TFY4235/FY8904 : Computational Physics (spring 2017)

Assignment 1 : Diffusion, Waves, Shock and Mathematical Subtleties…

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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 equation, the wave equation, Schrödinger's equation and Hopf's equation, also known as the inviscid Burgers' 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 a partial differential equation? Mathematics is full of surprises …

Relevant fields: All.

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

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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 models 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 at $x = x_0$.

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 $t = 0$, derive an equation that relates the rate of change of mass in the system to the flux at the boundary and discuss the different type of boundary conditions.

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

Task 2.6: For the three aforementioned schemes, study numerically the stability threshold. ($\star$) Explain the stability condition found numerically by rigorous mathematical arguments. Suggested reading: Chapters 1 and 2 in Ref. [1].

Task 2.7: First check for a satisfactory solution: is the condition suggested in Task 2.4 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 2.8: 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 τ by dimensional analysis as a function of D, and the length of the domain.

For the reflective and absorbing boundary problems, analytic solutions also exist. For a domain $[0, L]$[1], 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 2.9: Compare your numerical solutions to the exact solutions for the three schemes. You will study numerically how the error between the exact and numerical solution scales with the discretization steps. How do your results compare with the scaling of the truncature error expected by the analysis found in Chapter 2 of Ref. [1]?

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

Task 2.9 - bis: Same as Task 2.9 but only for the explicit scheme and keeping the ratio $\frac{D\delta t}{\delta x^2} = 1/6$, where δt and δx are respectively the time and spatial steps. ($\star$) Explain why the error decays faster in that case than for arbitrarily chosen discretization steps.

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).

Task 2.10: 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, in the case $x_0 = 0$ for $x \in \mathbb{R}$ and $t > 0$,

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

where

$$A_+(t) = 2\left[1 + \sqrt{\frac{D_-}{D_+}}\right]^{-1} \tag{2.10}$$

$$A_-(t) = A_+(t)\sqrt{\frac{D_-}{D_+}} . \tag{2.11}$$

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

Task 2.11: Once Task 2.10 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 (solutions given in complements);
- 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 Spectral theory and eigenvalue problem

3.1 Motivation

We consider Ω a domain of $\mathbb{R}^n$, of boundary $\partial\Omega$. Let $u(\mathbf{x}, t)$ denote a function depending on a time variable t and space variables $\mathbf{x}$. Imagine we are interesting in solving one of these equations of physical interest on this domain,

- the diffusion equation:
$$\frac{\partial u}{\partial t} = D\,\nabla^2 u \tag{3.1}$$
- the wave equation:
$$\frac{\partial^2 u}{\partial t^2} = c^2\,\nabla^2 u \tag{3.2}$$
- the Schrödinger equation:
$$i\hbar\,\frac{\partial u}{\partial t} = -\frac{\hbar^2}{2m}\,\nabla^2 u \tag{3.3}$$

given some initial conditions,

$$u(\mathbf{x}, 0) = u_{\text{in}}(\mathbf{x}), \qquad \forall\,\mathbf{x} \in \Omega, \tag{3.4}$$
$$\frac{\partial u}{\partial t}(\mathbf{x}, 0) = v_{\text{in}}(\mathbf{x}), \qquad \forall\,\mathbf{x} \in \Omega, \text{(for the wave equation)} \tag{3.5}$$

with Dirichlet boundary conditions

$$u(\mathbf{x}, y) = 0, \qquad \forall\,t > 0,\ \forall\,\mathbf{x} \in \partial\Omega. \tag{3.6}$$

You are most probably familiar with these equations, but we recall the possible physical meaning of each of them. As studied in the previous section, the diffusion equation could model here the diffusion of a chemical, or of temperature in a medium, with absorbent boundaries. The wave equation models the vibrations of a membrane ($n = 2$) which has been stretched and fixed at the boundary, like a drum for example. The Schrödinger equation describes the evolution of the wave function of a free particle in a box, the domain Ω.

It is worth noting the presence of the Laplace operator $\nabla^2 u = \sum_{i=1}^{n} \frac{\partial^2 u}{\partial x_i}$ in all these cases. This is a key observation that can be used to solve simultaneously the three above problems, as we motivate now.

Assume that we are looking for solutions of the form

$$u(\mathbf{x}, t) = \phi(t)\,w(\mathbf{x})\,, \tag{3.7}$$

then by plugging Eq. (3.7) into Eqs. (3.1,3.2,3.3) we get, at least formally,

- for the diffusion equation:
$$\frac{1}{D}\,\frac{\phi'}{\phi} = \frac{\nabla^2 w}{w}\,, \tag{3.8}$$
- for the wave equation:
$$\frac{1}{c^2}\,\frac{\phi''}{\phi} = \frac{\nabla^2 w}{w}\,, \tag{3.9}$$

- for the Schrödinger equation:

$$\frac{2m}{i\hbar}\frac{\phi'}{\phi} = \frac{\nabla^2 w}{w} \; . \tag{3.10}$$

In each of these last three equations, the left hand side is a function of time only and the right hand side is a function of position only. The only way this can hold for any time and at any position, is that both the left and right hand sides are constant, say $-\lambda$, with $\lambda \in \mathbb{R}$. Note that λ is an unknown. The convention for the minus sign will become clear below. Thus we must have

$$\frac{\phi'}{\phi} = -D\,\lambda \text{ or } = -\frac{i\hbar}{2m}\lambda\,, \qquad \text{(Diffusion and Shrödinger equations)} \tag{3.11}$$

$$\frac{\phi''}{\phi} = -c^2\,\lambda, \qquad \text{(Wave equation)} \tag{3.12}$$

and

$$-\,\nabla^2 w = \lambda w \; . \tag{3.13}$$

Eqs. (3.11,3.12) can be integrated simply as

$$\phi(t) = \phi_0\,\exp\left(-D\,\lambda\,t\right) \text{ or } = \phi_0 \exp\left(-\frac{i\hbar}{2m}\lambda\,t\right)\,, \qquad \text{(Diffusion and Shrödinger equations)} \tag{3.14}$$

$$\phi(t) = A\exp\left(i\,c\,\sqrt{\lambda}\,t + \varphi_0\right)\,, \qquad \text{(Wave equation)}\,. \tag{3.15}$$

We recognize the usual time dependencies for the diffusion equation and wave equations, namely an exponential decay in time for the first one and vibrations for the second one. If you are familiar with Quantum Mechanics, you will also recognize the time evolution phase factor $\exp\left(-i\frac{E}{\hbar}\,t\right)$ depending on energy $E = \frac{\hbar^2\lambda}{2m}$.

Now, the only problem that remains to be solved is the eigenvalue problem Eq. (3.13), i.e. finding the eigenvalues and corresponding eigenfunctions of the Laplace operator satisfying the boundary conditions. If we manage to find the eigenvalues $(\lambda_k)_{k\in\mathbb{N}}$ and corresponding eigenfunctions $(w_k)_{k\in\mathbb{N}}$ then we can expand the initial condition u_{in} on the complete set of eigenfunctions and apply the corresponding time dependency. For example, in the case of diffusion, if the expansion of the initial condition on the basis of eigenfunctions reads

$$u_{\text{in}} = \sum_k \alpha_k\,w_k\;, \tag{3.16}$$

then the solution is immediately given by

$$u(\mathbf{x},t) = \sum_k \alpha_k\,e^{-D\,\lambda_k\,t}\,w_k(\mathbf{x})\;. \tag{3.17}$$

You recognize here an equation similar to Eq. (2.5) used in the previous section to compare the numerical solution of the 1-dimensional diffusion equation $n = 1$. This is exactly the method used to find the exact solution as explained in details in the complements.

To sum up this motivation section, we can say that the three problem we started with can be solved once and for all if we manage to find the eigenvalues and eigenfunctions of the Laplace operator that satisfy the appropriate boundary conditions. In fact, this is in general the hard part of the problem, since in practice the boundary may be of arbitrary shape, which makes the resolution of the eigenvalue problem challenging.

Note that the eigenfunctions, also known as eigenmodes, are not simply mathematical commodities but also have a physical meaning. If we take the example of the two-dimensional drum, the eigenmodes are modes of resonant frequencies of the membrane.

In the following, we will restrict ourselves to a two-dimensional domain, and it may be helpful to think of the problem as finding the resonant modes of a drum with arbitrary shapes.

More details on the spectral theory can be found in Chapter 7 in Ref. [1], which has been a great source of inspiration for the present motivation.

3.2 Rectangular domain

We warm up with a good old academic exercise. We consider the eigenproblem of the Laplace operator with Dirichlet boundary conditions. The domain $\Omega = (0, L_x)\times(0, L_y)$, with $L_x, L_y > 0$, is a rectangle and the problem reads

$$-\nabla^2 u = \lambda u, \qquad \text{in } \Omega \tag{3.18a}$$
$$u = 0, \qquad \text{on } \partial\Omega \tag{3.18b}$$

where u is a function of position (x, y).

($\star$) **Task 3.1:** Show that the eigenvalues and corresponding normalized eigenmodes of the above problem read, for $k = (k_x, k_y) \in \mathbb{N}_*^2$,

$$\lambda_k = \left(\frac{k_x^2}{L_x^2} + \frac{k_y^2}{L_y^2}\right)\pi^2, \tag{3.19a}$$
$$u_k(x, y) = \frac{2}{\sqrt{L_x\, L_y}} \sin\left(\frac{k_x\,\pi\, x}{L_x}\right) \sin\left(\frac{k_y\,\pi\, y}{L_y}\right). \tag{3.19b}$$

For this, you can be inspired by what has been done in the complements for the diffusion problem in 1D. This result will be useful as a benchmark for your code.

Task 3.2: By applying a finite difference scheme on Eq. (3.18), explain how to write down the matrix system for which the eigenvalue problem must be solved for, and solve it numerically. You are allowed to use numerical libraries to solve the eigenproblem.

Task 3.3: Compare the numerical eigenvalues and eigenmodes to that of Eq. (3.19). Introduce a/some measure(s) of error between eigenmodes and estimate how it/they scale(s) with the discretization step h. (We will use for simplicity, $L_x = L_y = 1$, $\delta x = \delta y = h$.)

We consider now the following initial condition:

$$u_{\text{in}}(x, y) = \exp\left(-\frac{(\mathbf{r} - \mathbf{r}_0)^2}{\sigma}\right), \qquad \text{for } (x, y) \in \Omega\,, \tag{3.20}$$

which is intended to model how the membrane reacts to a rather concentrated deformation, how a concentrated concentration diffuses, how a concentrated wave function for a quantum particle evolves. You may choose: $\mathbf{r}_0 = (0.5, 0.5)$ and $\sigma = 0.001$. (In addition, for the wave equation we take $v_{\rm in} = 0$.)

Task 3.4: Project numerically the initial condition on the set of eigenmodes obtained from Task 3.2, i.e. compute the coefficients α_k of Eq. (3.16), i.e. perform

$$\alpha_k = \langle u_{\rm in}, w_k \rangle = \int_\Omega \bar{u}_{\rm in}(\mathbf{x})\, w_k(\mathbf{x})\, \mathrm{d}x\mathrm{d}y\ . \tag{3.21}$$

Here $\bar{f}$ denotes the complex conjugate of $u_{\rm in}$ (but we take $u_{\rm in}$ real so we do not really have to care about it here).

Task 3.5: Visualize the evolution of the solutions of the three problems (diffusion, wave and Schrödinger equation) by using the expansion in eingenmodes. You will precise the system of reduced units used.

Bonus tasks: If time allows, try to apply this method on a fractal boundary, for example that given in the exam in 2015:
`http://web.phys.ntnu.no/~ingves/Teaching/TFY4235/Exam/Exam_tfy4235_2015.pdf`

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 literally 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. In this subsection, we will take a constant speed such that $c > 0$. We will focus on the following schemes:

Upwind scheme:	$\frac{u_{i,n+1}-u_{i,n}}{\delta t} + c\,\frac{u_{i,n}-u_{i-1,n}}{\delta x} = 0\ ,$
Downwind scheme:	$\frac{u_{i,n+1}-u_{i,n}}{\delta t} + c\,\frac{u_{i+1,n}-u_{i,n}}{\delta x} = 0\ ,$
Explicit centered scheme:	$\frac{u_{i,n+1}-u_{i,n}}{\delta t} + c\,\frac{u_{i+1,n}-u_{i-1,n}}{2\delta x} = 0\ ,$
Implicit centered scheme:	$\frac{u_{i,n+1}-u_{i,n}}{\delta t} + c\,\frac{u_{i+1,n+1}-u_{i-1,n+1}}{2\delta x} = 0\ ,$
Lax-Friedrichs scheme:	$\frac{2u_{i,n+1}-u_{i+1,n}-u_{i-1,n}}{2\delta t} + c\,\frac{u_{i+1,n}-u_{i-1,n}}{2\delta x} = 0\ ,$
Lax-Wendroff scheme:	$\frac{u_{i,n+1}-u_{i,n}}{\delta t} + c\,\frac{u_{i+1,n}-u_{i-1,n}}{2\delta x} - \frac{c^2\delta t}{2}\,\frac{u_{i-1,n}-2u_{i,n}+u_{i+1,n}}{\delta x^2} = 0\ .$

Task 4.2: By using finite difference approximations seen in the lecture, explain how the four first schemes were obtained.

Task 4.3: Show that the Lax-Friedrichs scheme can be obtained as an average of two schemes: a scheme where $\partial u/\partial t$ is approximated by $\frac{u_{i,n+1}-u_{i+1,n}}{\delta t}$, and another one where $\partial u/\partial t$ is approximated by $\frac{u_{i,n+1}-u_{i-1,n}}{\delta t}$, and in both scheme a centered difference is used for $\partial u/\partial x$.

We derive here the Lax-Wendroff scheme for c constant in details as presented in [1]. 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

$$u(x,t+\delta t) = u(x,t) + \delta t\,\frac{\partial u}{\partial t}(x,t) + \frac{\delta t^2}{2}\,\frac{\partial^2 u}{\partial t^2}(x,t) + \mathcal{O}(\delta t^3)\,. \tag{4.4}$$

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).

$$u(x,t+\delta t) = u(x,t) - c\,\delta t\,\frac{\partial u}{\partial x}(x,t) + \frac{c^2\,\delta t^2}{2}\,\frac{\partial^2 u}{\partial x^2}(x,t) + \mathcal{O}(\delta t^3)\,. \tag{4.6}$$

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

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

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

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

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

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

Thus Eq. (4.6) becomes

$$\begin{aligned} u(x,t+\delta t) = u(x,t) &- \frac{c\,\delta t}{2\,\delta x}\,\left(u(x+\delta x,t) - u(x-\delta x,t)\right) \\ &+ \frac{c^2\,\delta t^2}{2\,\delta x^2}\,\left(u(x+\delta x,t) - 2\,u(x,t) + u(x-\delta x,t)\right) + \mathcal{O}(\delta t^3 + \delta t\,\delta x^2)\,. \end{aligned}$$

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 δt, space in step δx 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 4.4: Implement all the schemes. We will fix the domain of study to be $x \in (0, 1)$, we will use periodic boundary conditions, and you may play with different initial conditions. For each scheme, study numerically the stability, and the error between the exact and numerical solution. ($\star$) Explain your results by rigorous mathematical arguments. Suggested reading: Chapter 2 in Ref. [1].

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. 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 apparition of a shock wave for which the 'Hopf's' part of the equation is responsible.

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 4.5 - 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 4.6: 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

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

(Hint: use the conservative form.)

Task 4.7: 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 4.8**: 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 solutions, and weak entropy solutions of a PDE.
- Hyperbolic conservation laws, theory of distributions.

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.

6 Complements

6.1 What you will and will not find in these complements

These complements are intended to curious students who wish to know more about topics we have discussed in this assignment. There is material for everyone, for the ones who do not like to admit results and wonder how to *solve the diffusion equation exactly* with pen and paper, the ones who wish to read about the *method of characteristics* applied to the case of the advection equation and the Hopf equation that we have solved numerically and the ones who are not scared by mathematics and abstraction and wish to know how one can define a *generalized solution of a PDE for non-differentiable functions.* Although the first two complements are of interest if you plan to follow the course on Classical Transport Theory (TFY4275/FY8907) or simply study more about it, none of the following complements belong to the course curriculum in Computational Physics and some go far beyond it. Thus no stress if you have a look and do not get everything although the content has been written in details and at a not too abstract level.

However, it is worth mentioning that the last complement, about the notion of weak derivative and generalized solution of a PDE, which seems to be the more abstract one, that you might think as useless in practice, is actually at the core of a very powerful and successful method in Computational Physics and more generally engineering, namely the *variational approach* and the *finite element method*.

Unfortunately topics like consistency, precision, convergence and stability of finite difference schemes are not covered here. These have been sketched during the lectures or experienced by you with your simulations, or maybe in a previous course in numerical analysis if you took one. If you wish to know more about these interesting questions, which are fundamental for numerical simulations, we strongly recommend you to read chapter 2 in [1]. The book is available as an e-book with the library, and you may be able to read it online. All these notions are clearly (and rigorously) explained in a very pedagogical way by treating in great details different schemes for solving the diffusion equation that you are now familiar with. The variational approach and the finite element method are also covered in details in this book. You will recognize some ideas exposed here in the last complement if you are brave enough to read through it.

Finally, we will not expose here the resolution of the solution after the shock of the Hopf equation. We will simply sketch the rough idea. The reason for this is that this easily takes a full course on its own. We then refer to textbooks you may be interested to read. The resolution of the Hopf or inviscid Burgers equation is detailed in [2], and a course is dedicated to the topic at NTNU, (MA8103). We also give a short appetizer to the notion of weak solutions of a PDE and the theory of distribution that you can find in detail in textbooks such as [3, 4, 5] (or if you read French [6, 7]). A warning though if you plan to read [4], the text is very mathematical, so do not be fooled by its title. You may also consider following the course (Master/PhD level in Mathematics) on Distribution theory and Sobolev spaces with applications (MA8105), given at NTNU, if you feel like going deeper into the maths!

Enjoy and be brave!

6.2 Derivation of the exact solutions of the diffusion equation

In this complement we derive all the exact solutions used in the first problem of the assignment. All derivations, are adapted from the lecture notes, exercises or exam problems in the course in Classical Transport Theory (TFY4275/FY8907) given by Ingve in previous years [8].

Constant diffusivity profile and free boundary

We recall here the derivation of the solution of diffusion problem

$$\frac{\partial u}{\partial t} = D\,\frac{\partial^2 u}{\partial x^2}\,, \tag{6.1}$$

with constant diffusivity D. The initial condition is

$$\forall x \in \mathbb{R}, \qquad u(x,0) = \tilde{u}_0\,\delta(x - x_0)\,, \tag{6.2}$$

with $x_0 \in \mathbb{R}$ and the boundary conditions are

$$\forall t \in \mathbb{R}_+, \qquad \lim_{x\to\pm\infty} u(x,t) = 0\,. \tag{6.3}$$

We will use the so-called Fourier-Laplace transform technique. We recall these transforms and some useful properties[2]. For our purpose, it will be useful to define the transforms partially on each variable. We define the Fourier transform of f with respect to a spatial variable x by: $\forall k \in \mathbb{R}$,

$$\mathcal{F}_{[f]}(k,t) = \hat{f}(k,t) = \int_{-\infty}^{\infty} \mathrm{d}x\, f(x,t)\, e^{-ikx}\,, \tag{6.4}$$

and the inverse transform reads, $\forall x \in \mathbb{R}$,

$$\mathcal{F}^{-1}_{[\hat{f}]}(x,t) = f(x,t) = \frac{1}{2\pi}\int_{-\infty}^{\infty} \mathrm{d}k\, \hat{f}(k,t)\, e^{ikx}\,. \tag{6.5}$$

The reader will show by using a change of variable and integration by parts that the Fourier transform exhibits the following properties:

$$\mathcal{F}_{[f(x-x_0)]}(k,t) = e^{-ikx_0}\,\mathcal{F}_{[f]}(k,t) \tag{6.6}$$

$$\mathcal{F}_{[\partial_x f]}(k,t) = ik\,\mathcal{F}_{[f]}(k,t)\,. \tag{6.7}$$

To put these properties in words, the Fourier transform of a translated function is the Fourier transform of the non-translated function up to phase factor, and the Fourier transform of a derivative of a function is the Fourier transform of the function multiplied by ik. Furthermore, we define the Laplace transform of f, with respect to a time variable, as

$$\tilde{f}(x,s) = \mathcal{L}_{[f]}(x,s) = \int_0^{\infty} \mathrm{d}t\, f(x,t)\, e^{-st}, \qquad s \in \mathbb{C}\,. \tag{6.8}$$

We recall a useful property of the Laplace transform, that you will prove by integration by parts

$$\mathcal{L}_{[\partial_t f]}(x,s) = s\,\mathcal{L}_{[f]}(x,s) - f(x,0)\,. \tag{6.9}$$

Note the term $f(x,0)$, i.e. the *non-transformed* function evaluated at time $t = 0$. A useful inverse Laplace transform to know in our case, is

[2] at least formally. We do not wish to enter into the rigorous mathematical definitions and thus voluntarily skip the discussion on the space of functions or better, distributions, on which the transforms are defined.

$$\mathcal{L}^{-1}_{[\frac{1}{s+\alpha}]}(t) = e^{-\alpha t}\, H(t)\,, \tag{6.10}$$

for $\Re(s) > -\alpha$ and where H is the Heaviside step function. Note that α may depend on other variables, but we skipped the dependencies for clarity.

We now have all the tools we need to solve the free diffusion problem. First we take the Laplace transform of Eq. (6.1) with respect to time, which gives by using the property Eq. (6.9)

$$s\, \tilde{u}(x,s) - u(x,0) = D\, \frac{\partial^2 \tilde{u}}{\partial x^2}(x,s)\,. \tag{6.11}$$

This made the initial condition appear and thus by using Eq. (6.2) we get

$$s\, \tilde{u}(x,s) - \tilde{u}_0\, \delta(x-x_0) = D\, \frac{\partial^2 \tilde{u}}{\partial x^2}(x,s)\,. \tag{6.12}$$

Note that the $\tilde{}$ on $\tilde{u}_0$ does not correspond to any Laplace transform. It is just a scalar, the initial "mass", that we had chosen to denote this way. It is now time to take the Fourier transform with respect to space which yields

$$s\, \hat{\tilde{u}}(k,s) - \tilde{u}_0\, e^{-ikx_0} = D\,(ik)^2\, \hat{\tilde{u}}(k,s)\,. \tag{6.13}$$

Hence $\hat{\tilde{u}}(k,s)$ is solution of an algebraic equation and reads

$$\hat{\tilde{u}}(k,s) = \tilde{u}_0\, \frac{e^{-ikx_0}}{s + D\,k^2}\,. \tag{6.14}$$

Now we need to inverse transform the above expression. Note that the Laplace and Fourier transform had acted on independent variables and thus commute. By using the inverse Laplace transform given in Eq. (6.10) we obtain

$$\begin{aligned} \hat{u}(k,t) &= \tilde{u}_0\, e^{-ikx_0}\, \mathcal{L}^{-1}_{[\frac{1}{s+D\,k^2}]}(k,t) && (6.15)\\ &= \tilde{u}_0\, e^{-ikx_0 - Dk^2 t}\, H(t)\,. && (6.16) \end{aligned}$$

We take the inverse Fourier transform

$$\begin{aligned} u(x,t) &= \frac{1}{2\pi} \int_{-\infty}^{\infty} \mathrm{d}k\, \tilde{u}_0\, e^{ik(x-x_0) - Dk^2 t}\, H(t) && (6.17)\\ &= \frac{\tilde{u}_0}{\sqrt{4\pi D t}}\, \exp\left(-\frac{(x-x_0)^2}{4Dt}\right)\, H(t)\,. && (6.18) \end{aligned}$$

Here we recognized a Gaussian integral, and we leave the reader to check the last line by completing the square in the exponential and by using a change of variable. Since the solution was defined for positive time we can skip the Heaviside function and we get the announced result Eq. (2.4).

Constant diffusivity and reflective or absorbing boundaries

The diffusion problem on a bounded domain can be solved by expanding u in eigen-functions of the diffusion operator $D\frac{\partial^2}{\partial x^2}$. We note first that the family of functions

$$v_n^{\mathrm{r}}(x) = \begin{cases} \sqrt{\frac{1}{L}} & \text{for } n = 0 \\ \sqrt{\frac{2}{L}}\, \cos\left(n\pi\frac{x}{L}\right) & \text{for } n > 0 \end{cases} . \tag{6.19}$$

and

$$v_n^{\mathrm{a}}(x) = \begin{cases} 0 & \text{for } n = 0 \\ \sqrt{\frac{2}{L}}\, \sin\left(n\pi\frac{x}{L}\right) & \text{for } n > 0 \end{cases} . \tag{6.20}$$

are orthonormal families with respect to the scalar product

$$\langle f|g\rangle = \int_0^L \mathrm{d}x\, f(x)\, g(x)\,. \tag{6.21}$$

You will indeed verify that, for $n, m \in \mathbb{N}$,

$$\langle v_m^{\mathrm{r}}|v_n^{\mathrm{r}}\rangle = \delta_{n,m} \qquad \text{and,} \qquad \langle v_m^{\mathrm{a}}|v_n^{\mathrm{a}}\rangle = \delta_{n,m}\,. \tag{6.22}$$

Furthermore each function of $\{v_n^{\mathrm{r}}\}_{n\in\mathbb{N}}$ (resp. $\{v_n^{\mathrm{a}}\}_{n\in\mathbb{N}}$) satisfies by construction the reflective (resp. absorbing) boundary conditions, that is $\frac{\partial u}{\partial x} = 0$ on $\partial\Omega$ (resp. $u = 0$ on $\partial\Omega$). Moreover, we obtain by taking the second derivative of $v_n^{\mathrm{r,a}}$ that

$$D\,\frac{\partial^2 v_n^{\mathrm{r,a}}}{\partial x^2} = \lambda_n\, v_n^{\mathrm{r,a}}\,, \tag{6.23}$$

where

$$\lambda_n = -D\,\left(\frac{n\pi}{L}\right)^2\,. \tag{6.24}$$

In other words, $\{v_n^{\mathrm{r,a}}\}_{n\in\mathbb{N}}$ are eigen-functions of the diffusion operator.

Now we have all the tools we need to construct the solution of the diffusion problem on a bounded domain with either reflective or absorbing boundaries. The first step consists in expanding the solution on the set of eigen-functions:

$$u^{\mathrm{r,a}}(x,t) = \sum_{n=0}^{\infty} \alpha_n^{\mathrm{r,a}}(t|x_0, t=0)\, v_n^{\mathrm{r,a}}(x)\,. \tag{6.25}$$

The coefficients $\alpha_n^{\mathrm{r,a}}(t|x_0, t=0)$ are a priori time dependent and depend also on the initial condition, this is the reason for the notation $(t|x_0, t=0)$, i.e. time dependent and given a Dirac distribution centered at x_0 at time $t = 0$ as initial condition. We plug the expansion in the diffusion equation and obtain

$$\frac{\partial u^{\mathrm{r,a}}}{\partial t} = D\,\frac{\partial^2 u^{\mathrm{r,a}}}{\partial x^2} \tag{6.26}$$

$$\sum_{n=0}^{\infty} \frac{\mathrm{d}\alpha_n^{\mathrm{r,a}}}{\mathrm{d}t}\, v_n^{\mathrm{r,a}} = D\,\sum_{n=0}^{\infty} \alpha_n^{\mathrm{r,a}}\, \frac{\partial^2 v_n^{\mathrm{r,a}}}{\partial x^2} \tag{6.27}$$

$$\sum_{n=0}^{\infty} \frac{\mathrm{d}\alpha_n^{\mathrm{r,a}}}{\mathrm{d}t}\, v_n^{\mathrm{r,a}} = \sum_{n=0}^{\infty} \alpha_n^{\mathrm{r,a}}\, \lambda_n v_n^{\mathrm{r,a}}\,, \tag{6.28}$$

where have used last the property that $v_n^{\mathrm{r,a}}$ is an eigen-function of the diffusion operator Eq. (6.23). By taking the scalar product with $v_m^{\mathrm{r,a}}, m \in \mathbb{N}$, and using the orthonormality of the eigen-functions Eq. (6.22) we get

$$\sum_{n=0}^{\infty} \frac{\mathrm{d}\alpha_n^{\mathrm{r,a}}}{\mathrm{d}t} \langle v_n^{\mathrm{r,a}} | v_m^{\mathrm{r,a}} \rangle = \sum_{n=0}^{\infty} \alpha_n^{\mathrm{r,a}} \, \lambda_n \, \langle v_n^{\mathrm{r,a}} | v_m^{\mathrm{r,a}} \rangle \tag{6.29}$$

$$\frac{\mathrm{d}\alpha_m^{\mathrm{r,a}}}{\mathrm{d}t} = \lambda_m \, \alpha_m^{\mathrm{r,a}} \, . \tag{6.30}$$

The last equation shows that $\alpha_m^{\mathrm{r,a}}$ satisfies a first order ordinary differential equation with constant coefficient whose solution is given by

$$\alpha_m^{\mathrm{r,a}}(t|x_0, t=0) = \beta_m^{\mathrm{r,a}}(x_0) \, e^{\lambda_m t} \, , \tag{6.31}$$

with

$$\beta_m^{\mathrm{r,a}}(x_0) = \alpha_m^{\mathrm{r,a}}(0|x_0, t=0) \, . \tag{6.32}$$

Now the only unknowns left are the coefficients $\beta_m^{\mathrm{r,a}}(x_0)$ that we determine by using the initial condition, at $t = 0$ we have

$$\sum_{n=0}^{\infty} \beta_n^{\mathrm{r,a}}(x_0) \, v_n^{\mathrm{r,a}}(x) = \tilde{u}_0 \, \delta(x - x_0) \, , \tag{6.33}$$

and once more, by taking the scalar product with $v_m^{\mathrm{r,a}}, m \in \mathbb{N}$, and using the orthonormality of the eigen-functions Eq. (6.22) we get

$$\sum_{n=0}^{\infty} \beta_n^{\mathrm{r,a}}(x_0) \, \langle v_n^{\mathrm{r,a}} | v_m^{\mathrm{r,a}} \rangle = \tilde{u}_0 \, \langle \delta(x - x_0) | v_m^{\mathrm{r,a}} \rangle \tag{6.34}$$

$$\beta_m^{\mathrm{r,a}}(x_0) = \tilde{u}_0 \, v_m^{\mathrm{r,a}}(x_0) \tag{6.35}$$

where we have used the fundamental property of the Dirac distribution (and we assumed x_0 to be strictly inside Ω of course, otherwise the problem is pointless). Finally the expression of the solution reads as announced

$$u^{\mathrm{r,a}}(x,t) = \tilde{u}_0 \sum_{n=0}^{\infty} \exp\left(-\left(\frac{n\pi}{L}\right)^2 Dt \right) \, v_n^{\mathrm{r,a}}(x_0) \, v_n^{\mathrm{r,a}}(x) \, . \tag{6.36}$$

Note that when $t \to \infty$ all terms for $n > 0$ in the sum vanish due to the exponential factor (observe that $\lambda_n < 0$, see Eq. (6.24)) and only the $n = 0$ term remains which is 0 in the absorbing case and $\tilde{u}_0/L$ in the reflective case, as expected by our physical intuition.

Step diffusivity profile and free boundary

We sketch here how to derive the solution of

$$\frac{\partial u}{\partial t} = \frac{\partial}{\partial x} \left(D \, \frac{\partial u}{\partial x} \right) \, , \tag{6.37}$$

where

$$D(x) = \begin{cases} D_+ & \text{if } x \geq 0 \\ D_- & \text{if } x < 0 \end{cases} \, , \tag{6.38}$$

with $D_\pm \in \mathbb{R}_+^*$. The initial condition is[3]

$$\forall x \in \mathbb{R}, \qquad u(x,0) = \delta(x) \;, \tag{6.39}$$

and the boundary conditions are

$$\forall t \in \mathbb{R}_+, \qquad \lim_{x\to\pm\infty} u(x,t) = 0 \;. \tag{6.40}$$

The first idea one could have is to write Eq. (6.37) as

$$\frac{\partial u}{\partial t} = D' \, \frac{\partial u}{\partial x} + D \, \frac{\partial^2 u}{\partial x^2} \;, \tag{6.41}$$

but since the diffusivity is a step function, its derivative is given by the step formula

$$D'(x) = (D_+ - D_-)\delta(x) \;. \tag{6.42}$$

We will not enter into a rigorous derivation on how to handle this case using tools of distribution theory (we are physicists after all). Instead we will use physical intuition and state that the diffusivity is constant on both half line $\mathbb{R}_-^*$ and $\mathbb{R}_+^*$. Hence the diffusion equation reads

$$\frac{\partial u_\pm}{\partial t} = D_\pm \, \frac{\partial^2 u_\pm}{\partial x^2} \;, \tag{6.43}$$

respectively restricted on each half line. We then need to introduce a boundary condition at $x = 0$. This will be the continuity of the solution. The solution of the diffusion problem for a constant diffusivity hints us to look for a solution of the form

$$u_\pm(x,t) = \frac{A_\pm(t)}{\sqrt{4\pi D_\pm t}} \exp\left(-\frac{x^2}{4D_\pm t}\right) \;. \tag{6.44}$$

We recognize that it is constructed from the fundamental solution of the diffusion equation up to a time dependent amplitude factor $A_\pm$. Using the continuity of the solution at the origin one gets a relation between the amplitude factors.

$$\begin{align}
u_-(0,t) &= u_+(0,t) \tag{6.45}\\
\frac{A_-(t)}{\sqrt{4\pi D_- t}} &= \frac{A_+(t)}{\sqrt{4\pi D_+ t}} \tag{6.46}\\
A_-(t) &= A_+(t)\sqrt{\frac{D_-}{D_+}} \;. \tag{6.47}
\end{align}$$

To fully determine the solution, one need to solve for A_+ (or equivalently A_-) by using the normalization condition.

$$\begin{align}
1 &= \int_{-\infty}^{\infty} \mathrm{d}x \, u(x,t) \tag{6.48}\\
&= \int_{-\infty}^{0} \mathrm{d}x \, u_-(x,t) + \int_{0}^{\infty} \mathrm{d}x \, u_+(x,t) \tag{6.49}\\
&= \frac{A_-(t)}{\sqrt{4\pi D_- t}} \int_{-\infty}^{0} \mathrm{d}x \, e^{-\frac{x^2}{4D_- t}} + \frac{A_+(t)}{\sqrt{4\pi D_+ t}} \int_{0}^{\infty} \mathrm{d}x \, e^{-\frac{x^2}{4D_+ t}} \tag{6.50}
\end{align}$$

[3]The mass $\tilde{u}_0$ as been set to 1 for simplicity. This is equivalent to the change of variable $w = \frac{u}{\tilde{u}_0}$, i.e. a normalized density, but we will keep the same notations for clarity.

using a change of variable $y = \frac{x}{\sqrt{4D_\pm t}}$ one gets

$$1 = \frac{A_-(t)}{\sqrt{\pi}} \int_{-\infty}^{0} \mathrm{d}y \, e^{-y^2} + \frac{A_+(t)}{\sqrt{\pi}} \int_{0}^{\infty} \mathrm{d}y \, e^{-y^2} \tag{6.51}$$

$$= \frac{A_-(t)}{2} + \frac{A_+(t)}{2} \tag{6.52}$$

using Eq. (6.47) and solving for A_+ gives

$$A_+(t) = 2 \left[1 + \sqrt{\frac{D_-}{D_+}} \right]^{-1} \tag{6.53}$$

6.3 The method of characteristics

The advection equation

We refresh here the method of characteristics in the simple case of the advection equation with constant velocity field. We follow closely [6] to prove the following

Theorem

Let $u \in \mathcal{C}^1(\mathbb{R} \times \mathbb{R}_+)$ be a solution of the advection equation, i.e. that satisfies for all $t > 0$ and $x \in \mathbb{R}$,

$$\frac{\partial u}{\partial t}(x,t) + c \, \frac{\partial u}{\partial x}(x,t) = 0 \, , \tag{6.54}$$

with the initial condition,

$$u(x,0) = u^{\mathrm{in}}(x), \qquad \forall x \in \mathbb{R} \, . \tag{6.55}$$

Here $u^{\mathrm{in}} \in \mathcal{C}^1(\mathbb{R})$. The above problem admits a unique solution and we have an explicit formula for it which reads

$$u(x,t) = u^{\mathrm{in}}(x - c\,t) \, . \tag{6.56}$$

Proof

The proof consists in showing a necessary and sufficient condition. We will need to introduce the following $\mathcal{C}^1$ mapping

$$\gamma_y : \left\{ \begin{array}{ccc} \mathbb{R} & \to & \mathbb{R} \\ t & \mapsto & y + c\,t \end{array} \right. , \tag{6.57}$$

where $y \in \mathbb{R}$. The set $\{(t, \gamma_y(t)) | t \in \mathbb{R}\}$ is a line in $\mathbb{R} \times \mathbb{R}$ and is called characteristic curve, or simply characteristic, of the advection equation initiated at y. Note that the definition of γ_y has been chosen to fit the advection equation as it will become clear later. For another 1^{st} order PDE, γ_y would be different and the characteristics would not in general be lines.

Necessary condition for $u \in \mathcal{C}^1(\mathbb{R} \times \mathbb{R}_+)$ to be solution.

Let $u \in \mathcal{C}^1(\mathbb{R} \times \mathbb{R}_+)$ be a solution. Consider $y \in \mathbb{R}$, and $U_y \in \mathcal{C}^1(\mathbb{R}_+)$ defined for $t > 0$ by

$$U_y(t) = u(\gamma_y(t), t) \, . \tag{6.58}$$

The derivative of U_y reads

$$
\begin{aligned}
\frac{\mathrm{d}U_y}{\mathrm{d}t}(t) &= \frac{\partial u}{\partial t}(\gamma_y(t),t) + \frac{\mathrm{d}\gamma}{\mathrm{d}t}(t) \cdot \frac{\partial u}{\partial x}(\gamma_y(t),t) && (6.59)\\
&= \frac{\partial u}{\partial t}(\gamma_y(t),t) + c \cdot \frac{\partial u}{\partial x}(\gamma_y(t),t) && (6.60)\\
&= 0\,, && (6.61)
\end{aligned}
$$

since u is solution of the advection equation. Thus U_y is constant, i.e. u is constant along characteristics, i.e. for $t > 0$, $y \in \mathbb{R}$:

$$
u(y + c\,t, t) = U_y(t) = U_y(0) = u(y,0) = u^{\mathrm{in}}(y)\,. \tag{6.62}
$$

Now the change of variable $y + c\,t = x$ yields

$$
u(x,t) = u^{\mathrm{in}}(x - c\,t)\,. \tag{6.63}
$$

We have shown, that all solutions of the above advection problem is given by Eq. (6.87), and there exists thus *at most one solution.*

Sufficient condition.

We verify easily that u defined by Eq (6.87) is in $\mathcal{C}^1(\mathbb{R}\times\mathbb{R}_+)$ and satisfies the advection equation by plugging it in. There exist thus *at least one solution.*

Theorem proved. The important technique to remember from this proof is the introduction of the characteristic curves and to show that a solution is constant along these curves. We use below the same method on the Hopf equation to find a condition for the apparition of a shock in finite time as well as the time T at which the singularity arises.

The Hopf equation

Similarly to what we have done in the case of the advection equation, we introduce the function γ_y, $y \in \mathbb{R}$, defined by the implicit Cauchy problem

$$
\begin{aligned}
\gamma_y(0) &= y\,, && (6.64)\\
\gamma_y'(t) &= u(\gamma_y(t),t)\,, && (6.65)
\end{aligned}
$$

where u is a solution of the Hopf equation that we assume[4] to be $\mathcal{C}^2$. The function γ_y is, of course, constructed such that

$$
\begin{aligned}
\gamma_y''(t) &= \frac{\mathrm{d}}{\mathrm{d}t}u(\gamma_y(t),t) && (6.66)\\
&= \frac{\partial u}{\partial t}(\gamma_y(t),t) + \gamma_y'(t) \cdot \frac{\partial u}{\partial x}(\gamma_y(t),t) && (6.67)\\
&= \frac{\partial u}{\partial t}(\gamma_y(t),t) + u(\gamma_y(t),t) \cdot \frac{\partial u}{\partial x}(\gamma_y(t),t) && (6.68)\\
&= 0\,. && (6.69)
\end{aligned}
$$

Here we have used the chain rule for derivatives, Eq. (6.65), and the fact that u is a solution of the Hopf equation. Thus we observe that γ_y' is constant which means that u is constant along the characteristics $\{(\gamma_y(y),t)|t>0\}$, which in this case too are lines. Indeed we have

[4] this assumption will simplify the proof by allowing us to use Schwarz theorem to switch partial derivatives

$$u(\gamma_y(y),t) = \gamma_y'(t) = \gamma_y'(0) = u^{\mathrm{in}}(y)\,, \tag{6.70}$$

and by integration

$$\gamma_y(t) = y + u^{\mathrm{in}}(y)\,t\,. \tag{6.71}$$

Before going on with the condition for the apparition of shock, let us make a few remarks.

- Although the characteristics are lines as for the advection equation, the slopes $u^{\mathrm{in}}(y)$ of the characteristics are a priori different depending on the initial point y. Thus, depending on the initial condition, characteristics may intersect leading to a finite time at which it is not possible to recover the initial condition starting from the intersection point and going back in time.
- A solution of the Hopf equation, within the time $t < T$ where a unique solution is ensured, i.e. before characteristics intersect, cannot be expressed explicitly as we did for the advection equation. Indeed, we obtain an implicit equation which reads

  $$u(y + u^{\mathrm{in}}(y)\,t, t) = u^{\mathrm{in}}(y), \qquad t < T\,, \tag{6.72}$$

  and by change of variable $x = y + u^{\mathrm{in}}(y)\,t$ we get

  $$u(x,t) = u^{\mathrm{in}}(y(x,t))\,. \tag{6.73}$$

Let us now determine a condition of the apparition of a shock in finite time and compute this time. We define

$$w_\gamma(t) = \frac{\partial u}{\partial x}(\gamma_y(t),t)\,. \tag{6.74}$$

We analyze the derivative of w_γ

$$\begin{aligned}
w_\gamma'(t) &= \frac{\partial}{\partial t}\left[\frac{\partial u}{\partial x}\right](\gamma_y(t),t) + \gamma_y'(t)\cdot\frac{\partial^2 u}{\partial x^2}(\gamma_y(t),t) && (6.75)\\
&= \frac{\partial}{\partial x}\left[\frac{\partial u}{\partial t}\right](\gamma_y(t),t) + u(\gamma_y(t),t)\cdot\frac{\partial^2 u}{\partial x^2}(\gamma_y(t),t) && (6.76)\\
&= \frac{\partial}{\partial x}\left[-u\cdot\frac{\partial u}{\partial x}\right](\gamma_y(t),t) + u(\gamma_y(t),t)\cdot\frac{\partial^2 u}{\partial x^2}(\gamma_y(t),t) && (6.77)\\
&= -\left(\frac{\partial u}{\partial x}(\gamma_y(t),t)\right)^2 && (6.78)\\
&= -w_\gamma^2(t)\,. && (6.79)
\end{aligned}$$

Note here that we have used Schwarz theorem to switch the order of the derivatives in the second line. We used the fact that u is solution of the Hopf equation, simplified terms and recognize the square of w_γ. Thus w_γ satisfies a 1^{st} order non-linear ODE, that you may recognize as the Riccati equation:

$$w_\gamma' = -w_\gamma^2\,. \tag{6.80}$$

The Riccati equation is separable and can be solved in a straightforward way noticing that

$$1 = -\frac{w_\gamma'}{w_\gamma^2} = \frac{\mathrm{d}}{\mathrm{d}t}\left[\frac{1}{w_\gamma}\right]\,, \tag{6.81}$$

which gives by integration between 0 and t

$$t = \frac{1}{w_\gamma(t)} - \frac{1}{w_\gamma(0)}\,, \tag{6.82}$$

hence

$$w_\gamma(t) = \frac{w_\gamma(0)}{1 + w_\gamma(0)\,t}\,. \tag{6.83}$$

And now what? Well, we see that the solution w_γ is well behaved for all time if and only if $w_\gamma(0) \geq 0$. For $w_\gamma(0) < 0$ the solution will blow up a $t = -\frac{1}{w_\gamma(0)}$. Now recall the definition of w_γ, Eq. (6.74), as the spatial derivative of a solution of the Hopf equation along a characteristic issued from y. It thus means that $w_\gamma(0) = \frac{\partial u}{\partial x}(\gamma_y(0), 0) = (u^{\mathrm{in}})'(y)$ is *the slope of the initial profile at point y*. Conclusion:

A shock will appear in a finite if there exists a point with negative slope on the initial profile, i.e. if the profile is not monotonically increasing. In that case, the time T after which the solution of the Hopf equation is not defined in the regular sense is given by

$$T = \frac{1}{\sup_{x\in\mathbb{R}}\left[\max(0, -(u^{\mathrm{in}})'(x))\right]}\,. \tag{6.84}$$

6.4 A few words on generalized solutions of a PDE and invitation to the theory of distributions

In this complement, we introduce the notion of generalized solution of a PDE by considering the example of the advection equation. We will see how we can define a solution of PDE which does not have to be differentiable, which at first seems contradictory. Finally, we will introduce the notion of distributions (in the mathematical sense), which are very convenient mathematical objects for the studies of PDE. As a bonus, you will finally understand the "true nature" of the Dirac δ "function".

We follow quite closely the introduction given in [6].

Introduction to generalized solutions of a PDE via the example of the advection equation

We gently start by considering the advection equation again, now that we can solve it explicitly by using the method of characteristics, let us make use of this knowledge. Let $u \in \mathcal{C}^1(\mathbb{R}\times\mathbb{R}_+)$ be a solution (in the usual sense) of the advection equation, i.e. that basically u is differentiable and satisfies for all $t > 0$ and $x \in \mathbb{R}$,

$$\frac{\partial u}{\partial t}\,(x,t) + c\,\frac{\partial u}{\partial x}\,(x,t) = 0\,, \tag{6.85}$$

with the initial condition,

$$u(x,0) = u^{\mathrm{in}}(x), \qquad \forall x \in \mathbb{R}\,. \tag{6.86}$$

We have shown previously that if $u^{\mathrm{in}} \in \mathcal{C}^1(\mathbb{R})$, the above problem admits a unique solution and we have an explicit formula for it which reads

$$u(x,t) = u^{\mathrm{in}}(x - c\,t)\,. \tag{6.87}$$

The interpretation of this result was that the initial profile is translate of $c\,t$. We have seen too, when we sudied the Hopf's equation, that shock may arise for some PDEs. We felt the need to be able to define a solution which may not be differentiable. We can ask ourselves a similar question in the simple case of advection equation. Can we define a solution in some sense even if the initial profile is not differentiable? Since we have an explicit formula which gives a straightforward interpretation of the "effect" of the equation on the initial profile, we could still define Eq. (6.87) even for u^{in} non-differentiable, or even non-continuous. We will see now in which sense we can do that.

We start by considering a regular solution of the advection equation, $u \in \mathcal{C}^1(\mathbb{R} \times \mathbb{R}_+)$, the assertion u is solution of Eq. (6.85) is equivalent to u satisfies

$$\int_{\mathbb{R}} \int_{\mathbb{R}_+} \left(\frac{\partial u}{\partial t}(x,t) + c\,\frac{\partial u}{\partial x}(x,t) \right) \phi(x,t)\,\mathrm{d}t\,\mathrm{d}x = 0\,, \qquad \forall \phi \in \mathcal{C}_c^\infty(\mathbb{R} \times \mathbb{R}_+). \tag{6.88}$$

That Eq. (6.85) implies Eq. (6.88) is trivial, but the reciprocal implication lies on the fact that Eq. (6.88) must be satisfied *for all* functions ϕ taken in the space of infinitely differentiable function with compact support $\mathcal{C}_c^\infty(\mathbb{R})$. We recall that the support of a function ϕ is the closure of the set of elements for which ϕ is non zero, i.e. in our 1D case for functions from $\mathbb{R}$ to $\mathbb{R}$, $\mathrm{supp}(\phi) = \overline{\{x \in \mathbb{R} | \phi(x) \neq 0\}}$. So basically, what you should keep from this is that the functions $\phi \in \mathcal{C}_c^\infty(\mathbb{R})$ are "infinitely smooth" and vanish exactly as well as all their derivatives outside a segment $[a,b], a < b$ (segment which of course depends on ϕ).

By using Fubini's theorem we have

$$0 = \int_{\mathbb{R}} \int_{\mathbb{R}_+} \left(\frac{\partial u}{\partial t}(x,t) + c\,\frac{\partial u}{\partial x}(x,t) \right) \phi(x,t)\,\mathrm{d}t\,\mathrm{d}x \tag{6.89}$$

$$= \int_{\mathbb{R}} \int_{\mathbb{R}_+} \frac{\partial u}{\partial t}(x,t)\phi(x,t)\,\mathrm{d}t\,\mathrm{d}x + \int_{\mathbb{R}_+} \int_{\mathbb{R}} c\,\frac{\partial u}{\partial x}(x,t)\,\phi(x,t)\,\mathrm{d}x\,\mathrm{d}t\,. \tag{6.90}$$

By integrating by parts we can express

$$\int_{\mathbb{R}_+} \frac{\partial u}{\partial t}(x,t)\phi(x,t)\,\mathrm{d}t = \left[u(x,t)\,\phi(x,t)\right]_0^\infty - \int_{\mathbb{R}_+} u(x,t)\,\frac{\partial \phi}{\partial t}(x,t)\,\mathrm{d}t \tag{6.91}$$

$$= -\int_{\mathbb{R}_+} u(x,t)\,\frac{\partial \phi}{\partial t}(x,t)\,\mathrm{d}t\,. \tag{6.92}$$

Where the first term in the integration by parts vanishes since ϕ has compact support inside $\mathbb{R} \times \mathbb{R}_+^*$. Similarly

$$\int_{\mathbb{R}} c\,\frac{\partial u}{\partial x}(x,t)\,\phi(x,t)\,\mathrm{d}x = \left[c\,u(x,t)\,\phi(x,t)\right]_{-\infty}^\infty - \int_{\mathbb{R}_+} u(x,t)\,c\,\frac{\partial \phi}{\partial x}(x,t)\,\mathrm{d}x \tag{6.93}$$

$$= -\int_{\mathbb{R}_+} u(x,t)\,c\,\frac{\partial \phi}{\partial x}(x,t)\,\mathrm{d}x\,. \tag{6.94}$$

Plugging these back into Eq. (6.90) and regrouping the terms, we obtain

$$0 = \int_{\mathbb{R}} \int_{\mathbb{R}_+} \left(\frac{\partial u}{\partial t} + c\,\frac{\partial u}{\partial x} \right) \phi\,\mathrm{d}t\,\mathrm{d}x = -\int_{\mathbb{R}} \int_{\mathbb{R}_+} u \left(\frac{\partial \phi}{\partial t} + c\,\frac{\partial \phi}{\partial x} \right) \mathrm{d}t\,\mathrm{d}x \tag{6.95}$$

Therefore, the assertion $u \in \mathcal{C}^1(\mathbb{R} \times \mathbb{R}_+)$ is solution of Eq. (6.85) is also equivalent to u satisfies

$$\int_{\mathbb{R}}\int_{\mathbb{R}_+} u\, \left(\frac{\partial\phi}{\partial t} + c\,\frac{\partial\phi}{\partial x}\right)\,\mathrm{d}t\,\mathrm{d}x = 0\,, \qquad \forall\phi\in\mathcal{C}_c^\infty(\mathbb{R}_+\times\mathbb{R}). \tag{6.96}$$

And now what? Well, we notice that this last formulation does not make any use of the partial derivatives of u anymore. All derivatives have been switched from u to ϕ thanks to integration by parts. This is called the weak formulation of the PDE and is at the heart of the notion of weak derivatives and generalized solution of a PDE. Indeed, we can now define a generalized solution of the advection equation as a function u, which do not need to be differentiable, not even continuous, but satisfies Eq. (6.96) *for all* test functions $\phi\in\mathcal{C}_c^\infty(\mathbb{R}\times\mathbb{R}_+)$. This method can be generalized easily to any linear PDE, by using successive integration by parts.

Invitation to the theory of distributions[5]

The ideas of weak derivatives and generalized solutions of PDEs are mainly due to two mathematicians (among others), Jean Leray (1934) and the Serguei Sobolev (1936). The questions Leray and Sobolev wanted to answer were precisely the kind of questions we introduced here, namely on the regularity of solutions of PDEs and extension of regular solutions to non-regular ones in some sense. It is about 15 years later, that Laurent Schwartz developed the theory of distributions for which he was awarded the Fields Medal. Distribution theory sets a natural framework for the study of PDEs, although one can argue that one can avoid it in practice and use some nice functional spaces that give more constructive methods. This theory also gives a rigorous definition of strange but powerful formal objects used by physicists, like the Dirac δ-function.

Now enough History and let us define distributions. For simplicity we will work with functions from $\mathbb{R}\to\mathbb{R}$. First, we make a key observation. Consider a locally integrable function, $f\in L^1_{\mathrm{loc}}(\mathbb{R})$. We observe that the following integral

$$\int_{\mathbb{R}} f(x)\,\phi(x)\,\mathrm{d}x \tag{6.97}$$

is well defined for any test-function $\phi\in\mathcal{C}_c^\infty(\mathbb{R})$ and is linear in ϕ. This hint us to introduce the following linear form, or functional, T_f defined as

$$T_f : \begin{cases} \mathcal{C}_c^\infty(\mathbb{R}) & \to \quad \mathbb{R} \\ \phi & \mapsto \quad \int_{\mathbb{R}} f(x)\,\phi(x)\,\mathrm{d}x \end{cases}. \tag{6.98}$$

So to vulgarize a bit if you don't remember what is a functionals, T_f a mathematical "machine" that takes in a test function and gives out a number. We will denote the action of T_f on ϕ by the following bracket notation

$$\langle T_f,\phi\rangle = \int_{\mathbb{R}} f(x)\,\phi(x)\,\mathrm{d}x\,. \tag{6.99}$$

This of course recall the inner product in L^2. The linear functional T_f can also be shown to be continuous, and defines what is called a *regular distribution*. Now based on this idea, we give the general definition of a distribution.

Definition: *A distribution T is a linear continuous functional on the space of test-functions $\mathcal{C}_c^\infty(\mathbb{R})$.*

[5] An invitation only. We will give the fundamental ideas, rigorously, but without entering into too much details. We do not want to make a course on distribution theory here, but rather give an appetizer.

We have seen that any locally integrable function f defines a distribution, denoted T_f, but these are not the only ones. There are distributions which cannot be constructed from any functions, the most striking example being the Dirac mass at a point x_0, δ_{x_0} defined as

$$\langle \delta_{x_0}, \phi \rangle = \phi(x_0), \qquad \forall \phi \in \mathcal{C}_c^\infty(\mathbb{R}) \, . \tag{6.100}$$

In this framework the Dirac mass is straightforward to define and we now see the link with the formal notation used by physicists by analogy with regular distributions Eq. (6.99), we can "imagine" (although we can show it does not exist) a kind of function δ such that

$$\int_{\mathbb{R}} \delta(x - x_0)\, \phi(x)\, \mathrm{d}x = \phi(x_0) \, . \tag{6.101}$$

Thus although physicists manipulate the Dirac mass as a function, because it is practical, we have to keep in mind that mathematically, the Dirac mass is a distribution, i.e. a linear continuous functional, and that talking about the value of a distribution at a point has no meaning, since it acts on a test-function.

Derivatives

We now come to the last paragraph we will write about distributions in this complement, and not the least. Indeed, we will see now why are distributions so convenient to work with for PDEs. It is simply due to the fact that distributions are infinitely differentiable, in the sense that we now give.

We start again to play with a regular distribution T_f associated to a differentiable function f. Assuming the derivative f' in L^1_{loc}, f' also defines a distribution $T_{f'}$ whose action on a test-function reads

$$\langle T_{f'}, \phi \rangle = \int_{\mathbb{R}} f'(x)\, \phi(x)\, \mathrm{d}x \, . \tag{6.102}$$

By integration by part one gets

$$\begin{aligned}
\langle T_{f'}, \phi \rangle &= [f\,\phi]_{-\infty}^{\infty} - \int_{\mathbb{R}} f(x)\, \phi'(x)\, \mathrm{d}x && (6.103)\\
&= -\int_{\mathbb{R}} f(x)\, \phi'(x)\, \mathrm{d}x && (6.104)\\
&= -\langle T_f, \phi' \rangle \, . && (6.105)
\end{aligned}$$

Here we used the fact that ϕ has a bounded support, thus the integrated term vanishes. We then use the last equation has the definition of the derivative for any distribution (and by construction it will correspond to the usual derivative on differentiable functions by integration by part). The derivative of distribution T is defined by

$$\langle T', \phi \rangle = -\langle T, \phi' \rangle \, , \qquad \forall \phi \in \mathcal{C}_c^\infty(\mathbb{R}) \, , \tag{6.106}$$

and we can verify that the functional defined above is still a distribution. Notice thus that distributions are infinitely differentiable. We now understand clearly the point of starting with infinitely smooth test-functions on compact supports and defining the space of distribution by a duality argument.

6.5 After the shock ?

As promised, a very few words on how to treat the Hopf problem after the shock. One idea is to realize that the Hopf equation has a conservative form and use argument such as the Rankine-Hugoniot to find the velocity of the shock front as averages of velocities upstream and downstream from the shock. One can show that this can be viewed as simple application of the step, or jump formula for derivation of regular distributions associated to discontinuous functions.

Another approach, more thorough, consists in introducing a viscosity (or diffusive) term in the Hopf equation and we obtain the so-called Burgers' equation

$$\frac{\partial u}{\partial t} + u\,\frac{\partial u}{\partial x} = \frac{\epsilon}{2}\,\frac{\partial^2 u}{\partial x^2}\,. \tag{6.107}$$

Here $\epsilon > 0$. If we hide the $u\,\frac{\partial u}{\partial x}$ term, we recognize the diffusion equation we have studied previously and which has the nice property of smearing irregularities. Remember that starting with a δ distribution, the diffusion equation had the effect of smoothing it instantly. The idea here that the diffusive term will prevent for shock to appear by smearing out the profile u if it tends to become too sharp.

The idea now is to solve Eq. (6.107), and show that in the limit $\epsilon \to 0$, the solution we obtain u_ϵ converges to a generalized solution of the Hopf equation in the sense of weak entropy solution [2, 6].

Physicists will argue that in real life we always have some viscosity anyway ...

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