Computational Physics (TFY4235/FY8904) - Assignment 1

Diffusion, Waves, Shock and Mathematical Subtleties ...

Soft deadline: 15.02.24

January 19, 2024

**Abstract**

In this assignment we will solve numerically a few classic partial differential equations (PDEs) describing a time evolution of a system, and which play an important role in all fields of Physics and other sciences. We will be interested in the diffusion, the wave and the Hopf's equation, also known as the inviscid Burger's equation. The latter will give us a perfect opportunity to raise an important problem in the study of PDEs in general, namely the regularity of the solutions. We will see for example that the space of differentiable functions is not sufficient to describe solutions of PDEs and that we will even feel the need to consider non continuous functions as a solution of a PDE. How can a non continuous function, and therefore not differentiable, be a solution of partial differential equation? Mathematics is full of surprises ...

**Relevant fields**: All.

**Mathematical and numerical methods**: PDE, finite difference, linear algebra, method of characteristics.

**Authors**: Jean-Philippe Banon, Ingve Simonsen.

**Contacts**: Jonas Frafjord (jonas.frafjord@ntnu.no), Raffaela Cabriolu (raffaela.cabriolu@ntnu.no).

# 1 Introduction

Partial differential equations are used in almost every sciences to model very diverse phenomena. The diffusion of a chemical, the motion of a fluid, the waves propagating on the surface of water, the propagation of light, the dynamics of galaxy, the weather, the spread of an epidemy, and many other phenomena can be described by PDEs. In the lectures, you have seen (or will see) three basic second order PDEs that one often encounters in Physics, and other sciences, namely the diffusion, the wave and the Poisson equation. The first two describe time evolution of a system and the third a stationary state. We will focus on the first two as well as the most elementary first order PDE, the advection equation, which we will eventually modify to get the Hopf's equation. The Hopf's equation is a first order non-linear PDE which plays a central role in the understanding of shock phenomena.

The three problems can be treated independently.

Tasks preceded by ($\star$) require some mathematical analysis. They can be skipped at first but we encourage you to work on these tasks when the numerics is under control.

# 2 The diffusion equation

## 2.1 The equation

The diffusion equation is often used to describe the evolution of the density of a substance in a solvent (a drop of ink in water, a polluant in a lake or in the ground, ...), the evolution of the temperature in a medium, or the spread of an epidemy for example. Realistic problems will most probably take into account several mechanisms and couple the diffusion process with advection if we consider the flow of a river or with reaction for instance in chemistry where several substances might be present and react. Here we will focus on pure diffusion. To fix the ideas, let us assume that $u(x,t)$ is the density of ink in water, or the temperature along a bar of metal, at a position $x$ and at time $t$, and we consider a 1D problem for simplicity. The evolution of $u$ is then given by the diffusion equation

$$\frac{\partial u}{\partial t} = \frac{\partial}{\partial x}\left(D\,\frac{\partial u}{\partial x}\right) . \tag{2.1}$$

Here $D$ is the so-called diffusion constant, which might in principle depend on the position, time and even the density $u$ but the latter will lead to non-linear PDE. For this reason we prefer the term of diffusivity for $D$. In this problem we will only deal with $D$ being constant or position dependent.

We now need to give a set of initial and boundary conditions in order to solve a specific problem.

## 2.2 Numerical resolution

We consider now a few problems for you to solve.

**Constant diffusivity**

In the case of constant diffusivity Eq. (2.1) reads

$$\frac{\partial u}{\partial t} = D\,\frac{\partial^2 u}{\partial x^2} . \tag{2.2}$$

We consider an initial condition of the form

$$u(x,0) = \tilde{u}_0\,\delta(x-x_0) , \tag{2.3}$$

which model a sudden spil of 'mass' $\tilde{u}_0$ concentrated in an infinitely small volume at $x = x_0$. Here we recall that $\delta(x-x_0)$ denotes the Dirac delta distribution centered an $x = x_0$.

**Task 2.1**: What are the dimensions of $D$ and $\tilde{u}_0$ expressed in time, length and $[u]$ (dimension of $u$)? Has $\delta(x-x_0)$ a dimension?

**Task 2.2**: For an unbounded system, say modelling a drop of ink in a lake, what are the boundary conditions?

**Task 2.3**: Same question, for a system bounded to $[a,b]$, where $a,b \in \mathbb{R}, a < b$, with (i) reflective boundaries at $a$ and $b$, say modelling a drop of ink in a glass of water, (ii) perfectly absorbent boundaries.

**Task 2.4**: Assuming that the only source was the one at time $t = 0$, write an equation that translate the conservation of the total 'mass' $\tilde{u}_0$.

**Task 2.5**: Write down and implement a Crank-Nicolson scheme to solve numerically the two problems mentioned above (i.e. bounded with either reflective or absorbing boundaries). Get help from the slides of the lecture[1]. You will treat with great care and justification the numerical implementation of the Dirac-$\delta$. To solve the linear system that you will end up with, you may implement your own tridiagonal solver or use one from a library.

**Bonus task**: For the brave, also implement the Euler explicit and implicit schemes and study the numerical stability threshold.

**Task 2.6**: First check for a satisfactory solution: is the condition suggested in task 4 satisfied? Discuss.

The unbounded problem can be solved analytically, and we have, for $x \in \mathbb{R}$ and $t > 0$,

$$u(x,t) = \frac{\tilde{u}_0}{\sqrt{4\pi D t}} \exp\left(-\frac{(x-x_0)^2}{4Dt}\right) . \tag{2.4}$$

**Task 2.7**: Do you expect the above solution to be a good approximation for the bounded problems? Discuss the validity and quality of the approximation with respect to the parameters at hand (time, length of the domain, diffusion constant). Check if the above solution and your numerical solutions match in the region of validity you have identified. Hint: the validity region can be expressed as a short time condition $t < \tau$ where you will estimate $\tau$ by dimensional analysis as a function of $D$, and the length of the domain.

For the reflective and absorbing boundary problems, analytic solutions also exists. For a domain $[0, L]^2$, we have, for $x \in [0, L]$ and $t > 0$,

$$u(x,t) = \tilde{u}_0 \sum_{n=0}^{\infty} \exp\left(-\left(\frac{n\pi}{L}\right)^2 Dt\right) v_n(x_0)\, v_n(x) , \tag{2.5}$$

where the $(v_n)_{n\in\mathbb{N}}$ are the so called, eigenfunctions of the diffusion operator satisfying the boundary conditions, and defined as

*Reflective boundaries*

$$v_n(x) = \begin{cases} \sqrt{\frac{1}{L}} & \text{for } n = 0 \\ \sqrt{\frac{2}{L}} \cos\left(n\pi \frac{x}{L}\right) & \text{for } n > 0 \end{cases} . \tag{2.6}$$

*Absorbing boundaries*

$$v_n(x) = \begin{cases} 0 & \text{for } n = 0 \\ \sqrt{\frac{2}{L}} \sin\left(n\pi \frac{x}{L}\right) & \text{for } n > 0 \end{cases} . \tag{2.7}$$

**Task 2.8**: Compare your numerical solutions to the exact solutions.

### Space dependent diffusivity

Let the diffusivity be position dependent, $D = D(x)$. The relevant equation to solve is then the original one, Eq. (2.1).

[1] see blackboard for slides.

[2] one can easily translate this case to $[a, b]$ by translation, and dilatation

**Task 2.9**: Derive a Crank-Nicolson scheme in this case, implement it and solve the problems again with a constant diffusivity, and a step profile of diffusivity.

$$D(x) = \begin{cases} D_+ & \text{if } x \geq 0 \\ D_- & \text{if } x < 0 \end{cases} , \tag{2.8}$$

where $D_+, D_- \in \mathbb{R}_+$. This could model for example the diffusion of temperature in a bar composed of one material, say copper, on one half and another one, say iron, on the other half.

Do you get back the same solution as before in the case of constant diffusivity? For a step diffusivity profile an exact solution can be derived for the unbounded problem and reads, for $x \in \mathbb{R}$ and $t > 0$,

$$\frac{u(x,t)}{\tilde{u}_0} = \begin{cases} \frac{A_+(t)}{\sqrt{4\pi D_+ t}} \exp\left(-\frac{(x-x_0)^2}{4D_+ t}\right) & \text{if } x \geq 0 \\ \frac{A_-(t)}{\sqrt{4\pi D_- t}} \exp\left(-\frac{(x-x_0)^2}{4D_- t}\right) & \text{if } x < 0 \end{cases} , \tag{2.9}$$

where

$$A_+(t) = 2\left[1 + \operatorname{erf}\left(\frac{x_0}{\sqrt{4D_+ t}}\right) + \sqrt{\frac{D_-}{D_+}}\, e^{\frac{(D_+ - D_-)x_0^2}{4D_+ D_- t}} \left(1 - \operatorname{erf}\left(\frac{x_0}{\sqrt{4D_- t}}\right)\right)\right]^{-1} \tag{2.10}$$

$$A_-(t) = A_+(t)\sqrt{\frac{D_-}{D_+}} \exp\left(\frac{(D_+ - D_-)x_0^2}{4D_+ D_- t}\right) . \tag{2.11}$$

Does your numerical solution match the solution to the unbounded problem for short time?

**Task 2.10**: Once task 2.9 is under control, play with profiles for both the initial condition and the diffusivity profile of increasing level of 'wildness', i.e. try both a differentiable profile, a continuous but non differentiable profile and a non continuous profile (i.e. like the step but you could add more steps for fun), and describe with your own words the regularisation properties of the diffusion equation.

**Bonus tasks**: If time allows and you would like to get a deeper understanding of the diffusion equation or wish to investigate, you can:

- ($\star$) derive all exact solutions suggested in this problem;
- extend to the two dimensional problem (i.e. 2D in space);
- investigate the diffusion-reaction equation

$$\frac{\partial u}{\partial t} = \nabla \cdot (D\, \nabla u) + R(u) . \tag{2.12}$$

  where $R$ is a functional modeling the reaction term. You will find different interesting functionals to investigate by a quick literature search.

# 3 The wave equation

## 3.1 The equation

The wave equation, as the name indicates, is often used to model wave phenomena such a mechanical wave propagating along string, deformation wave on a membrane, pressure waves in a gas, and even electromagnetic waves to some extend. The wave equation reads

$$\frac{\partial^2 u}{\partial t^2} - c^2 \, \Delta u = 0 \, . \tag{3.1}$$

Here $|c|$ is the speed of the wave. In this assignment, we consider a two dimensional problem, i.e. a typical model of membrane wave.

## 3.2 Numerical resolution

**Shape of a square drum**

We consider the problem suggested in the lecture slides. The vibration of a square membrane is described by the following partial differential equation, for $t > 0, (x, y) \in \Omega = [0, 1]^2$,

$$\frac{\partial^2 u}{\partial t^2} = c^2 \left( \frac{\partial^2 u}{\partial x^2} + \frac{\partial^2 u}{\partial y^2} \right) \, , \tag{3.2}$$

and the initial and boundary conditions read

$$\begin{aligned} u(0, x, y) &= \sin(\pi x) \, \sin(2\pi y), && \text{for } (x, y) \in \Omega \\ u(t, x, y) &= 0, && \text{for } t \geq 0, \ (x, y) \in \partial\Omega \\ \tfrac{\partial u}{\partial t}(0, x, y) &= 0, && \text{for } (x, y) \in \Omega \, . \end{aligned} \tag{3.3}$$

**Task 3.1**: Implement the finite difference scheme presented in the lecture slides. We will choose for simplicity the same spacial step along the $x$ and $y$ direction, $\delta x = \delta y = h$.

**Task 3.2**: Run your program and plot $u(t, x, y)$ at different times. You may want to make an animation to appreciate the evolution of the membrane deformation in time. Compare your numerical result with the exact solution given in the lecture slides.

**Task 3.3**: Study numerically the stability threshold

$$\frac{h}{\delta t} > \frac{c}{\sqrt{2}} \, . \tag{3.4}$$

**Water waves or not water waves?**

We consider now the following initial condition:

$$u(0, x, y) = \exp\left( -\frac{(\mathbf{r} - \mathbf{r}_0)^2}{\sigma} \right) , \qquad \text{for } (x, y) \in \Omega \, , \tag{3.5}$$

which is intended to model how the membrane react to a rather concentrated deformation. You may choose: $\mathbf{r}_0 = (0.5, 0.5)$ and $\sigma = 0.001$.

**Task 3.4**: Run your program for this new initial condition, and describe the solution. We wish to simulate the surface of water waves in a swimming pool when a stone is thrown in it. Do you think the previous model describes well this situation? Which physical effects are missing in your opinion?

**Bonus tasks**: If time allows and you would like to get a deeper understanding of the wave equation or wish to investigate, you can:

- change the shape of the boundary, make it circular for example (drums are usually circular).
- ($\star$) find the eigen-modes for the circular drum;
- use the eigenmodes as initial conditions, and visualize how the shape of the drum evolves in time;
- adapt the scheme so that it solves the wave equation with spatially dependent velocity

$$\frac{\partial^2 u}{\partial t^2} = \nabla \cdot \big(c^2(x,y)\nabla u\big) \ . \tag{3.6}$$

# 4 Hopf's equation and shock

## 4.1 Back to basics: the advection equation

We gently start this last section with probably the most simple PDE you may know, the advection equation, also known as the transport equation.

$$\frac{\partial u}{\partial t} + c\,\frac{\partial u}{\partial x} = 0 \tag{4.1}$$

with initial condition, for $x \in \mathbb{R}$,

$$u(x, 0) = u_0(x)\,. \tag{4.2}$$

Here $c \in \mathbb{R}$ plays the role of a velocity which litteraly transports the initial profile $u_0$ as you may already know. The method of characteristics gives us the explicit solution, for $x, t \in \mathbb{R}$,

$$u(x, t) = u_0(x - ct)\,. \tag{4.3}$$

($\star$) **Task 4.1**: Prove Eq. (4.3) using the methods of characteristics.

There exist many numerical schemes to solve the advection equation, also in more complicated cases where the velocity field may depend on the position for instance. Here we will focus on the Lax-Wendroff scheme which we will derive for $c$ constant. In a further subsection you will adapt this derivation to a non-linear case. We start by a Taylor expansion of $u$ to second order in time

$$u(x, t + \delta t) = u(x, t) + \delta t\,\frac{\partial u}{\partial t}(x, t) + \frac{\delta t^2}{2}\,\frac{\partial^2 u}{\partial t^2}(x, t) + o(\delta t^2)\,. \tag{4.4}$$

Now the game is to replace all the time derivatives on the right hand side with spatial derivatives using the advection equation Eq. (4.1). In particular, we need an expression for $\frac{\partial^2 u}{\partial t^2}$ that we get by taking the time derivative of Eq. (4.1)

$$\frac{\partial^2 u}{\partial t^2} = -c\,\frac{\partial}{\partial t}\left[\frac{\partial u}{\partial x}\right] = -c\,\frac{\partial}{\partial x}\left[\frac{\partial u}{\partial t}\right] = c^2\,\frac{\partial^2 u}{\partial x^2}\,. \tag{4.5}$$

Notice just as a curiosity that if $u$ is solution of the advection equation, then $u$ is also solution of the wave equation. Then using the above equation and the advection equation, we can replace all the time derivatives by spatial derivatives in Eq. (4.4).

$$u(x, t + \delta t) = u(x, t) - c\,\delta t\,\frac{\partial u}{\partial x}(x, t) + \frac{c^2\,\delta t^2}{2}\,\frac{\partial^2 u}{\partial x^2}(x, t) + o(\delta t^2)\,. \tag{4.6}$$

We can approximate the term $\frac{\partial u}{\partial x}$ by a central difference of step $\delta x$

$$\frac{\partial u}{\partial x}(x, t) = \frac{u(x + \delta x, t) - u(x - \delta x, t)}{2\,\delta x} + o(\delta x^2)\,. \tag{4.7}$$

and similarly for the term $\frac{\partial^2 u}{\partial x^2}$. We will detail though the latter so that you can use the same idea later in the non-linear case. We use a central difference approximation for the outer derivative but with step $\delta x/2$ which reads

$$\frac{\partial}{\partial x}\left[\frac{\partial u}{\partial x}\right](x, t) = \frac{\frac{\partial u}{\partial x}(x + \delta x/2, t) - \frac{\partial u}{\partial x}(x - \delta x/2, t)}{\delta x} + o(\delta x^2)\,, \tag{4.8}$$

and once more for each 1st order derivatives at the numerator

$$\frac{\partial^2 u}{\partial x^2}(x, t) = \frac{u(x + \delta x, t) - 2\,u(x, t) + u(x - \delta x, t)}{\delta x^2} + o(\delta x^2)\,. \tag{4.9}$$

Thus Eq. (4.6) becomes

$$\begin{aligned}u(x,t+\delta t) = u(x,t) &- \frac{c\,\delta t}{2\,\delta x}\,\left(u(x+\delta x,t) - u(x-\delta x,t)\right)\\ &+ \frac{c^2\,\delta t^2}{2\,\delta x^2}\,\left(u(x+\delta x,t) - 2\,u(x,t) + u(x-\delta x,t)\right) + o(\delta t^2) + o(\delta x^2)\,.\end{aligned}$$

This gives the so-called Lax-Wendroff scheme which is of order 2 both in space and time

$$u_{i,n+1} = u_{i,n} - \frac{c\,\delta t}{2\,\delta x}\,\left(u_{i+1,n} - u_{i-1,n}\right) + \frac{c^2\delta t^2}{2\,\delta x^2}\left(u_{i+1,n} - 2\,u_{i,n} + u_{i-1,n}\right)\,. \tag{4.10}$$

where time as been discretized in step $\delta t$, space in step $\delta x$ and the approximation of the solution on the space-time grid at point $(i\,\delta x, n\,\delta t)$ is $u_{i,n}$ $(i,n \in \mathbb{Z})$.

**Task 4.2**: Implement the Lax-Wendroff scheme and compare the numerical solution to the exact solution. You may take any initial condition you like. Study the stability of the scheme.

## 4.2 Hopf's equation, a non-linear sister of the advection equation

We now consider the Hopf's equation which looks formally similar to the advection equation but the velocity field is now $u$ itself.

$$\frac{\partial u}{\partial t} + u\,\frac{\partial u}{\partial x} = 0\,. \tag{4.11}$$

The Hopf's equation is thus non-linear and we will study the effect of this non-linearity. The Hopf's equation as it stands in Eq. (4.11) is rather a prototypical equation and does not really describe any specific physical system. Nonetheless its left hand side is often present (up to some constants taking care of the dimensions) to equations encountered in fluid mechanics, in particular to model the behaviour of an incompressible and non-viscous shallow fluid[3]. A more realistic PDE for this kind of problems may contain other terms as well, describing surface tension, external forces, viscosity, compressibility, dispersion, etc ... Here we are particularly interested in studying the effect of shock for which the 'Hopf's' part of the equation is responsible. Then to fix the ideas, we could say that $u(x,t)$ model the height of water at position $x$ and time $t$ and the height is transported by a velocity field proportional to the height itself $v(x,t) = k\,u(x,t)$ but for simplicity we take $k = 1$ [4]. The problem you will study is then basically that of the apparition of a tsunami (in a very very very over-simplified way).

## 4.3 Numerical resolution ... at least up to a critical time

As any first order PDE, the Hopf's equation could be solved by the method of characteristics, we will use this method later and rather start naively by a numerical approach.

**Task 4.3 - conservative form**: Show that for $u \in \mathcal{C}^1(\mathbb{R}^2, \mathbb{R})$, Eq. (4.11) is equivalent to the following conservative equation

$$\frac{\partial u}{\partial t} + \frac{1}{2}\,\frac{\partial u^2}{\partial x} = 0\,. \tag{4.12}$$

**Task 4.4**: Review the derivation presented in section 4.1 to derive a Lax-Wendroff scheme for the Hopf's equation. Show that you get a scheme which reads as

[3] Note that an ocean can be viewed in first approximation as an incompressible, inviscid shallow water since its depth is much smaller than its width.

[4] we could anyway go back to this case from $k \neq 1$ by a change of time or spatial scale

$$u_{i,n+1} = u_{i,n} - \frac{\delta t}{4\,\delta x}\,\left(u_{i+1,n}^2 - u_{i-1,n}^2\right) \\ + \frac{\delta t^2}{8\,\delta x^2}\left[(u_{i+1,n} + u_{i,n})(u_{i+1,n}^2 - u_{i,n}^2) - (u_{i,n} + u_{i-1,n})(u_{i,n}^2 - u_{i-1,n}^2)\right] \,. \tag{4.13}$$

(Hint: use the conservative form.)

**Task 4.5**: Implement the Lax-Wendroff scheme and run simulations with initial and boundary conditions of your choice. The only constraint we impose on an initial condition is that it should be smooth enough, say $\mathcal{C}^1$, so that the PDE description make sense, at least for the start. Describe the solution, understand or get a feeling of what is the effect of the Hopf's equation on the initial profile and explain it in your own words. Conjecture a simple condition on the initial profile for a shock to develop in finite time.

As you have realized in the previous task, the Hopf's equation may lead to a shock, i.e. a solution which becomes singular at a certain point in time. In the case we studied, the slope may become infinite at some point and the description of the evolution of the system as a PDE breaks down. Your numerical job is done for this assignment and we will embark now into more theoretical and mathematical considerations.

($\star$) **Task 4.6**: By using the method of characteristics, derive the condition you have conjectured in the previous task, i.e. a condition on the initial condition $u_0(x)$ which leads to a singular solution in a finite time. In that case, derive the time $T$ up to which the method of characteristics ensures you a unique well behaved solution. Check that the time you derived is consistent with the time you can estimate from your simulation.

## 4.4 ... and after the shock? On the regularity of solutions

($\star$) **Bonus tasks**: What happens after the shock? How can we deal with a discontinuous and therefore non differentiable solution for a PDE? If you find these intriguing questions interesting, consider the following literature search:

- Rankine-Hugoniot equation.
- Notion of weak solution of a PDE.
- Theory of distributions and PDE analysis.

# 5 Report

Write a report of your work (maximum 6 pages). The report is expected to take the form of a scientific article, containing an abstract, a short introduction, the modeling of the problem, a few words on its numerical resolution, your results and discussion, a conclusion and references. The tasks are here to guide you, and you should not write your answers task by task in the report, but rather select the important pieces of information showing in a concise way how you dealt with the problem, and critically discuss your results. Your codes are not expected in the report, but must be attached to it if it is delivered during the exam. Codes must be clear, and commented.