Numerical Solution of PDEs using Spectral Theory

Erik Liodden[a]

[a] *Institutt for fysikk, Norges Teknisk-Naturvitenskapelige Universitet, N-7491 Trondheim, Norway.*

Abstract

This problem set is about solving various PDEs directly and by using spectral theory and discuss the advantage of using spectral theory.

1. Introduction

Many physical systems can be described using Partial Differential Equations, or PDEs. This could be simulating the diffusion of a chemical in a liquid, the motion of a gas, the weather, the motion of waves an many more systems. Three main classes of PDEs are the Diffusion equation, the Wave equation and the Schrodinger equation.

2. The Diffusion equation

The concentration of inc in water after some time t given some initial condition can be described using the diffusion equation. The diffusion equation in 1D is given by

$$\frac{\partial u}{\partial t} = \frac{\partial}{\partial x}\left[D(x)\frac{\partial u}{\partial x}\right] \tag{1}$$

Where $u = u(x,t)$. $D(x)$ is the diffusion constant and is in general dependent of position.

2.1. Constant diffusivity

Assume $D(x) = D = constant$, and the initial condition is a drop of inc at position x_0. The problem now becomes

$$\begin{cases} \dfrac{\partial u}{\partial t} = D\dfrac{\partial^2 u}{\partial x^2}, \\ u(x,0) = \tilde{u}_0\delta(x-x_0) \end{cases}$$

The $\delta(x-x_0)$ is the Dirac delta function. If the system was unbounded, e.g. the ocean, the boundary conditions would be $\lim_{x\to\pm\infty} u(x,t) = 0$. On the other hand, if the system is bounded to a region $[a,b]$, two normal boundary conditions would be the Dirichlet problem

$$u(a,t) = u(b,t) = 0$$

and the Neumann problem

$$\frac{\partial}{\partial x}u(a,t) = \frac{\partial}{\partial x}u(b,t) = 0.$$

Both the Dirichlet and Neumann problem can be solved numerically using the explicit/implicit Euler scheme or the Crank-Nicolson scheme which is a combination of those two. The explicit Euler scheme approximates the derica-tives as

$$\frac{\partial u(x_i,t_j)}{\partial t} \approx \frac{u_{i,j+1} - u_{i,j}}{\Delta t} \tag{2}$$

and

$$\frac{\partial^2 u(x_i,t_j)}{\partial x^2} \approx \frac{u_{i+1,j} - 2u_{i,j} + u_{i-1,j}}{\Delta x^2} \tag{3}$$

where $u(x_i,t_j) = u_{i,j}$. The implicit euler is solved the same way, but changing $j \to j+1$ in the approximation of $\frac{\partial^2}{\partial x^2}$.

The exact solution to the unbounded diffusion problem is given by

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

Figures 1 and 2 shows the solution to the Dirichlet problem with constant diffusivity.

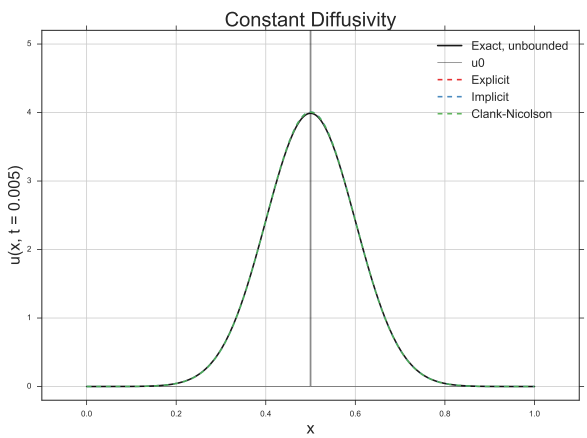

Figure 1: Constant Diffusivity $D = 1$. Dirichlet boundary conditions. $t = 0.005$.

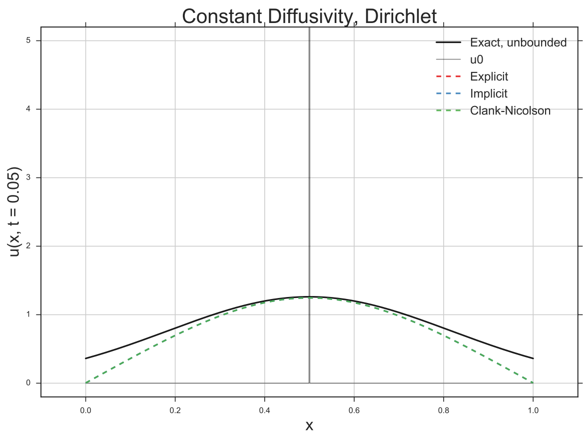

Figure 2: Constant Diffusivity $D = 1$. Dirichlet boundary conditions. $t = 0.05$.

Figures 3 and 4 shows the solution to the Neumann problem with constant diffusivity.

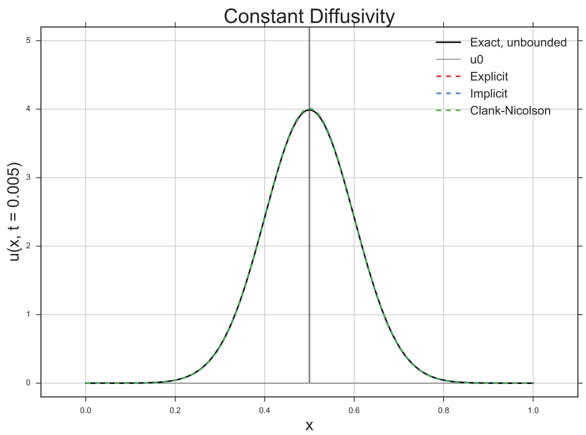

Figure 3: Constant Diffusivity $D = 1$. Neumann boundary conditions. $t = 0.005$.

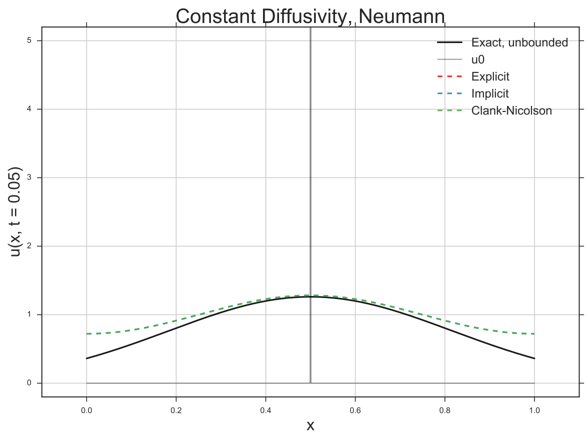

Figure 4: Constant Diffusivity $D = 1$. Neumann boundary conditions. $t = 0.05$.

2.2. Position dependent diffusivity $D = D(x)$

The diffusivity D can in principal be position dependent, $D = D(x)$. Foe example if you have two different metals jouned together. Figures 5 and 6 shows the solution to the Dirichlet and Neumann problem with diffusivity given by

$$D(x) = \begin{cases} 1, & x < 0.5 \\ 4, & x > 0.5 \end{cases}$$

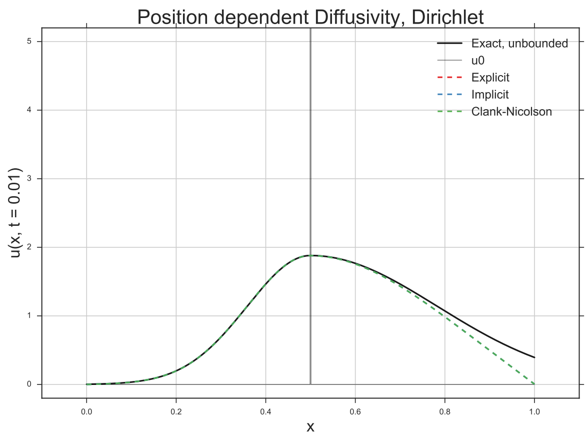

Figure 5: Variable diffusivity D. Dirichlet boundary conditions. $t = 0.01$.

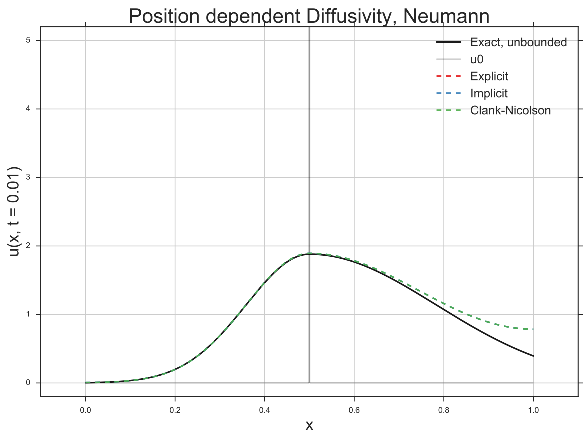

Figure 6: Variable diffusivity D. Neumann boundary conditions. $t = 0.01$.

3. Spectral theory

Consider a domain $\Omega \in \mathbb{R}^n$. The diffusion equation

$$\frac{\partial u}{\partial t} = D\Delta u$$

the wave equation

$$\frac{\partial^2 u}{\partial t^2} = c^2 \Delta u$$

and the Schrodinger equation

$$i\hbar \frac{\partial u}{\partial t} = -\frac{\hbar^2}{2m}\Delta u$$

with the initial conditions

$$\begin{cases} u(\mathbf{x}, 0) = u_0(\mathbf{x}), & \forall \mathbf{x} \in \Omega \\ \dfrac{\partial u(\mathbf{x}, 0}{\partial t} = v_0(\mathbf{x}), & \forall \mathbf{x} \in \Omega \end{cases}$$

with the Dirichlet boundary condition

$$u(\mathbf{x}, t) = 0, \quad \forall t > 0, \forall \mathbf{x} \in \partial\Omega$$

can all be solved almost simultaneously using spectral theory. By look for solutions on the form $u(\mathbf{x}, t) = \phi(t)w(\mathbf{x})$, and substituting this into the above equations we get for the diffusion equation

$$\frac{1}{D}\frac{\phi'}{\phi} = \frac{\Delta w}{w}$$

for the wave equation

$$\frac{1}{c^2}\frac{\phi''}{\phi} = \frac{\Delta w}{w}$$

and for the Schrodinger equation

$$\frac{2m}{i\hbar}\frac{\phi'}{\phi} = \frac{\Delta w}{w}$$

. Since the left side of all equations are only dependent on time, and the right hand side is only dependent on position, they must both be equal a constant, $-\lambda$.

This gives the following solution for the time dependency

$$\phi(t) = \begin{cases} \phi_0 \exp(-D\lambda t), & \text{Diffusion eqn.} \\ \phi_0 \exp\left(-\dfrac{i\hbar}{2m}\lambda t\right), & \text{Schrodinger eqn.} \\ A\exp(-ic\sqrt{\lambda}t + \phi_0), & \text{Wave eqn.} \end{cases}$$

This leaves the position dependency, which is the same eigenvalue problem for all

$$-\Delta w = \lambda w \tag{5}$$

Solving this will give the eigenvalues $(\lambda_k)_{k\in\mathbb{N}}$ with the corresponding eigenvectors $(w_k)_{k\in\mathbb{N}}$. The eigenvectors forms a complete orthonormal set, and we can find the general solution by projecting the initial condition on the eigenspace and apply the time dependency

$$u(\mathbf{x}, t) = \sum_k \langle u_0, w_k \rangle \phi(t) w_k \tag{6}$$

where u_0 is the initial condition and $\langle u_0, w_k \rangle$ is an inner product defined in Hilbert space.

3.1. Numerical resolution

The eigenvalue problem (5) is in general challenging to solve numerically, so I have used libraries, in particular `SciPy` [2]. To simplify, the domain is a 2D domain defined as $\Omega = [0, 1]^2$. The domain is divided into a grid of equal size in x and y direction. The 2D problem is converted to a 1D problem by mapping $(i, j) \to k$. The first eigenmodes of the system is shown in fig. 7 with arbitrary units.

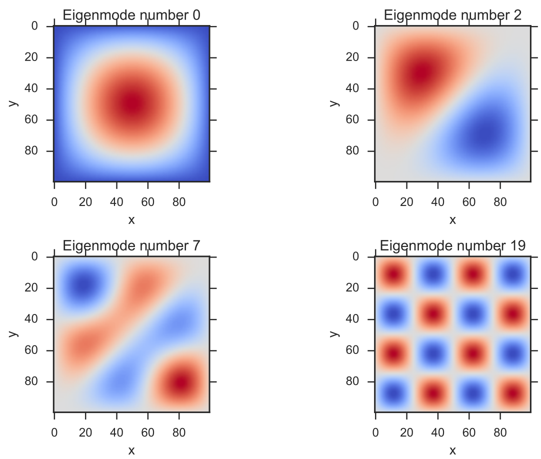

Figure 7: Eigenmode 0, 2, 7 and 19

By setting the initial condition to

$$u_0(\mathbf{x}) = \exp\left(-\frac{(\mathbf{r} - \mathbf{r}_0)^2}{\sigma}\right)$$

with $\mathbf{r}_0$ as distance to the the center $(0.5, 0.5)$. The spectral resolution to this initial condition is shown in fig. 8.

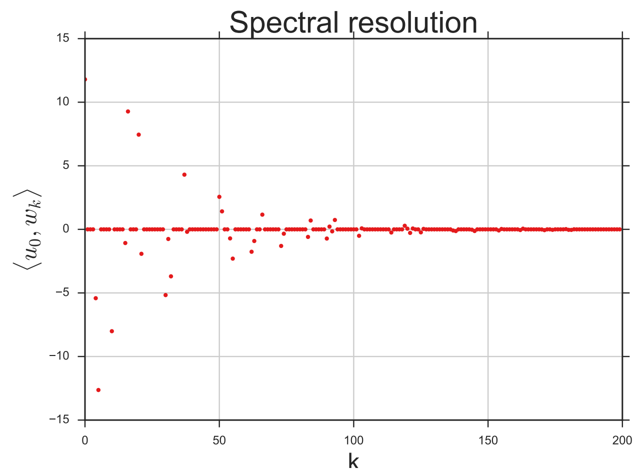

Figure 8: Spectral resolution of the initial condition as a Gaussian centered around $(0.5, 0.5)$ and $\sigma = 0.01$. The coefficiens goes to 0 as k gets large as expected.

The time evolution of the Schrodinger equation is shown in fig. 9

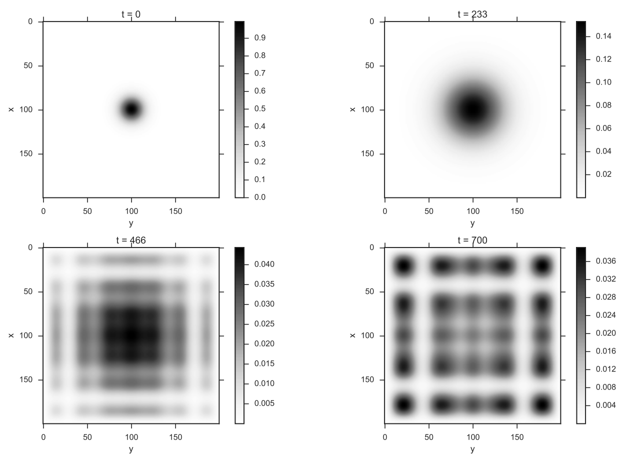

Figure 9: Time-evolution (in terms of probability distribution) of the Schrodringer equation, with initial condition as a Gaussian centered around $(0.5, 0.5)$ and $\sigma = 0.01$.

The time evolution of the diffusion equation is shown in fig. 10

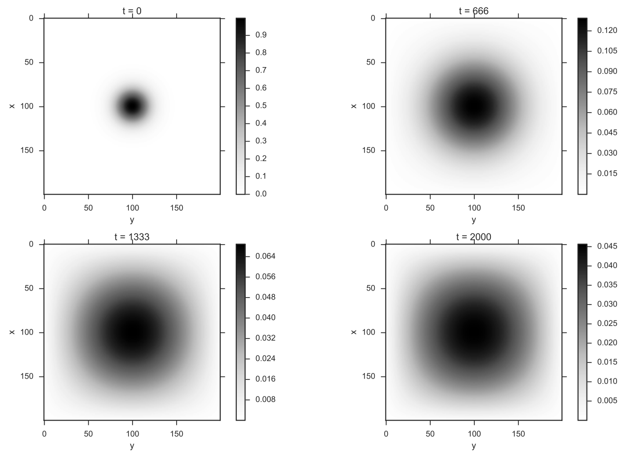

Figure 10: Time-evolution of the diffusion equation, with initial condition as a Gaussian centered around $(0.5, 0.5)$ and $\sigma = 0.01$.

The time evolution of the wave equation is shown in fig. 11

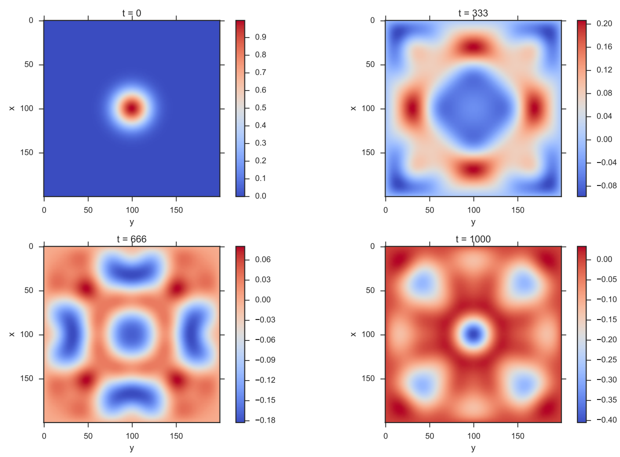

Figure 11: Time-evolution of the wave equation, with initial condition as a gaussian centered around $(0.5, 0.5)$ and $\sigma = 0.01$.

4. Hopf's equation

4.1. Linear case

A simple PDE is the advection equation, or the transport equation, given by:

$$\begin{cases} \dfrac{\partial u}{\partial t} + c\dfrac{\partial u}{\partial x} = 0 \\ u(x, 0) = u_0(x) \end{cases}$$

This equation has the exact solution

$$u(x, t) = u_0(x - ct)$$

There exists many schemes to solve this problem. Some of these schemes are the Upward, Downward, Explicit, Implicit, Lax-Friedrichs and Lax-Wendroff as defined in [1]. By setting periodic boundary conditions and the initial condition to

$$u_0(x) = \max(1 - (4(x - 0.5))^2, 0)$$

the different schemes gives the following results

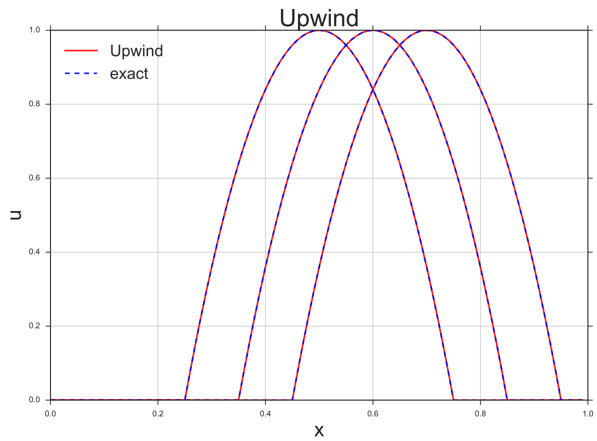

Figure 12: Upwind scheme. $\Delta x = 0.01$, $\Delta t = 0.01$. Sample times, $t \in \{0, 0.1, 0.2\}$. x and u in arbitrary units.

The upwind scheme gives the exact solution when $\Delta x = \Delta t$

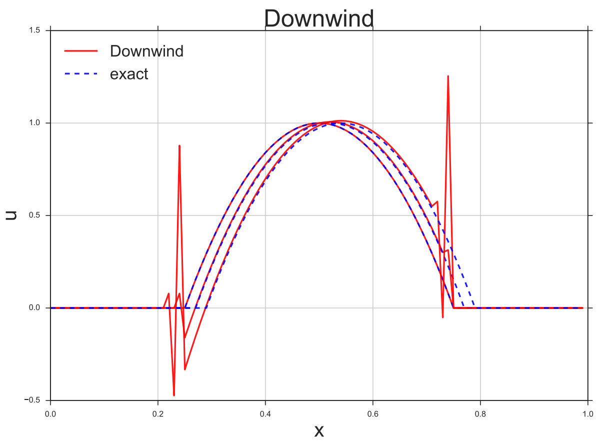

Figure 13: Downwind scheme. $\Delta x = 0.01$, $\Delta t = 0.01$. Sample times, $t \in \{0, 0.02, 0.04\}$. x and u in arbitrary units.

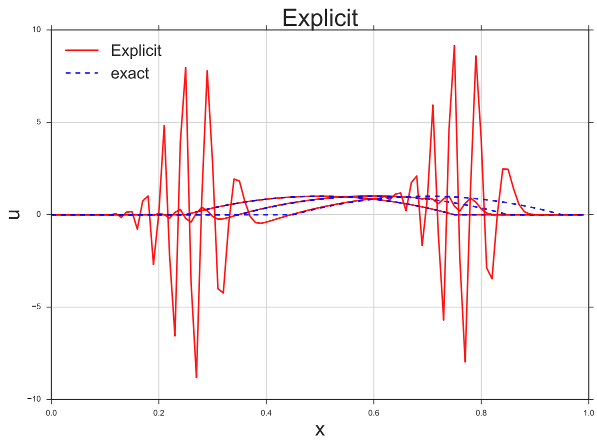

Figure 14: Explicit scheme. $\Delta x = 0.01$, $\Delta t = 0.01$. Sample times, $t \in \{0, 0.1, 0.2\}$. x and u in arbitrary units.

The downwind scheme fig. 13 and the explicit scheme fig. 14 have some instability issues around the endpoints.

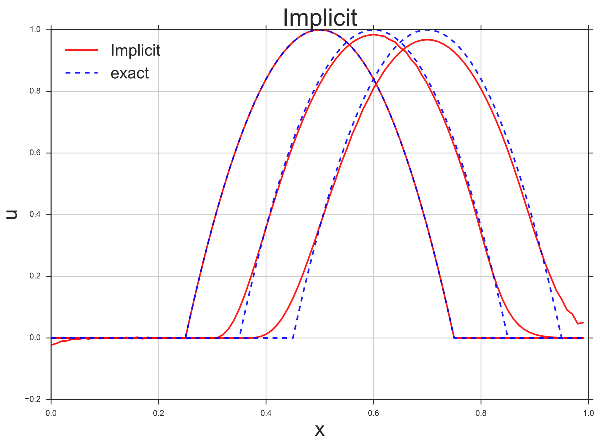

Figure 15: Implicit scheme. $\Delta x = 0.01$, $\Delta t = 0.01$. Sample times, $t \in \{0, 0.1, 0.2\}$. x and u in arbitrary units.

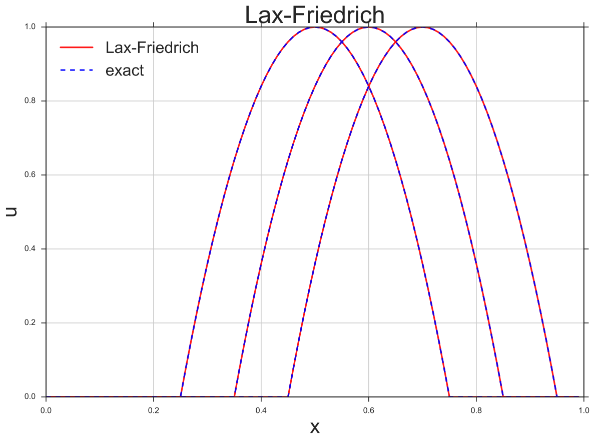

Figure 16: Lax-Friedrich scheme. $\Delta x = 0.01$, $\Delta t = 0.01$. Sample times, $t \in \{0, 0.1, 0.2\}$. x and u in arbitrary units.

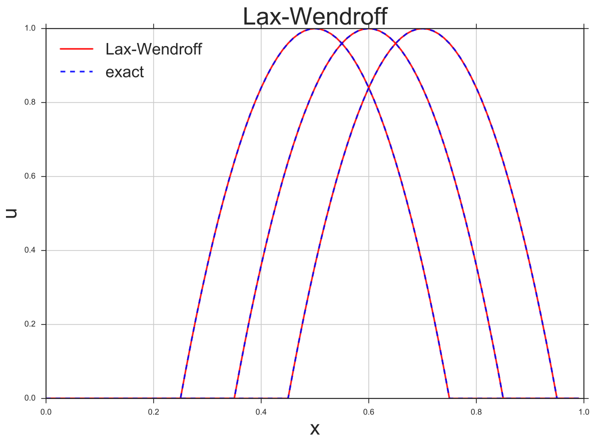

Figure 17: Lax-Wendroff scheme. $\Delta x = 0.01$, $\Delta t = 0.01$. Sample times, $t \in \{0, 0.1, 0.2\}$. x and u in arbitrary units.

Both the Lax-Friedrich scheme in fig. 16 and the Lax-Wendroff scheme in fig. 18 gives the exact solution when $\Delta x = \Delta t = 0.01$.

4.2. Non-linear case

A non-linear version of the Hopf's equation is

$$\begin{cases} \dfrac{\partial u}{\partial t} + u\dfrac{\partial u}{\partial x} = 0 \\ u(x,0) = u_0(x) \end{cases}$$

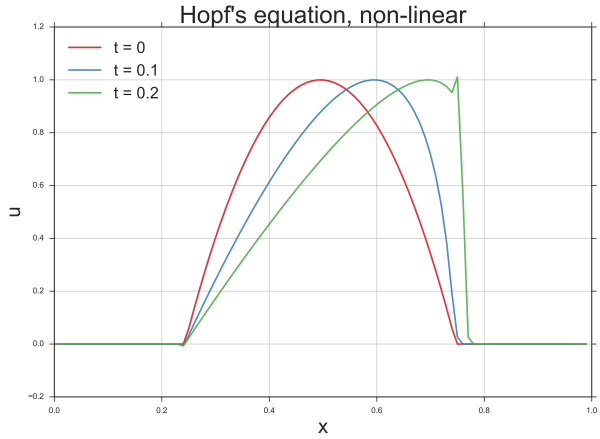

Figure 18: Non-linear Hopf's Equation solved using the explicit euler scheme. $\Delta x = 0.01$, $\Delta t = 0.01$. Sample times, $t \in \{0, 0.1, 0.2\}$. x and u in arbitrary units.

5. Conclusion

There are many ways to solve a PDE, and if it is linear, it is quite efficient to solve it using linear algebra. Non-linear PDEs are more difficult and require more iterative methods. I have also seen that by using spectral theory, one are able to solve a large group of PDEs at the same time.

References

[1] Problem Set 3, TFY4235, April 2016
[2] `http://www.scipy.org/`, v. 0.17