Solving the diffusion equation

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Abstract

This report investigates the numerical solution of partial differential equations (PDEs) commonly found in various fields, including the heat/diffusion, wave, and Hopf's equations. Utilizing finite difference methods implemented in C and utilizing the GNU Scientific Library (GSL). The rapport compares numerical solutions to analytical solutions. Focusing on the diffusion equation initially, attention is given to different boundary conditions (BC). The Crank-Nicolson method is highlighted for its stability and conservativeness. Further exploration includes the effects of a non-constant diffusivity, revealing insights into diffusive behaviors. The wave equation is subsequently examined, showcasing the numerical and analytical solutions. Lastly, the Hopf equation is investigated, applaying lax-wendrof scheme. The solution of the Hopfs equation show non-uniform wavefront movement and the influence of wave density on velocity.

1 Introduction

In almost evry field one fines partial differential equations (PDEs) describing pyhsical phenomena. Through numerical methods, one gains the capability to analyze and predict the behavior of complex systems that may lack analytical solutions. In this report the Heat/diffusion, Wave and Hopf's equations are studied. Finite difference methods are deployed to solve these equations. The methods are implemented in C and the packages GNU Scientific Library (GSL), and Blas are used to solve the linear systems of equations. The results are compared to analytical solutions.

2 Method

2.1 Diffusion equation

Starting with an examination of the diffusion equation, represented by

$$\frac{\partial u}{\partial t} = \frac{\partial}{\partial x}\big(D(x)\frac{\partial u}{\partial x}\big)$$

If $D(x)$ is constant with respect to x, the equation is simplified to

$$\frac{\partial u}{\partial t} = D\frac{\partial^2 u}{\partial x^2}$$

Rescaling this equation it becomes

$$\frac{\partial u}{\partial t} = T_0\frac{D}{L^2}\frac{\partial^2 u}{\partial x^2}$$

The constants tells us that D has the units $\frac{m^2}{s}$. The diffusion process is one where consentraion of matter is spread out.

When the initial mass is small compared to the domain size, boundary conditions take the form $u(0,t) = u(L,t) \approx 0$. Extending this further, in an infinite domain, $lim_{x\to\pm\infty}u(x,t) = 0$. In a finite domain where all matter exits at the boundary, Dirichlet Bc are encountered: $u(0,t) = u(L,t) = 0$. When there is no leakage (no flux) at the boundary, Neumann BC arise: $\frac{\partial u}{\partial x}(0,t) = \frac{\partial u}{\partial x}(L,t) = 0$.

2.1.1 Numerical implementation

The choice of method here is important, since selecting the wrong method might prevent capturing the behavior of the system. For example, using an explicit method such as forward Euler would be unstable. Opting for an implicit method like backward Euler is better, as it is stable; however, it is also dissipative, and thus mass won't be conserved. The Crank-Nicolson method is both stable and conservative, making it a good choice. Taking the avrage of a forward and a backward difference, we get the Crank-Nicolson method. The Crank-Nicolson method is a second order accurate in both time and sapce.

$$-\frac{\alpha}{2}u_{n+1}^{i-1} + (1+\alpha)u_{n+1}^{i} - \frac{\alpha}{2}u_{n+1}^{i+1} = \frac{\alpha}{2}u_{n}^{i-1} + (1-\alpha)u_{n}^{i} + \frac{\alpha}{2}u_{n}^{i+1}$$

The following equation can be written in matrix form $Au^{n+1} = Bu^n$, where A and B are tridiagonal matrices.

$$A = \begin{bmatrix} 1+\alpha & -\frac{\alpha}{2} & \dots & 0 \\ -\frac{\alpha}{2} & \ddots & \ddots & \vdots \\ \vdots & \ddots & \ddots & -\frac{\alpha}{2} \\ 0 & \dots & -\frac{\alpha}{2} & 1+\alpha \end{bmatrix} \quad \text{and} \quad B = \begin{bmatrix} 1-\alpha & \frac{\alpha}{2} & \dots & 0 \\ \frac{\alpha}{2} & \ddots & \ddots & \vdots \\ \vdots & \ddots & \ddots & \frac{\alpha}{2} \\ 0 & \dots & \frac{\alpha}{2} & 1-\alpha \end{bmatrix}$$

the solution can be obtained in $O(n)$ operations using the Thomas algorithm.

2.2 Non constant diffusion coefficient

Ensuring a constant diffusivity across an entire domain often lacks realism as different mediums may exhibit varying diffusivity constants. Numerically speaking there are two ways of discretizing the diffusion equation if $D(x)$ is not constant. One way of discretizing would be to apply the derivative using the chain rule leaving us with

$$\frac{\partial u}{\partial t} = \frac{\partial}{\partial x}\big(D(x)\frac{\partial u}{\partial x}\big) = D_x u_x + D u_{xx}$$

Subsequently, one would typically apply the chain rule to simplify the equation. However, this approach may not always be suitable, as indiscriminate application of the chain rule can result in issues of mass conservation. Depending on the context, this may or may not pose a problem. Alternatively, another method of discretizing the equation can circumvent this issue. By applying central differences each derivative instead of the chain rule, one can effectively avoid the problem. This yields the resulting equation.

$$\big(-\beta D_- u_{i-1}^{n+1} + (\beta\Delta D + 1)u_i^{n+1} - \beta D_+ u_{i+1}^{n+1}\big) = \big(\beta D_- u_{i-1}^{n} + (1-\beta\Delta D)u_i^{n} + \beta D_+ u_{i+1}^{n}\big)$$

where $D_- = D_{i-\frac{1}{2}}$, $D_+ = D_{i+\frac{1}{2}}$, $\Delta D = \big(D_{i-\frac{1}{2}} + D_{i+\frac{1}{2}}\big)$ and $\beta = \frac{\Delta t}{2(\Delta x)^2}$

2.3 Wave equation

The wave equation, a fundamental concept in physics, it describes the behavior of waves propagating through a medium. The wave equation

$$\frac{\partial u}{\partial t} - c^2\nabla^2 u = 0$$

will be solved for two diffrent inial values/conditons.

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

and the initial condition

$$u(x,y,0) = \exp(-\frac{(r-r_0)^2}{\sigma}) \text{ where } r = x^2 + y^2 \text{ and } r_0 = (0.5, 0.5)$$

One can discretizing the PDE with central differences in both time and space resulting in the following scheme:

$$u_{n+1}^{i,j} = -u_{n-1}^{i,j} + (1-2\beta)^2 u_n^{i,j} + \beta(u_n^{i+1,j} + u_n^{i-1,j} + u_n^{i,j+1} + u_n^{i,j-1})$$

combined with the boundary condition we get the following matrix equation:

$$\vec{u} = \vec{u}^{n-1} + A\vec{u}^n \text{ where } u^{-1} = -\vec{u}^0 + A\vec{u}^0$$

where u is a vector of length N, and A is of the size $N^2 \times N^2$.

2.4 Hopf equation

Implementing a Lax-Wendroff scheme to solve $\frac{\partial u}{\partial t} + \frac{1}{2}\frac{\partial u^2}{\partial x} = 0$ involves changing the order of derivatives. This alteration assumes that the solution is sufficiently smooth, which may not always be the case depending on the initial data. However, this potential issue can be circumvented by avoiding such initial data selections. Introducing some notation, $\otimes$ signifies element-wise multiplication. Additionally, when a vector v is denoted as v^2, it indicates $v = [v_1^2, v_2^2, \ldots, v_n^2]$. This notation facilitates expressing the scheme in the following form:

$$\vec{u}_{n+1} = \vec{u}_n - \sigma \hat{B}\vec{u}_n^2 + 2\sigma^2(-B\vec{u}_n \otimes \vec{u}_n^2 + B\vec{u}_n^2 \otimes \vec{u}_n + A\vec{u}_n^3)$$

Here, matrix A is tridiagonal, featuring -2 on the diagonal and 1 on both the subdiagonal and superdiagonal. Matrix B is bidiagonal, with zeros on the main diagonal and ones on both the subdiagonal and superdiagonal. Matrix $\hat{B}$ is identical to B, except the lower diagonal entries are negative.

3 Results and Discussion

3.1 Diffusion equation

To verify the correctness of the Crank Nicolson method's implementation, the conservation of mass can be examined for the Neumann case. The total mass of the system is simply given by

$$\int_a^b u(x,t)\ dx = C\ \forall\ t$$

where C is some constant that is dependent on the initail condtions. Δt is the size of the time step, and N is the number of grid points, while D is the speed at which diffusion happens.

	Neumann results		
	$\alpha = 0.05$	$\alpha = 0.26$	$\alpha = 0.46$
t = 0.25	564.189575	564.189575	564.189575
t = 0.50	564.189575	564.189575	564.189572
t = 0.75	564.189577	564.1896	564.189578
t = 1.00	564.1896	564.1896	564.189575

Table 1: The table shows the total mass of the system for different values of α. Frome the data one can infer the numericall method is able to conserve the mass. The values $\Delta t = 10^{-4}$, N = 51 were used for the simulations.

	Dirichlet results		
	$\alpha = 0.05$	$\alpha = 0.26$	$\alpha = 0.46$
t = 0.25	564.189575	564.189575	564.189575
t = 0.50	427.846755	56.4628050	7.58511100
t = 0.75	257.768862	4.44055500	0.08014500
t = 1.00	154.461671	0.34922500	0.00084200

Table 2: The table shows the total mass of the system for different values of α. The mass is vanishing faster for larger values of D. The values $\Delta t = 10^{-4}$, $N = 51$ were used for the simulations.

3.1.1 Unbounded analytical solution

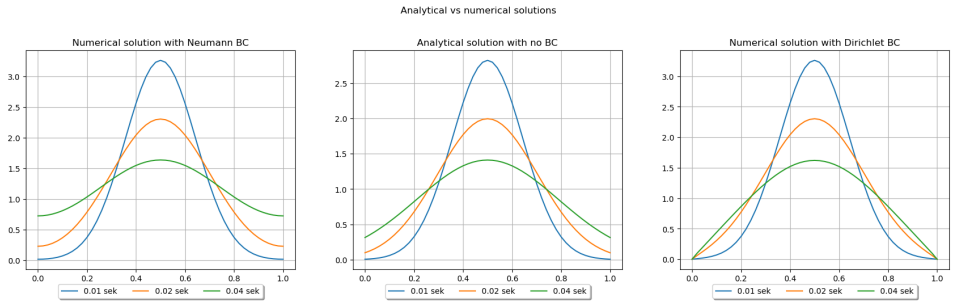


Figure 1: The analytical solution for the unbounded diffusion equation compared to the numerical solution.

The analytical solution of the unbounded diffusion equation serves as a reliable approximation for the numerical solution in general. However, this approximation doesn't hold true for all time instances. As information reaches the boundary, discrepancies between the three solutions emerge. The time it takes for these differences to manifest is directly related to the distance from the boundary and the speed of the diffusion process.

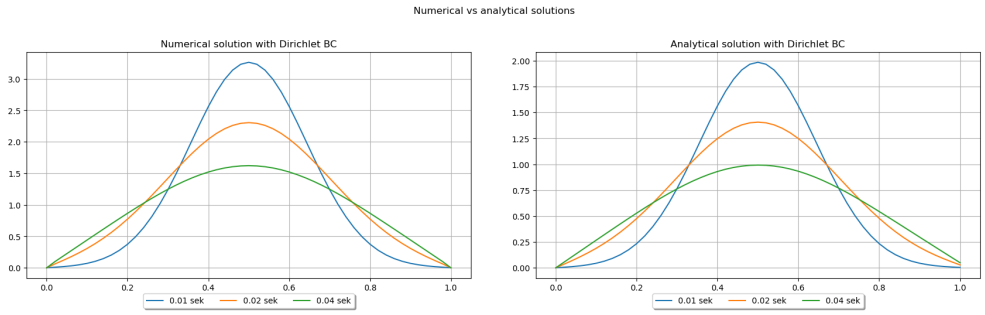


Figure 2: The analytical solution for the bounded diffusion equation compared to the numerical solution with diriclet BC.

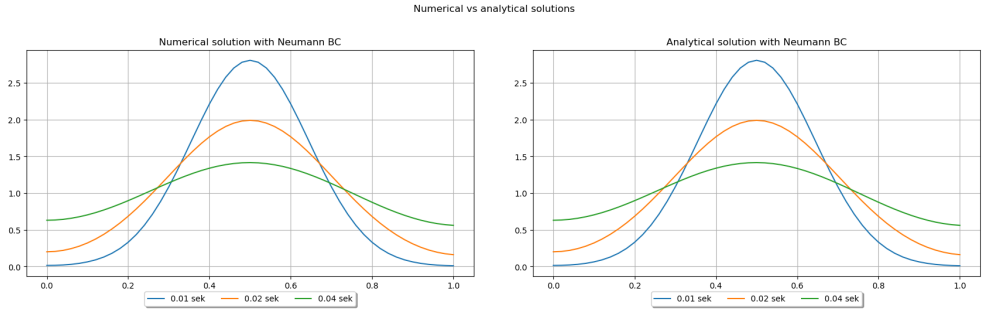


Figure 3: The analytical solution for the bounded diffusion equation compared to the numerical solution with neumann BC.

3.1.2 Bounded analytical solution

The analytical solution appears to match both solutions for the two different BC. However, there is a minor scaling discrepancy in the numerical solution with Dirichlet BC.e

3.2 Non constant diffusion coefficient

The following distribution is applied for the diffusivity:

$$D(x) = \frac{a}{1 + e^{-b(x-c)}} + d$$

As the parameter b increases, the diffusivity tends towards resembling a step function. The sigmoid function, characterized by infinitely many continuous derivatives, is a favorable choice for modeling smooth diffusivity. Later the parameter b in such a manner that the sigmoid function closely resembles its typical behavior. With this choice of diffusivity. The bellow figure shows the effects of a non constant diffusivity for diffrent BC. There seems to be a scaling issue with the analytical solution. However, one is still able to see the same main effect accross the diffrent boundaty conditions. namely, where the diffusivity is greater the solution is more spread out. This is aspecially clear for the Neumann BC. As the Neumann solution is very close to a stedy state for $x > 0.5$.

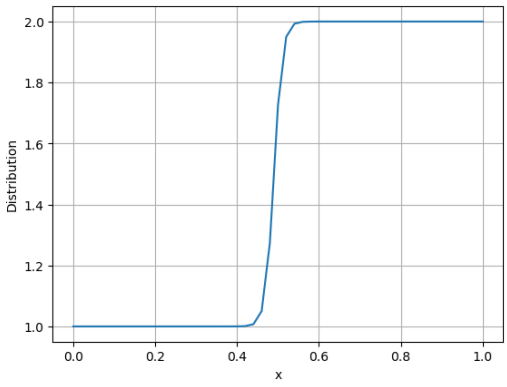


Figure 4: The following parameters are used: a=1, b=100, c=0.5, d=1

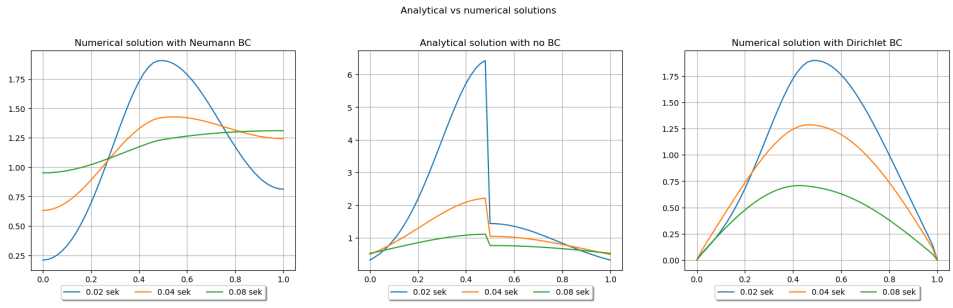


Figure 5: Solution to diffusion equation with above diffusivity

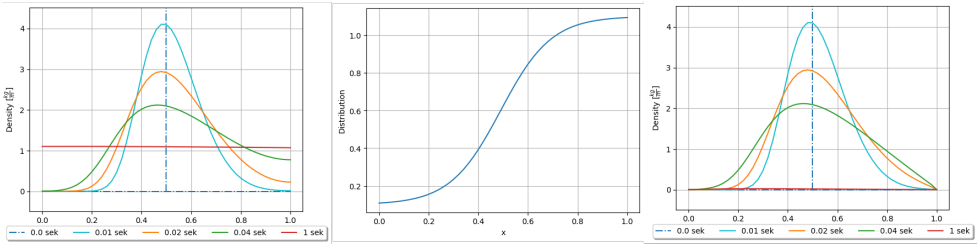
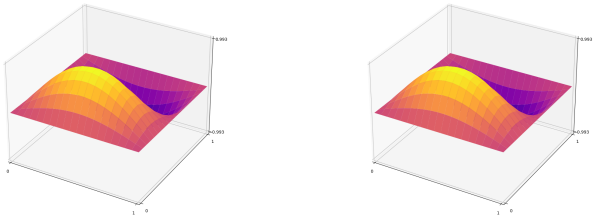


Figure 6: The leftmost plot depicts Neumann boundary conditions, the middle plot shows diffusion distribution with parameters: $a = 1$, $b = 10$, $c = 0.5$, $d = 0.1$. The rightmost plot has Dirichlet boundary conditions.

3.3 Wave equation

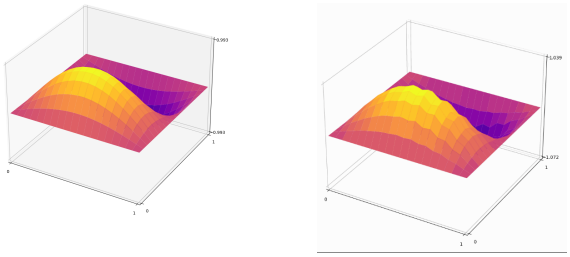


(a) Analytic solution (animation)

(b) Numerical solution (animation)

Figure 7: Pameter for (animation) was h = 0.05, dt = 0.02

The numerical and analytical solutions appear visually identical. Any perceived differences in speed are attributable to animation artifacts rather than disparities in the solutions themselves. Notably, the solution exhibits oscillatory behavior as expected. An examination of numerical stability can be done by generating plots with diffrent grid sizes.



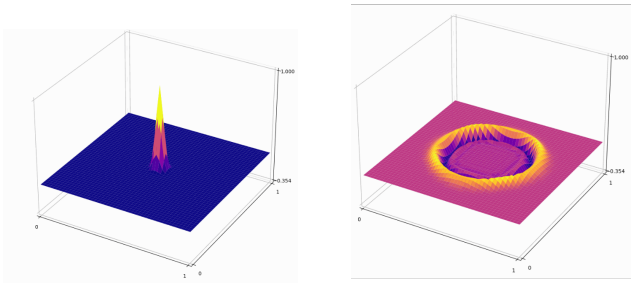
(a) Stabil solution (animation)

(b) Unstabil solution (animation)

Figure 8: Stabil and Unstabil plots

The onset of instability becomes perceptible as the animation draws to a close. Towards the end of the animation, waves and spikes begin to emerge on the primary wave. This occurs when h and t are selected such that the following inequality is not met:

$$\frac{h}{\delta t} < \sqrt{2}c$$



(a) $t = 0$ (animation) (b) $t > 0$ (animation)

Figure 9: Simulation of rock dropped into water

The inital data does a god job of representing a rock thrown into water. The waves propagate outwards from the point of impact, and the waves are reflected at the boundary. The waves have to go diffrent length, this results in the waves being out of phase after the reflection making intresing patterns. As the waves are being disspersed trhough the liquid the energy seems to be dissapation, this however should not happen as the differantional equation we are solving is not taking friction into account. It is rather an effect of the energy in the waves becomin more and more spread out as the waves propagate.

3.4 The advection equation

As the name inplies this equation transports quantitys. The quantity is the inital data.

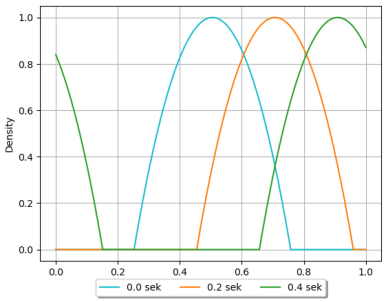
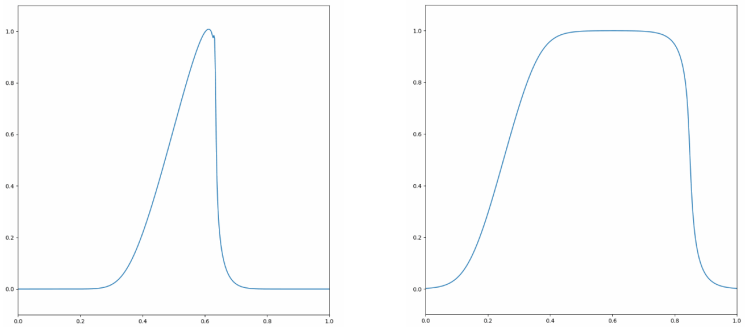


Figure 10: (animation)

The BC here was choocen to be periodic. $u(0,t) = u(1,t)$ This BC lets the simulation run indefinitely as the method never breacks down.

3.5 Hopf equation



(a) Sharp wave (animation) (b) Wide wave (animation)

Figure 11: Effect of hopfs Eq

In the animation, it is evident that both the sharp and broad wave fronts exhibit non-uniform movement. The centrum of the wavefront advances more rapidly than the remainder. Specifically, the densest region of

the wavefront has highest velocity. When the wave cathes up to the front, the solutoin breaks down as shocks appear. This behavior of this shock can be characterized by the Rankine–Hugoniot conditions.

$$\frac{F(u_-) - F(u_+)}{u_- - u_+} = \frac{\frac{1}{2}(u_-^2 - u_+^2)}{u_- - u_+} = \frac{1}{2}(u_- + u_+) = \dot{s}$$

From the Rankine–Hugoniot fomrula the shock wave is expected to move along the function by $\frac{1}{2}(u_- + u_+)t$. Notably, this behavior appears to be highly contingent upon the initial conditions. However, it is noteworthy that in the context of the aforementioned animation, this phenomenon occurs notably when the peak surpasses the leading edge.

4 Conclusion

This report delves into the implications of non-constant diffusivity on solutions, analyzing how it alters the approach. Furthermore, the stability of solutions to the wave equation under varying initial data conditions is explored. Lastly, the investigation of the Hopf equation involves a scheme assuming initial data to be C^2,otherwise introducing artifacts into the solution. The emergence of shocks as the wave catches up to itself is observed, highlighting their effects on the system.