Delta D = D_{i-\frac{1}{2}} + D_{i+\frac{1}{2}}.$$

The same can be done for the backward Euler (implicit) scheme, and as normal combine the two to get the Crank-Nicolson scheme with space-dependent diffusivity

$$\begin{aligned} -\tilde{\alpha}D_{i-\frac{1}{2}}u_{i-1}^{n+1} + (1 + \tilde{\alpha}\Delta D_i)u_i^{n+1} - \tilde{\alpha}D_{i+\frac{1}{2}}u_{i+1}^{n+1} \\ = \tilde{\alpha}D_{i-\frac{1}{2}}u_{i-1}^n + (1 - \tilde{\alpha}\Delta D_i)u_i^n + \tilde{\alpha}D_{i+\frac{1}{2}}u_{i+1}^n, \end{aligned} \quad (9)$$

where $\tilde{\alpha} = \Delta t/2(\Delta x)^2$. The exact solution can be derived from the unbounded problem and is, for $x \in \mathbb{R}$ and $t > 0$, and is presented in Appendix A Eq. (27).

2.2. The wave equation

2.2.1. The equation. Waves are a natural phenomena that occurs in many systems, for example waves in water, wave propagation on a string or deformation of a membrane such as a drum. These waves can be modelled by the wave equation

$$\frac{\partial^2 u}{\partial t^2} - c^2 \Delta u = 0, \quad (10)$$

where c is the speed of the wave u . In this paper we consider a two-dimensional wave such that $u = u(t, x, y)$ where t is the time. Membrane of a square drum To model vibrations on a square membrane, such as a drum, we use the following PDE

$$\frac{\partial^2 u}{\partial t^2} = c^2 \left(\frac{\partial^2 u}{\partial x^2} + \frac{\partial^2 u}{\partial y^2} \right), \quad (11)$$

which is valid for $t > 0$ and $(x, y) \in \Omega = [0, 1]^2$ [1]. To solve the time evolution of this equation we implement a numerical scheme with a centered finite difference approximation that reads

$$\begin{aligned} u_{i,j}^{n+1} = -u_{i,j}^{n-1} + (1 - 2\beta)2u_{i,j}^n \\ + \beta(u_{i+1,j}^n + u_{i-1,j}^n + u_{i,j+1}^n + u_{i,j-1}^n), \end{aligned} \quad (12)$$

where the grid constant is the same in both spatial directions, $\delta x = \delta y = h$, and $\beta = c^2 \Delta^2 / h^2$ [3]. This stability of this implementation is heavily dependent on the stability threshold [1]

$$\frac{h}{\delta t} > \frac{c}{\sqrt{2}} \quad (13)$$

The initial and boundary conditions of the vibrations are

$$\begin{cases} u(0, x, y) = \sin(\pi x) \sin(2\pi y), & \text{for } (x, y) \in \Omega \\ u(t, x, y) = 0, & \text{for } t \geq 0, (x, y) \in \partial\Omega \\ \frac{\partial u}{\partial t}(0, x, y) = 0, & \text{for } (x, y) \in \Omega. \end{cases} \quad (14)$$

These initial and boundary conditions have the analytical solution

$$u(x, y, t) = \cos(\lambda_{12}t) \sin(\pi x) \sin(2\pi y), \quad (15)$$

where $\lambda_{12} = \sqrt{5}\pi$ when $c = 1$ [3].

2.2.2. Waves in water. Another interesting case to study is the evolution of the waves in water created when a stone is thrown in. A simplification of the initial condition is

$$u(0, x, y) = \exp\left(-\frac{(\mathbf{r} - \mathbf{r}_0)^2}{\sigma}\right), \quad \text{for } (x, y) \in \Omega, \quad (16)$$

which for low σ models quite concentrated deformations [1].

2.3. Hopf's equation and shock

2.3.1. Advection. To transport an initial profile u_0 one can use the advection equation

$$\frac{\partial u}{\partial t} + c \frac{\partial u}{\partial x} = 0. \quad (17)$$

This transports the initial condition $u(x, t = 0) = u_0(x)$ for $x \in \mathbb{R}$ with the velocity $c \in \mathbb{R}$. Numerically, the advection equation can be solved with the Lax-Wendroff scheme

$$u_{i,n+1} = u_{i,n} - \frac{c\delta t}{2\delta x}(u_{i+1,n} - u_{i-1,n}) + \frac{c^2\delta t^2}{2\delta x^2}(u_{i+1,n} - 2u_{i,n} + u_{i-1,n}). \quad (18)$$

The numerical solution can also be compared with the exact solution, which is the initial profile translated by ct , $u(x, t) = u_0(x - ct)$. [1]

2.3.2. Hopf's equation. The advection equation considers a constant velocity c . If the velocity field is u itself, we get the Hopf's equation

$$\frac{\partial u}{\partial t} + u \frac{\partial u}{\partial x} = 0. \quad (19)$$

This equation can be used to model a simplified version of the height of a tsunami wave $u(x, t)$ at position x at time t [1]. The height of the wave is transported by a velocity $v(x, t) = u(x, t)$.

When u is scalar valued, we have that

$$u \frac{\partial u}{\partial x} = \frac{1}{2}(2u) \frac{\partial u}{\partial x} = \frac{1}{2} \frac{\partial u^2}{\partial x}. \quad (20)$$

Using Eq. (20) we get the conservative form of the Hopf's equation (19)

$$\frac{\partial u}{\partial t} + \frac{1}{2} \frac{\partial u^2}{\partial x} = 0. \quad (21)$$

Using the conservative form we can derive a Lax-Wendroff scheme for the Hopf's equation which reads [1]

$$u_{i,n+1} = u_{i,n} - \frac{\delta t}{4\delta x}(u_{i+1,n}^2 - u_{i-1,n}^2) + \frac{\delta t^2}{8\delta x^2}[(u_{i+1,n} + u_{i,n})(u_{i+1,n}^2 - u_{i,n}^2) - (u_{i,n} + u_{i-1,n})(u_{i,n}^2 - u_{i-1,n}^2)]. \quad (22)$$

The Hopf's equation may lead to a situation where the solution becomes singular at a point in time. This can happen due to the slope becoming infinite and thus the PDE can no longer describe the system, and the phenomena is called shock.

3. Results

3.1. Diffusion

The Crank-Nicolson scheme were used to numerically solve the diffusion process with the Dirac delta initial condition in Eq. (3). Firstly, the time evolution of the diffusion equation in an unbounded system is presented in Figure 1 at time $t = 0.1$ ms with constant diffusivity $D = 1 \mu\text{m}/\text{ms}$. The unbounded solution is given by Eq. (23), and it satisfies the condition for validity given by Eq. (5). Bounded systems with both reflective and absorbing boundaries were also simulated with the same diffusion constant. Figure 2 and 3 presents the solution after time $t = 0.5$ for the reflective boundary and absorbing boundary respectively. The exact solutions for bounded scenarios are given by Eq. (24), and the numerical system solves Eq. (6) as the subsequent matrix problem. Conservation of mass for the bounded cases were analyzed with Eq. (4) and in relation to Figure 2 and 3 the deviation from $\tilde{u}_0 = 1.0$ after $t = 0.1$ ms

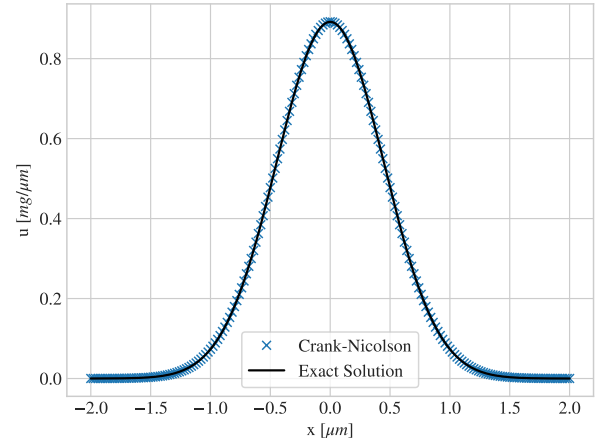


Figure 1. Density of ink u in water for the exact solution and Crank-Nicolson scheme with initial condition $u(x, 0) = \tilde{u}_0\delta(x)$ after time $t = 0.1$ ms, in an unbounded system.

were found to be $3 \cdot 10^{-14}$ mg for the system with reflective boundaries. The system with absorbent boundaries had a total mass of 0.917 mg.

The position dependent diffusivity in Eq. (7) was implemented with the Crank-Nicolson scheme in Eq. (9) and has the exact solution given in Eq. (27). Firstly, when using a constant diffusion, the new scheme gave the same answer as the previous scheme which was implemented only for constant diffusivity. The simulated diffusion process with step diffusivity after $t = 0.2$ ms is presented in Figure 4 with the exact solution and the step diffusivity profile $D(x)$. Furthermore, several diffusivity-profiles were investigated. A continuous and differentiable profile, a continuous but not differentiable profile and a not continuous profile are presented in Figures 5, 6 and 7 respectively.

3.2. Waves

The wave equation were solved for a system simulating vibrations on a drum. Using Eq. (12) with the initial- and boundary conditions in Eq. (14) the evolution of the system were solved numerically and presented in Figure 8 along with the exact solution in Eq. (15).

To simulate waves in water, the concentrated initial deformation in Eq. (16). The time evolution of the system is presented in Figure 9.

The numerical stability of the scheme in Eq. (13) were investigated and it was found that when $h/\delta t$ is lower than $2c/\sqrt{2}$ the numerical solution does not hold. This is two times the original stability criterion in Eq. (13). Figure 12 in Appendix B shows several simulations to the same time point of one "period" for different stability parameter values.

3.3. Advection and Shock

An initial gaussian wave is transported by the Lax-Wendroff scheme in Eq. (18) and the time evolution is presented in Figure 10. The same figure also shows the exact solution which is simply the translation of the initial profile. Transporting a wave can also be modelled by the Hopf's equation which gives the numerical Lax-Wendroff scheme in Eq. (22). A gaussian wave is transported by this equation is presented in Figure 11.

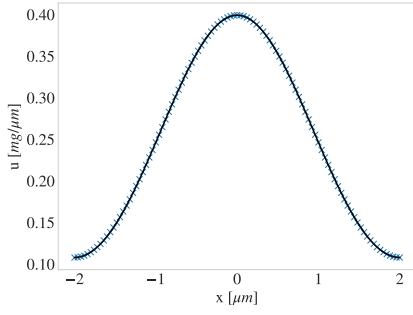


Figure 2. Density of ink u in water for the exact solution and Crank-Nicolson scheme with initial condition $u(x, 0) = \tilde{u}_0\delta(x)$ after time $t = 0.5$ ms. The system has reflective boundaries.

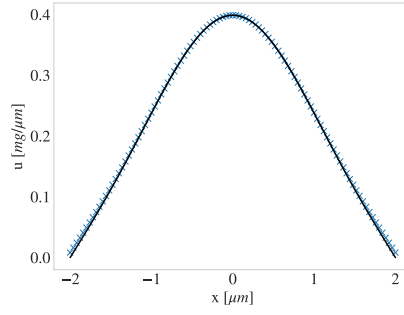


Figure 3. Density of ink u in water for the exact solution and Crank-Nicolson scheme with initial condition $u(x, 0) = \tilde{u}_0\delta(x)$ after time $t = 0.5$ ms. The system has absorbing boundaries.

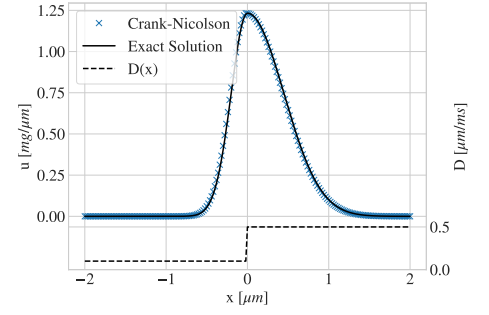


Figure 4. Density of ink u in water for the exact solution and Crank-Nicolson scheme with initial condition $u(x, 0) = \tilde{u}_0\delta(x)$ after time $t = 0.2$ ms. The diffusivity profile is the dashed line with scale on the right side.

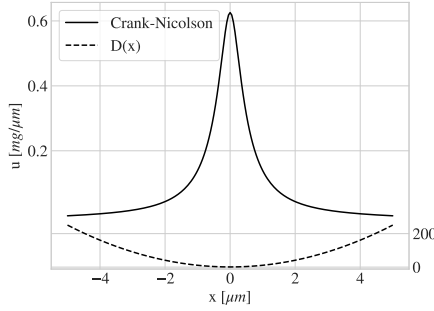


Figure 5. Density of ink u in water (solid line) simulated with the Crank-Nicolson scheme with initial condition $u(x, 0) = \tilde{u}_0\delta(x)$ after time $t = 0.09$ ms. The diffusivity profile is the dashed line with scale on the right side.

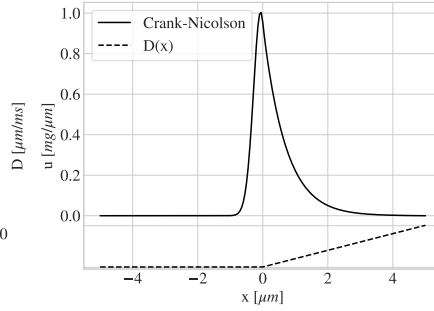


Figure 6. Density of ink u in water (solid line) simulated with the Crank-Nicolson scheme with initial condition $u(x, 0) = \tilde{u}_0\delta(x)$ after time $t = 0.3$ ms. The diffusivity profile is the dashed line with scale on the right side.

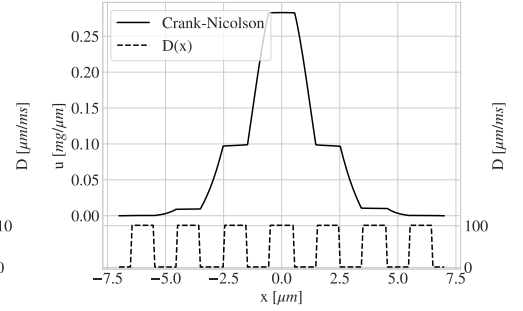


Figure 7. Density of ink u in water (solid line) simulated with the Crank-Nicolson scheme with initial condition $u(x, 0) = \tilde{u}_0\delta(x)$ after time $t = 1.9$ ms. The diffusivity profile is the dashed line with scale on the right side.

4. Discussion

4.1. Diffusion

An unbounded system with constant diffusivity is presented in Figure 1. The numerical solution matches the exact solution, which supports the validity of the numerical model. It is important to note that the analytical solution is only valid for times less than $L/D = 2$ ms, after which the diffusion should reach the boundaries and thus get unwanted effects. The figure also shows that the density u is flat before the edges meaning no density has come as far. This shows that an unbounded system can be implemented as a bounded system as long as there are no effects from the boundary.

Figure 2 shows the numerical and exact solution after time $t = 0.1$ ms with constant diffusivity. The numerical scheme gives the same solution as the exact solution, notably after the diffusion has reached the boundaries. Since the boundaries are perfectly reflective, all the mass should be contained in the system, and with a small deviation of $3 \cdot 10^{-14}$. This means the mass is conserved more or less perfectly, which is the wanted behavior. The same parameters were used for the system with fully absorbent boundaries, which is presented in Figure 3. The numerical solution matches the exact solution except for a very small deviation close to the boundaries. This might suggest that the boundary conditions are slightly wrong. Since the diffusion has interacted with the boundaries, the mass will be absorbed by the boundaries and the total mass is expected to decrease over time. The total integrated mass of the system is 0.917 mg after 0.5 ms, which shows that the boundaries work in the correct way relative to the reflective case.

Systems with space-dependent diffusivity were also investigated. Firstly, the new scheme in Eq. (9) were verified by using a constant diffusivity and receiving the same answer as Eq. (6) which was implemented for a constant diffusivity. The step diffusivity profile presented in Figure 4 were solved both with the exact solution and the numerical Crank-Nicolson scheme, and both yield the same results. From the diffusion equation (1) we can see that a higher diffusivity D gives a faster rate of change in density u . This behaviour can be seen in the solution of the system as the ink (density) has more greatly extended on the side with higher diffusivity. If one were to consider a system of two joined metal bars and modelling the temperature, this would mean that the bar with higher diffusivity would more rapidly spread the heat out and thus have worse insulating capabilities.

To test the system further, several different diffusivity-profiles were implemented. A continuous and differentiable profile $D(x) = x^2$ was simulated and presented in Figure 5. This system gives a very low diffusivity at the center and higher the further it diffuses, and the density u shows a very high peak with long tails. A continuous but non-differentiable profile as presented in Figure 6. On the left side with very low constant diffusivity we get the same behaviour as in the step diffusivity profile. However, on the right side where the diffusivity is continuously rising, the density shows the same behavior as the $D(x) = x^2$ profile. Observing the same behavior as the previous cases supports the scheme's validity. Lastly, a diffusivity-profile with many steps is presented in Figure 7. This system clearly shows the differences between high and

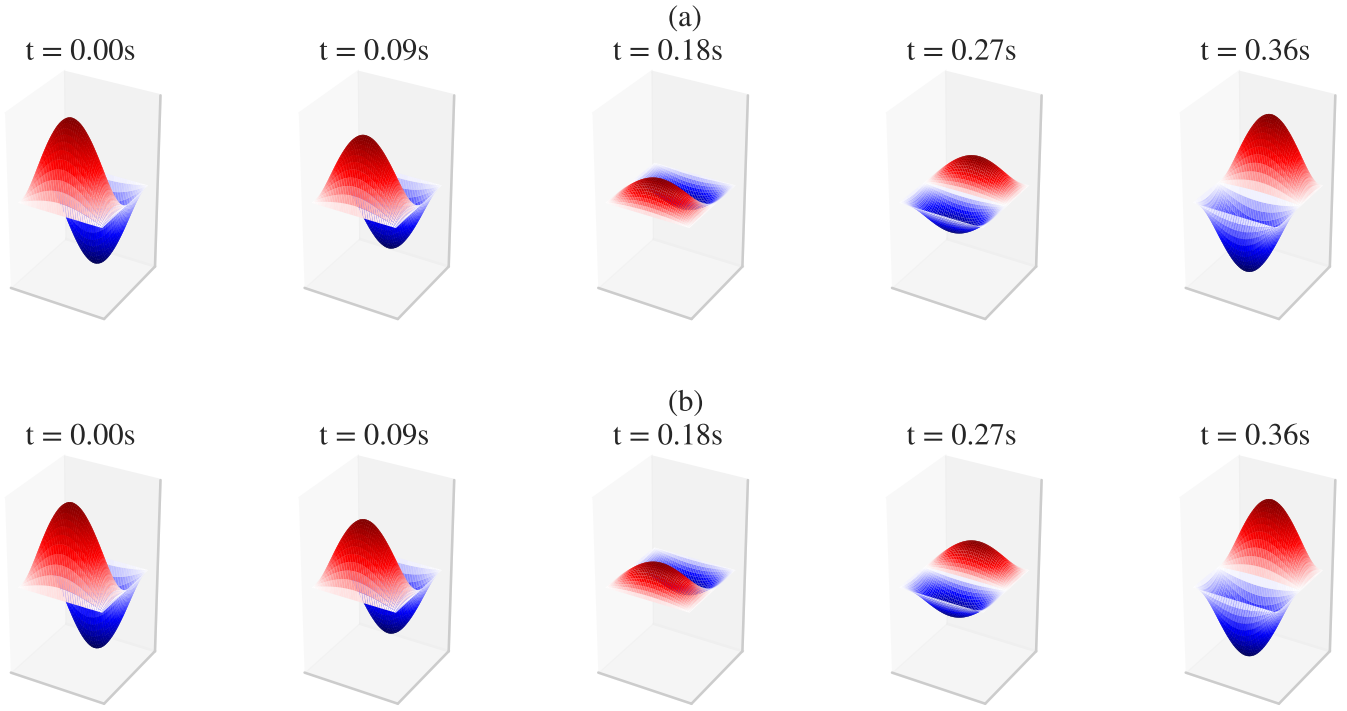


Figure 8. (a) The time evolution of vibrations on a drum at different times t . The x - and y -axis span from 0 to 1, while the z -axis span from -1 to 1. The color of the wave is red when above zero and blue when below zero. The exact solution is presented in (b).

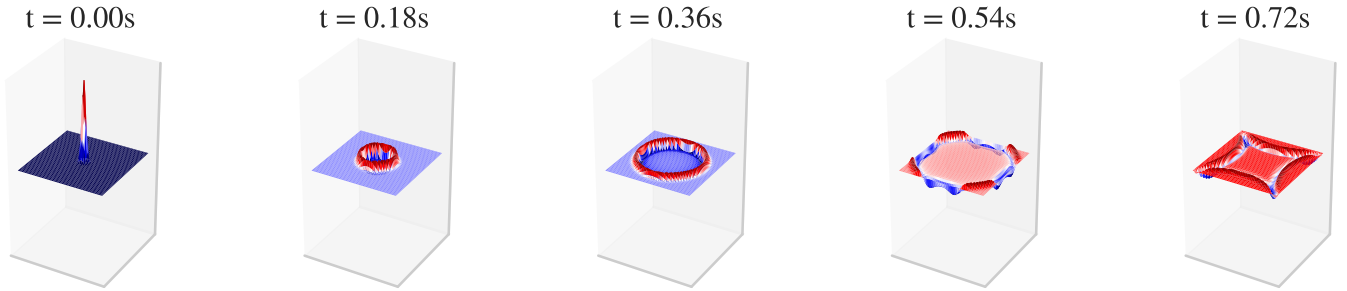


Figure 9. Time evolution of a wave after a concentrated initial condition in the center. The x - and y -axis span from 0 to 1, while the z -axis span from -1 to 1. The color of the wave is red when above zero and blue when below zero.

low diffusivity as we see that the density spreads fast with high diffusivity and slowly with low diffusivity.

4.2. Waves

To simulate vibrations on a square drum the wave equation (10) with initial and boundary conditions (14). The numerical finite difference scheme in Eq. (12) is compared with the exact solution from Eq. (15) in Figure 8. We can see that the numerical solution is equal to the exact solution. The wave on the drum has an oscillating behavior and the figure shows half a period. The numerical stability of this method is investigated in Figure 12 in Appendix B. Here it shows that the numerical method is stable for $h/\delta t > 2c/\sqrt{2}$ which is twice the amount in Eq. (13). This is quite interesting and suggests that there either is something wrong with the implementation of the scheme, or simply a small constant missing in the code. The latter might be more reasonable due to the verification when comparing the solution to the exact solution.

A stone dropped in water was simulated with the initial condition in Eq. (16) and the results were presented in Figure 9. We see that the initial wave spreads out radially without

losing any height before it hits the boundaries of the system. This suggests that there is no or little dispersion in the system which is a physical effect that is missing. The wave then reflects perfectly off the boundaries and inwards again. If the system had dispersion we should have noticed that the wave dies out eventually, but the simulation gives no notion of this.

4.3. Hopf

The Lax-Wendroff scheme in Eq. (18) was used to transport an initial Gaussian wave as presented in Figure 10. The numerical scheme gave the same answer as the exact solution. The scheme was then further developed for Hopf's equation and applied to an initial Gaussian wave. The results of this experiment are presented in Figure 11. By the first and second time in the figure, we note that the wave is tilted in the direction it is moving. This is due to the velocity-dependency of the wave. The higher up in the wave, the faster it is transported and thus we see the tilt. Eventually, since the higher points in the wave are transported faster, they will overcome the lower points and we get the shock behavior we see after $t = 0.14$ s and onwards.

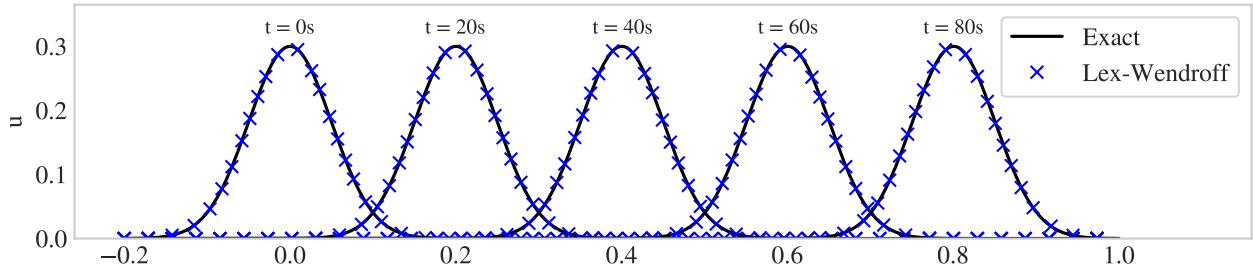


Figure 10. Time evolution of a gaussian wave at different times t for the Lax-Wendroff scheme for the advection equation and the exact solution.

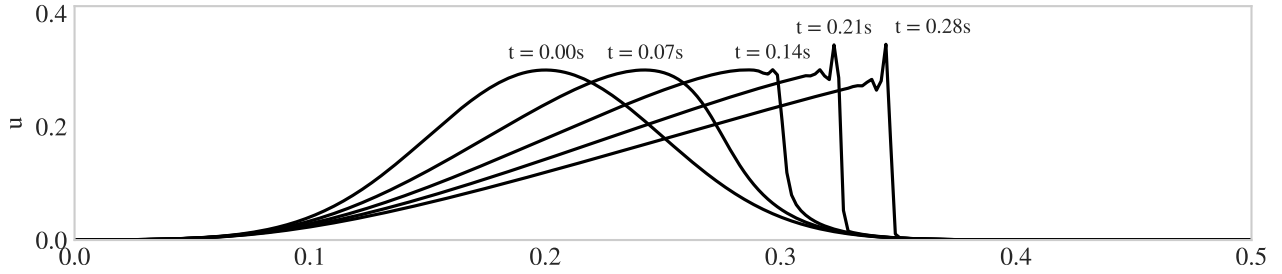


Figure 11. Time evolution of a gaussian wave at different times t for the Lax-Wendroff scheme for Hopf's equation and the exact solution.

5. Conclusion

Solving the diffusion problem for both constant and space-dependent diffusivity gave insights into the behavior of diffusion of a Dirac delta initial condition. The unbounded system with constant diffusivity was implemented as a bounded system and was found to give good estimates as long as the density does not reach the boundaries. For both reflective and absorbent boundaries, the numerical solution gave the same answer as the exact solution. The reflective boundaries conserved the total mass, while the system with absorbing boundaries saw a decrease in total mass when the boundary effects came in contact with the mass. Further space-dependent diffusivity profiles were investigated and it was found that higher diffusivity gave more rapid diffusion. The experiments show that the diffusion process regulates the density by smoothing it out.

The numerical stability of the scheme used to simulate the vibrations of a drum was found to be twice the expected amount and is most likely due to a small typo in the code rather than the numerical scheme given that the scheme gave the exact analytical solution. Water waves were also simulated with the same method, and it was found that the system most likely does not exhibit dispersion which is a crucial physical phenomenon when modelling waves.

Lastly, the transportation of a wave was experimented with, with both the advection equation and Hopf's equation. In Hopf's equation, the wave over time exhibits shock due to the higher points in the wave being transported faster than the lower points.

References

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A. Exact solutions

This Appendix presents some exact solutions given in [1]. When modelling a drop of ink in water and using the Dirac delta function as the initial profile, the unbounded problem has the analytical solution

$$u(x, t) = \frac{\tilde{u}_0}{\sqrt{4\pi Dt}} \exp\left(-\frac{(x - x_0)^2}{4Dt}\right). \quad (23)$$

The bounded problem with both reflective and absorbing boundaries has the exact solution

$$u(x, t) = \tilde{u}_0 \sum_{n=0}^{\infty} \exp\left(-\left(\frac{n\pi}{L}\right)^2 Dt\right) v_n(x_0) v_n(x). \quad (24)$$

The eigenfunctions of the diffusion operator $(v_n)_{n \in \mathbb{N}}$, are defined for the reflective boundaries as

$$v_n(x) = \begin{cases} \sqrt{\frac{1}{L}}, & \text{for } n = 0 \\ \sqrt{\frac{2}{L}} \cos\left(n\pi \frac{x}{L}\right), & \text{for } n > 0, \end{cases} \quad (25)$$

and for absorbing boundaries as

$$v_n(x) = \begin{cases} 0, & \text{for } n = 0 \\ \sqrt{\frac{2}{L}} \sin\left(n\pi \frac{x}{L}\right), & \text{for } n > 0, \end{cases} \quad (26)$$

For a space dependent diffusivity profile $D(x)$ with the step diffusivity in Eq. (7) has the exact solution

$$\frac{u(x, t)}{\tilde{u}_0} = \begin{cases} \frac{A_+(t)}{\sqrt{4\pi D_+ t}} \exp\left(-\frac{(x-x_0)^2}{4D_+ t}\right), & \text{if } x \leq 0 \\ \frac{A_-(t)}{\sqrt{4\pi D_- t}} \exp\left(-\frac{(x-x_0)^2}{4D_- t}\right), & \text{if } x > 0, \end{cases} \quad (27)$$

where

$$A_+(t) = 2 \left[1 + \left(\frac{x_0}{4D_+ t} \right) + \xi \right]$$

$$\xi = \left[\sqrt{\frac{D_-}{D_+}} e^{\frac{(D_+ - D_-)x_0^2}{4D_+ D_- t}} \left(1 - \operatorname{erf}\left(\frac{x_0}{\sqrt{4D_- t}}\right) \right) \right]^{-1}$$

$$A_-(t) = A_+(t) \sqrt{\frac{D_-}{D_+}} \exp\left(\frac{(D_+ - D_-)x_0^2}{4D_+ D_- t}\right).$$

B. Additional results

Numerical analysis of the finite difference scheme for vibrations on a square drum were performed by studying the simulation for different stability parameters in Eq. (13). The results are presented in Figure 12.

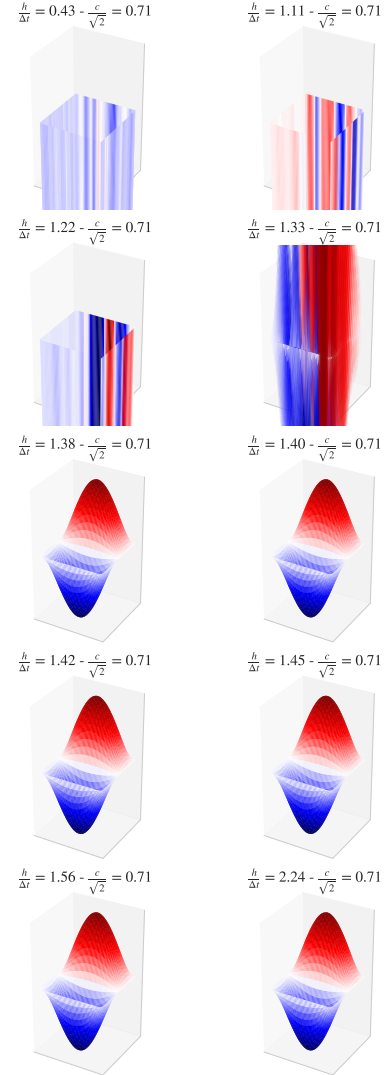


Figure 12. Time evolution of a wave simulating vibrations on a drum simulated for different stability parameters after one full period of the wave. The x - and y -axis span from 0 to 1, while the z -axis span from -1 to 1 . The color of the wave is red when above zero and blue when below zero.