PDEs and Numerical Methods

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Intro and Basics

1.1 Class notes

Chapter 1

Some basic notions about PDEs

1.1 ODEs and PDEs

Definition 1.1. A **differential equation** is a relationship involving a function u and (some of) its derivatives. It is called an **ordinary differential equation (ODE)** if u depends on one single variable, or a **partial differential equation (PDE)** if u depends on several variables.

Examples

- $-u''(x) + x^2\, u'(x) - x\, u(x) = \sin x$ *is an ODE.*
- $\dfrac{\partial^2 u}{\partial x^2}(x,y,z) + \dfrac{\partial u}{\partial y}(x,y,z)\dfrac{\partial u}{\partial z}(x,y,z) = 0$ *is a PDE.*

1.2 Usual partial differential operators

Definition 1.2. Let $u : \Omega \subset \mathbb{R}^n \to \mathbb{R}$. The **directional (or Gâteaux) derivative** of u at point $\mathbf{x} \in \Omega$ in direction $\mathbf{d} \in \mathbb{R}^n$ is

$$\frac{\partial u}{\partial \mathbf{d}}(\mathbf{x}) = \lim_{\alpha \to 0} \frac{u(\mathbf{x} + \alpha \mathbf{d}) - u(\mathbf{x})}{\alpha}$$

Examples

- *A partial derivative is a directional derivative in a direction belonging to the canonical basis.*
- *Let* $u(x,y) = x^2 - 2xy + y$ *and* $\mathbf{d} = (1,2)$. *The directional derivative of* u *in direction* $\mathbf{d}$ *is*

$$\frac{\partial u}{\partial \mathbf{d}}(\mathbf{x}) = -2x - 2y + 2$$

Definition 1.3. Let $u : \Omega \subset \mathbb{R}^n \to \mathbb{R}$. The **gradient** of u at point $\mathbf{x}$ is

$$\text{grad } u(\mathbf{x}) = \nabla u(\mathbf{x}) = \begin{pmatrix} \dfrac{\partial u}{\partial x_1}(\mathbf{x}) \\ \vdots \\ \dfrac{\partial u}{\partial x_n}(\mathbf{x}) \end{pmatrix}$$

Theorem 1.1. An important relation: $\dfrac{\partial u}{\partial \mathbf{d}}(\mathbf{x}) = \nabla u(\mathbf{x}).\ \mathbf{d}$

Definition 1.4. Let $\mathbf{u} : \Omega \subset \mathbb{R}^n \to \mathbb{R}^n$ denoted by $\mathbf{u}(\mathbf{x}) = \begin{pmatrix} u_1(x_1, \dots, x_n) \\ \vdots \\ u_n(x_1, \dots, x_n) \end{pmatrix}$.

The **divergence** of $\mathbf{u}$ is: $\text{div}\, \mathbf{u} = \displaystyle\sum_{i=1}^{n} \frac{\partial u_i}{\partial x_i}$. It can also be denoted formally by $\nabla.\mathbf{u}$

Definition 1.5. Let $\mathbf{u} : \Omega \subset \mathbb{R}^3 \to \mathbb{R}^3$. The **curl** of $\mathbf{u}$ is defined by:

$$\text{curl}\, \mathbf{u} = \begin{pmatrix} \dfrac{\partial u_3}{\partial x_2} - \dfrac{\partial u_2}{\partial x_3} \\ \dfrac{\partial u_1}{\partial x_3} - \dfrac{\partial u_3}{\partial x_1} \\ \dfrac{\partial u_2}{\partial x_1} - \dfrac{\partial u_1}{\partial x_2} \end{pmatrix}$$

It can also be denoted formally by $\nabla \wedge \mathbf{u}$.

Definition 1.6. Let $u : \Omega \subset \mathbb{R}^n \to \mathbb{R}$. The **Laplacian** of u is defined by $\Delta u = \displaystyle\sum_{i=1}^{n} \frac{\partial^2 u}{\partial x_i^2}$

It can also be defined for $\mathbf{u} : \Omega \subset \mathbb{R}^n \to \mathbb{R}^n$ by $\Delta \mathbf{u} = \begin{pmatrix} \Delta u_1 \\ \vdots \\ \Delta u_n \end{pmatrix}$

Δu is sometimes denoted by $\nabla^2 u$.

1.3 Green formulas

Let Ω an open bounded subset of $\mathbb{R}^n$, with a piecewise smooth boundary $\partial\Omega$. The external normal vector to $\partial\Omega$ is denoted by $\mathbf{n}$. So called **Green formulas**[1] are actually particular cases

[1] e.g. Gauss (or Ostrogradsky, or divergence) theorem, Stokes theorem, Green-Riemann theorem...

of integration by parts.

The basic Green formula reads:

$$\int_\Omega \frac{\partial u}{\partial x_k}\, v \, d\mathbf{x} = -\int_\Omega u\, \frac{\partial v}{\partial x_k}\, d\mathbf{x} + \int_{\partial\Omega} u\, v\, (\mathbf{e}_k.\mathbf{n})\, d\mathbf{s}$$

where $\mathbf{e}_k$ is the unit vector in direction x_k, and where u and v are continuously differentiable functions on $\overline{\Omega}$.

All other formulas derive from it, like for instance:

$$\int_\Omega \Delta u\, v\, d\mathbf{x} = -\int_\Omega \nabla u\,.\nabla v\, d\mathbf{x} + \int_{\partial\Omega} \frac{\partial u}{\partial \mathbf{n}}\, v\, d\mathbf{s}$$

$$\int_\Omega u\, \mathrm{div}\,\mathbf{E}\, d\mathbf{x} = -\int_\Omega \nabla u.\mathbf{E}\, d\mathbf{x} + \int_{\partial\Omega} u\, (\mathbf{E}.\mathbf{n})\, d\mathbf{s}$$

1.4 Some definitions related to PDEs

Definition 1.7. Like for ODEs, the **order** of a PDE is the highest degree of derivation that appears in the PDE.

Definition 1.8. Like for ODEs, a PDE is **linear** iff the relation is linear w.r.t. u and its partial derivatives. The PDE is said to be **non linear** otherwise.

Definition 1.9. Like for ODEs, a PDE is **quasi linear** if each nonlinear term is actually a n^{th} derivative multiplied by a coefficient which depends only on $\mathbf{x}$, u and its derivatives up to order $n-1$.

Examples

- *The inviscid Burgers equation* $\dfrac{\partial u}{\partial t} + u\,\dfrac{\partial u}{\partial x} = f$ *is a non linear first order PDE. It is actually a quasi linear PDE.*
- *The transport-diffusion equation* $\dfrac{\partial u}{\partial t} + \mathbf{c}\,.\nabla u - \nu\,\Delta u = f$ *is a linear second order PDE.*

Definition 1.10. A PDE that involves the time variable is a **time-dependent** (or evolution) equation. Otherwise it is a **steady-state** (or time-independent, or stationary) equation.

Definition 1.11. PDEs are generally complemented with **boundary conditions (BCs)**, prescribed on the limits of the domain, and with an **initial condition** (generally the value of the solution at the initial time) if the PDE is time-dependent.

Some usual boundary conditions are:

Dirichlet $\quad u = g \quad \text{on } \partial\Omega$

Neumann $\quad \dfrac{\partial u}{\partial \mathbf{n}} = g \quad \text{on } \partial\Omega$

Robin (or Fourier) $\quad \dfrac{\partial u}{\partial \mathbf{n}} + r\,u = g \quad \text{on } \partial\Omega$

Mixed Dirichlet-Neumann $\quad \begin{cases} u = g \text{ on } \Gamma_0 \\ \dfrac{\partial u}{\partial \mathbf{n}} = h \text{ on } \Gamma_1 \end{cases} \quad$ where $\Gamma_0 \cup \Gamma_1 = \partial\Omega$ and $\Gamma_0 \cap \Gamma_1 = \emptyset$

Definition 1.12. A steady-state PDE with boundary conditions is also called a **boundary value problem**.
A time-dependent PDE with initial conditions is also called an **initial value problem**, or a **Cauchy problem**.

Definition 1.13. A problem (PDE + initial and/or boundary conditions) is **well-posed** (in the sense of Hadamard) iff it has a unique solution, that continuously depends on the "parameters" of the problem (shape of the domain, coefficients in the equation, initial and/or boundary conditions...). Otherwise the problem is said to be **ill-posed**.

This continuous dependence is a crucial property for numerical simulation, since numerical solutions result from perturbations of the original problem. It is thus a necessary condition for numerical solutions to hopefully be correct approximations of the true solution.

1.5 Classification of PDEs

Many PDEs can roughly be classified into three main categories, which can generally be loosely described as follows:

- **elliptic**: time-independent, describing smooth equilibrium states
- **parabolic**: time-dependent and diffusive
- **hyperbolic**: time-dependent and wave-like, with finite speed of propagation

This classification can be made mathematically precise in particular for second order linear PDEs. Let consider such a PDE on $\Omega \subset \mathbb{R}^n$:

$$\sum_{i=1}^{n}\sum_{j=1}^{n} a_{ij}(\mathbf{x})\frac{\partial^2 u}{\partial x_i \partial x_j} + \sum_{i=1}^{n} b_i(\mathbf{x})\frac{\partial u}{\partial x_i} + c(\mathbf{x})u = f \qquad (E)$$

The quadratic form corresponding to its second order part is

$$Q_{\mathbf{x}}(X_1, \dots, X_n) = \sum_{i=1}^{n} \sum_{j=1}^{n} a_{ij}(\mathbf{x}) X_i X_j$$

(E) is said to be:

elliptic at point $\mathbf{x}$ iff $Q_{\mathbf{x}}$ is definite (positive or negative)

parabolic at point $\mathbf{x}$ iff $Q_{\mathbf{x}}$ is positive or negative, but not definite

hyperbolic at point $\mathbf{x}$ iff $Q_{\mathbf{x}}$ is neither definite, nor positive or negative

Examples

- *The wave equation* $\dfrac{\partial^2 u}{\partial t^2} - c^2 \Delta u = 0$ *is a hyperbolic equation.*
- *The Laplace equation* $\Delta u = 0$ *is an elliptic equation.*
- *The diffusion equation* $\dfrac{\partial u}{\partial t} - \nu \Delta u = 0$ *is a parabolic equation.*
- *The equation* $x \dfrac{\partial^2 u}{\partial x^2} + y \dfrac{\partial^2 u}{\partial y^2} = 0$ *is elliptic for* $xy > 0$, *parabolic for* $xy = 0$, *and hyperbolic for* $xy < 0$.
- *The Schrödinger equation* $\dfrac{\partial u}{\partial t} - i\nu \Delta u = 0$ *does not fall in the preceding classes, due to its non real coefficient.*

We will study typical equations of each of these three categories in the following chapters.

1.6 Fourier analysis of PDEs

As will be seen in the following chapters, Fourier analysis is a powerful tool for studying PDEs and their approximations (see Appendix A for some reminders on Fourier series and Fourier transforms).

The basic idea is that a linear homogeneous (i.e. with a null right-hand side) PDE with constant coefficients has **plane-wave solutions** of the form $u(\mathbf{x}, t) = e^{i(\mathbf{k}.\mathbf{x} + \omega t)}$, $\mathbf{k} \in \mathbb{R}^n, \omega \in \mathbb{C}$ (or $u(\mathbf{x}) = e^{i\mathbf{k}.\mathbf{x}}$ if it is a steady-state equation). Another point of view, for time-dependent PDEs, consists in observing that if an initial data $u_0(\mathbf{x}) = e^{i\mathbf{k}.\mathbf{x}}$ is supplied to such an equation, then it has a solution $u(\mathbf{x}, t) = e^{i\omega t} u_0(\mathbf{x})$ (where ω depends on $\mathbf{k}$), i.e. the initial condition multiplied by an oscillatory factor. Characterizing $\mathbf{k}$ and ω provides information on the equation.

1.2 Techniques : Change of Variables

1.2.1 Change of Variables for ODE's

We can transform a DE into a easier problem using this method. For instance, consider the following problem

Example 1.2.1 (Change of Variables). *We have the problem*

$$y' = F\left(\frac{y}{x}\right)$$

. Since this is homogenous we can rewrite the equation in the form of

$$v(x) = \frac{y}{x} \implies y = xv$$

Using the product rule we get

$$y' = v + xv'$$

Using the substitution this gives us

$$\begin{aligned} v + xv' &= F(v) \\ xv' &= F(v) - v \qquad \implies \qquad \frac{dv}{F(v) - v} = \frac{d}{x} \end{aligned}$$

Which is seperable.

Example 1.2.2 (Change of Variables). *Another problem is*

$$y' = G\left(ax + by\right)$$

which can be solved with

$$u = ax + by \implies u' = a + by'$$

which gives

$$u' = a + G(u) \implies \frac{du}{a + bG(u)} = dx$$

1.2.2 Change of Variables for PDE

Example 1.2.3 (Change Of Variables). *Consider the function*

$$2\frac{dz}{dx} - \frac{dz}{dy} = 0, \qquad \text{with } z = f(x + 2y) \tag{1.1}$$

Let $u = x + 2y$ then we can compute the derivatives using the chain rule.

$$\frac{\partial f}{\partial x} = \left(\frac{\partial f}{\partial u}\right)\left(\frac{\partial u}{\partial x}\right) = f'(u)(1) = f'(u)$$
$$\frac{\partial f}{\partial y} = \left(\frac{\partial f}{\partial u}\right)\left(\frac{\partial u}{\partial y}\right) = 2f'(u)$$

Putting those into the equation we get

$$2f'(u) - 2f'(u) = 0$$

Using the same function. We can also make the change of variables using $t = x + 2y$ and $s = x$. Taking the derivatives we get

$$\frac{\partial z}{\partial x} = \frac{\partial z}{\partial t}\frac{\partial t}{\partial x} + \frac{\partial z}{\partial s}\frac{\partial s}{\partial x} = \frac{\partial z}{\partial t} + \frac{\partial z}{\partial s}$$
$$\frac{\partial z}{\partial y} = \frac{\partial z}{\partial t}\frac{\partial t}{\partial y} + \frac{\partial z}{\partial s}\frac{\partial s}{\partial y} = 2\frac{\partial z}{\partial t}$$

Putting those two into the equations gives us

$$\frac{\partial z}{\partial s} = 0$$

which shows that z does not depend on s, thus, any function of the form $z = f(t)$ satisfies the equation.

Example 1.2.4 (Change of Variables : 2nd Order PDE)**.** *Find the formula for $\frac{\partial^2 z}{\partial r^2}, \frac{\partial^2 z}{\partial \theta^2}, \frac{\partial^2 z}{\partial r \partial \theta}$ if $z = f(x, y)$ and $x = r\cos\theta$ and $y = r\sin\theta$.*
Let $\xi = f(x, y)$ with $x = r\cos\theta$ and $y = r\sin\theta$ The chain rule gives us :

$$\begin{aligned}
\frac{\partial \xi}{\partial r} &= \frac{\partial f}{\partial x}\frac{\partial x}{\partial r} + \frac{\partial f}{\partial y}\frac{\partial y}{\partial r} \\
&= \frac{\partial f}{\partial x}\cos\theta + \frac{\partial f}{\partial y}\sin\theta \\
&\textit{and} \\
\left(\frac{\partial}{\partial r}\right)\left(\frac{\partial \xi}{\partial r}\right) &= \frac{\partial}{\partial x}\left(\frac{\partial \xi}{\partial r}\right)\left(\frac{\partial x}{\partial r}\right) + \frac{\partial}{\partial y}\left(\frac{\partial \xi}{\partial r}\right)\left(\frac{\partial y}{\partial r}\right) \\
&= \left(\frac{\partial^2 f}{\partial x^2}\cos\theta + \frac{\partial^2 f}{\partial y \partial x}\sin\theta\right)\cos\theta + \left(\frac{\partial^2 f}{\partial x \partial y} + \frac{\partial^2 f}{\partial y^2}\sin\theta\right)\sin\theta \\
&= \cos^2\theta f_{xx} + 2f_{xy}\cos\theta\sin\theta + \sin^2\theta f_{yy}
\end{aligned}$$

The difficult with these is using the chain rule for higher order derivatives.

1.2.3 Chain Rule

We begin with the chain rule for single variable functions.

Theorem 1.2.5 (Chain Rule Single Variable)**.**

$$(f \circ g)'(x) = f'(g(x))g'(x)$$

Thus, for a second order derivative we have

$$(f \circ g)''(x) = \frac{d}{dx}\left[f'(g(x))g'(x)\right] = f''(g(x))g'(x)g'(x) + f'(g(x))g''(x)$$

$$= f''(g(x))\left[g'(x)\right]^2 + f'(g(x))g''(x)$$

Or, using Leibniz notation :

$$\frac{d^2 f}{dx^2}\big(g(x)\big)\left[\frac{dg}{dx}\right]^2 + \frac{df}{dx}\big(g(x)\big)\frac{d^2 g}{dx^2}$$

Theorem 1.2.6 (Chain Rule for Multivariable Functions)**.**

$$\frac{\partial f}{\partial r} = \frac{\partial f}{\partial x}\frac{\partial x}{\partial r} + \frac{\partial f}{\partial y}\frac{\partial y}{\partial r}$$

We can achieve a second order derivative using this rule.

$$\frac{\partial^2 f}{\partial r^2} = \frac{\partial}{\partial r}\left[\frac{\partial f}{\partial x}\frac{\partial x}{\partial r}\right] + \frac{\partial}{\partial r}\left[\frac{\partial f}{\partial y}\frac{\partial y}{\partial r}\right]$$

We first investigate the first term. We need to use the chain rule for $\frac{\partial f}{\partial x}$.

$$\frac{\partial}{\partial r}\left[\frac{\partial f}{\partial x}\right] = \frac{\partial}{\partial x}\left(\frac{\partial f}{\partial x}\frac{\partial x}{\partial r}\right) + \frac{\partial}{\partial x}\left(\frac{\partial f}{\partial y}\frac{\partial y}{\partial r}\right)$$

$$= \frac{\partial^2 f}{\partial x^2}\frac{\partial x}{\partial r} + \frac{\partial^2 f}{\partial x \partial y}\frac{\partial y}{\partial r}$$

Thus,

$$\frac{\partial}{\partial r}\left[\frac{\partial f}{\partial x}\right]\frac{\partial x}{\partial r} = \left(\frac{\partial^2 f}{\partial x^2}\frac{\partial x}{\partial r} + \frac{\partial^2 f}{\partial x \partial y}\frac{\partial y}{\partial r}\right)\frac{\partial x}{\partial r} + \frac{\partial f}{\partial x}\frac{\partial^2 x}{\partial r^2}$$

The other right hand expression of the original equation is found using the same methods :

$$\frac{\partial}{\partial r}\left[\frac{\partial f}{\partial y}\frac{\partial y}{\partial r}\right] = \left(\frac{\partial^2 f}{\partial y^2}\frac{\partial x}{\partial r} + \frac{\partial^2 f}{\partial y \partial x}\frac{\partial y}{\partial r}\right)\frac{\partial r}{\partial r} + \frac{\partial f}{\partial y}\frac{\partial^2 y}{\partial r^2}$$

1.3 Problem Set 1

PDEs and numerical methods - Some introductory exercises

The goal of these exercises is to get used to some usual vocabulary, notions and tools frequently encountered when dealing with PDEs.

Reminder: *A* ***differential equation*** *is a relationship involving a function u and its derivatives. It is an* ***ordinary differential equation (ODE)*** *if u depends on only one variable, or a* ***partial differential equation (PDE)*** *if u depends on several variables.*

Exercise 1 Solve the PDE: $\dfrac{\partial^2 u}{\partial y^2}(x,y) = 1$

Exercise 2 *Some tools for solving PDEs: change of variables*

2.1 Look for solutions of $\quad x\,\dfrac{\partial u}{\partial x} + y\,\dfrac{\partial u}{\partial y} = u \quad$ as $u(x,y) = f(x^2+y^2)$.

2.2 Same question for the PDE $x\,\dfrac{\partial u}{\partial x} + y\,\dfrac{\partial u}{\partial y} = \lambda\, u$, where λ is a real constant.

2.3 Let $u : \mathbb{R}^n \to \mathbb{R}$ and $\lambda \in \mathbb{R}$. Solve the PDE $\displaystyle\sum_{i=1}^{n} x_i\,\frac{\partial u}{\partial x_i} = \lambda\, u$

Exercise 3 *Some tools for solving PDEs : change of variables*

Look for solutions for the PDE $x\,\dfrac{\partial u}{\partial x} + y\,\dfrac{\partial u}{\partial y} = 0$ under the form $u(x,y) = f\left(\dfrac{x}{y}\right)$.

Exercise 4 *Some tools for solving PDEs : change of variables*

Look for solutions of $\dfrac{\partial^2 u}{\partial x^2} - \dfrac{\partial^2 u}{\partial y^2} = 0$ using the change of variables $(X,Y) = (x+y, x-y)$.

Exercise 5 *Some tools for solving PDEs : Fourier transform*

Let consider the PDE $\dfrac{\partial u}{\partial t}(x,t) - \nu\dfrac{\partial^2 u}{\partial x^2}(x,t) = 0$ $(x \in \mathbb{R}, t > 0, \nu > 0)$ with the initial condition $u(x,0) = u_0(x)$. Solve this equation using a Fourier transform.

Reminder: the Fourier transform of f is $\widehat{f}(\xi) = \int_{\mathbb{R}} f(x)\, e^{-2i\pi x\xi}\, dx$, and $\widehat{e^{-x^2/a^2}} = \sqrt{\pi} a\, e^{-\pi^2\, a^2\, \xi^2}$.

Exercise 6 *Partial differential operators*

6.1 Let $\varphi : \mathbb{R}^3 \to \mathbb{R}$. Compute $\mathrm{curl}(\nabla\varphi)$.

6.2 Let $\varphi : \mathbb{R}^n \to \mathbb{R}$. Compute $\mathrm{div}(\nabla\varphi)$.

6.3 Let $\psi : \Omega \subset \mathbb{R}^2 \to \mathbb{R}$, $(u,v) = (\partial\psi/\partial y, -\partial\psi/\partial x)$ is the *velocity field derived from the stream-function* ψ. Prove that the velocity field is everywhere tangent to the isolines of ψ. Compute the divergence of the velocity field.

Exercise 7 *Proof of the basic Green formula in the 2D case*

The aim of this exercise is to prove the basic Green formula

$$\int_\Omega \frac{\partial u}{\partial x_k}\, v\, dx = -\int_\Omega u\, \frac{\partial v}{\partial x_k}\, dx + \int_{\partial\Omega} u\, v\, (e_k.n)\, ds$$

where e_k is the unit vector in direction x_k, in the 2D-case ($\Omega \subset \mathbb{R}^2$).
7.1 Prove this formula for Ω being the reference triangle (i.e. with nodes (0,0), (1,0) and (0,1)).
7.2 Discuss the extension of this result to any domain Ω with sufficiently smooth boundary

Exercise 8 *Green formulas*

Perform an integration by parts for the following expressions:

8.1 $\displaystyle\int_\Omega \operatorname{div}(\mathbf{E}(\mathbf{x}))\,d\mathbf{x}$ with $\mathbf{E} : \Omega \subset \mathbb{R}^n \to \mathbb{R}^n$

8.2 $\displaystyle\int_\Omega \operatorname{div}(k(\mathbf{x})\,\nabla u(\mathbf{x}))\,d\mathbf{x}$ with $u : \Omega \subset \mathbb{R}^n \to \mathbb{R}$

8.3 $\displaystyle\int_\Omega \sum_{i=1}^n \alpha_i \frac{\partial u}{\partial x_i}\,\frac{\partial v}{\partial x_i}$ with $u, v : \Omega \subset \mathbb{R}^n \to \mathbb{R}$ and $\alpha_1, \dots, \alpha_n$ given real numbers.

Exercise 9 *Boundary conditions and well-posedness*

9.1 Let the ODE $u''(x) = 0$ in $]a, b[$. Find its solution(s), considering the following different boundary conditions:
- **9.1.a** Dirichlet conditions: $u(a) = \alpha, u(b) = \beta$
- **9.1.b** Neumann conditions: $u'(a) = \alpha, u'(b) = \beta$
- **9.1.c** Robin conditions: $u'(a) + \lambda u(a) = \alpha, u'(b) + \lambda u(b) = \beta$ $(\lambda \neq 0)$
- **9.1.d** Mixed conditions: $u'(a) = \alpha, u(b) = \beta$

9.2 Let consider the Poisson equation $\Delta u = f$ on $\Omega \subset \mathbb{R}^n$. Study the unicity of its solution(s), considering the following different boundary conditions:
- **9.2.a** Dirichlet conditions: $u = g$ on $\partial\Omega$
- **9.2.b** Neumann conditions: $\dfrac{\partial u}{\partial n} = h$ on $\partial\Omega$
- **9.2.c** Mixed conditions: $u = g$ on Γ_0, $\dfrac{\partial u}{\partial n} = h$ on Γ_1, where $\Gamma_0 \cup \Gamma_1 = \partial\Omega$ and $\Gamma_0 \cap \Gamma_1 = \emptyset$

Exercise 10 *Characterization of a PDE*
For each of the following PDEs, give as many indications as possible on its nature: order, linear or not, with or without right hand side, stationary or not, elliptic/parabolic/hyperbolic...

10.a $\displaystyle\frac{\partial u}{\partial t}(x,t) + u^2(x,t)\,\frac{\partial u}{\partial x}(x,t) = 0 \qquad (x \in \mathbb{R}, t > 0)$

10.b $\displaystyle\sum_{i=1}^n \alpha_i^2\,\frac{\partial^2 u}{\partial x_i^2}(\mathbf{x}) = f(\mathbf{x}) \qquad (\mathbf{x} \in \mathbb{R}^n)$

10.c $\displaystyle\frac{\partial^2 u}{\partial t^2}(\mathbf{x},t) - c^2 \sum_{i=1}^n \frac{\partial^2 u}{\partial x_i^2}(\mathbf{x},t) = f(\mathbf{x},t) \qquad (\mathbf{x} \in \mathbb{R}^n, t > 0, c \neq 0 \text{ given})$

10.d $\displaystyle\frac{\partial u}{\partial t}(\mathbf{x},t) - \nu \sum_{i=1}^n \frac{\partial^2 u}{\partial x_i^2}(\mathbf{x},t) = f(\mathbf{x},t) \qquad (\mathbf{x} \in \mathbb{R}^n, t > 0, \nu > 0 \text{ given})$

10.e $\displaystyle\frac{\partial^2 u}{\partial y^2}(x,y) + y\,\frac{\partial^2 u}{\partial x^2}(x,y) = 0$

10.f $\displaystyle x^2\,\frac{\partial^2 u}{\partial x^2}(x,y) + 2xy\,\frac{\partial^2 u}{\partial x\,\partial y}(x,y) + y^2\,\frac{\partial^2 u}{\partial y^2}(x,y) = f(x,y)$

1.4 Solutions to Problem Set 1

1.4.1 Exercise 1

Solution is simple :

$$\begin{aligned}
\frac{\partial^2 u}{\partial y^2} u &= 1 \\
\int \frac{\partial^2 u}{\partial y^2} u &= \int 1 dy \\
\frac{\partial u}{\partial y} &= y + c(x) \\
\int \frac{\partial u}{\partial y} &= \int y + c(x) dy \\
u &= \frac{1}{2} y^2 + y c(x) + d(x)
\end{aligned}$$

1.4.2 Exercise 2 : Change of variables

2.1

Look for solutions of $x\frac{\partial u}{\partial x} + y\frac{\partial u}{\partial y} = u$ for $u(x,y) = f(x^2+y^2)$
First we take the x variable :

$$\frac{\partial u}{\partial x} = \frac{\partial f}{\partial x} = \left(f'\right)(2x)$$

Simlarly for the y variable :

$$\frac{\partial u}{\partial y} = \frac{\partial f}{\partial y} = \left(f'\right)(2y)$$

Plugging back into the equation :

$$2x^2 f' + 2y^2 f' = f$$

which can be solved thusly :

$$
\begin{aligned}
2f'\left(x^2+y^2\right) &= f \\
&\text{Let } x^2+y^2=r \\
\frac{f'}{f} &= \frac{1}{2r} \\
\int \frac{f'}{f} &= \int \frac{1}{2r} \\
\ln(f) &= \frac{1}{2}\ln(r)+c \\
f &= e^{\ln(r)/2}e^c \\
f &= A\sqrt{r} \quad \text{where } A=e^c
\end{aligned}
$$

This finally gives us the solution

$$u(x,y) = A\sqrt{x^2+y^2} \quad A \in \mathbb{R}$$

2.2

Same question for the PDE $x\frac{\partial u}{\partial x} + y\frac{\partial u}{\partial y} = \lambda u$ where $\lambda \in \mathbb{R}$ and constant. We begin with the relation

$$2rf' = \lambda u$$

which gives $2rf' = \lambda f$ allowing us to solve.

$$
\begin{aligned}
2rf' &= \lambda f \\
\frac{f'}{f} &= \frac{\lambda}{2r} \\
\int \frac{f'}{f} &= \int \frac{\lambda}{2r} \\
\ln(f) &= \frac{\lambda}{2}\ln(r) \\
f &= Ar^{\lambda/2}
\end{aligned}
$$

Finally,

$$u(x,y) = A\left(x^2+y^2\right)^{\lambda/2}$$

2.3

Let $u : \mathbb{R} \to \mathbb{R}$ and $\lambda \in \mathbb{R}$. Solve

$$\sum_{i=1}^{n} x_i \frac{\partial u}{\partial x_i} = \lambda u \tag{1.2}$$

We first begin with the basic relations

$$f(x_1^1 + \cdots + x_n^2) = u(x_1, \cdots, x_n)$$

The left hand side of 1.2 elementwise then becomes

$$\left(2x_i^2\right) f'$$

then the entire expression is

$$\sum_{i=1}^{n} \left(2x_i^2\right) \left(f'\right) = \lambda u$$

then

$$\left(2f'\right) \|x\|^2 = \lambda f$$

replacing $\|x\|^2 = r$ we get

$$\frac{f'}{f} = \frac{\lambda}{2} r$$

$$\ln\left(f\right) = \frac{\lambda}{2} \ln\left(r\right)$$

$$f = r^{\lambda/2}$$

So we finally have,

$$\left(\|x\|^2\right)^{\lambda/2} = \|x\|^{\lambda}$$

and our solution is

$$u = \|x\|^{\lambda}$$

3

Look for solutions for the PDE $x\frac{\partial u}{\partial x} + y\frac{\partial u}{\partial y} = 0$ under the form $u(x,y) = f\left(\frac{x}{y}\right)$.

We first look for x :

$$\frac{\partial f}{\partial x} = \frac{f'}{y}$$

for y :

$$\frac{\partial f}{\partial y} = \frac{-xf'}{y^2}$$

Plugging in to the original equation we get

$$f'\frac{x}{y} - \frac{x}{y}f' = 0$$

$$f'\left(\frac{x}{y} - \frac{x}{y}\right) = 0$$

which has ∞ many solutions.

Exercise 4

Look for solutions of $\frac{\partial^2 u}{\partial x^2} - \frac{\partial^2 u}{\partial y^2} = 0$ using $(X, Y) = (x + y, x - y)$.

$$\frac{\partial^2 f}{\partial x} - \frac{\partial^2 f}{\partial y^2} = 0$$

We first compute the left hand side

$$\begin{aligned}\frac{\partial^2 f}{\partial x} &= \frac{\partial}{\partial x}\left(\frac{\partial f}{\partial x}\right) \\ &= \frac{\partial}{\partial x}\left(\frac{\partial f}{\partial X}\frac{\partial X}{\partial x} + \frac{\partial f}{\partial Y}\frac{\partial Y}{\partial x}\right) \\ &= \frac{\partial}{\partial x}\left(\frac{\partial f}{\partial X} + \frac{\partial f}{\partial Y}\right)\end{aligned}$$

each of these can be a bit tricky. We refer to 1.2.6 in order to see that

$$\begin{aligned}\frac{\partial}{\partial x}\left(\frac{\partial f}{\partial X}\right) &= \frac{\partial}{\partial X}\left(\frac{\partial f}{\partial X}\frac{\partial X}{\partial x} + \frac{\partial f}{\partial Y}\frac{\partial Y}{\partial x}\right) \\ &= \frac{\partial^2 f}{\partial X^2}(1) + \frac{\partial^2 f}{\partial X \partial Y}(1)\end{aligned}$$

Similarly, for the right hand side

$$\begin{aligned}\frac{\partial}{\partial x}\frac{\partial f}{\partial Y} &= \frac{\partial}{\partial Y}\left(\frac{\partial f}{\partial X}\frac{\partial x}{\partial x} + \frac{\partial f}{\partial Y}\frac{\partial Y}{\partial x}\right) \\ &= \frac{\partial^2 f}{\partial Y \partial X}(1) + \frac{\partial^2 f}{\partial Y^2}(1)\end{aligned}$$

This leaves us with

$$\frac{\partial^2 f}{\partial x^2} = \frac{\partial^2 f}{\partial X^2} + \frac{\partial^2 f}{\partial X \partial Y} + \frac{\partial^2 f}{\partial Y \partial X} + \frac{\partial^2 f}{\partial Y^2}$$

For the second term,

$$\begin{aligned}\frac{\partial^2 f}{\partial y^2} &= \frac{\partial}{\partial y}\left(\frac{\partial f}{\partial y}\right) \\ &= \frac{\partial}{\partial y}\left(\frac{\partial f}{\partial X}\frac{\partial X}{\partial x} + \frac{\partial f}{\partial Y}\frac{\partial Y}{\partial y}\right) \\ &= \frac{\partial}{\partial y}\left(\frac{\partial f}{\partial X} - \frac{\partial f}{\partial Y}\right)\end{aligned}$$

Thus,

$$\begin{aligned}\frac{\partial}{\partial y}\left(\frac{\partial f}{\partial X}\right) &= \frac{\partial}{\partial X}\left(\frac{\partial f}{\partial X}\frac{\partial X}{\partial y} + \frac{\partial f}{\partial Y}\frac{\partial Y}{\partial y}\right)\\ &= \frac{\partial}{\partial X}\left(\frac{\partial f}{\partial X} - \frac{\partial f}{\partial Y}\right)\\ &= \frac{\partial^2 f}{\partial X^2} - \frac{\partial^2 f}{\partial X \partial Y}\end{aligned}$$

and,

$$\begin{aligned}\frac{\partial}{\partial y}\left(\frac{\partial f}{\partial Y}\right) &= \frac{\partial}{\partial Y}\left(\frac{\partial f}{\partial X}\frac{\partial X}{\partial y} + \frac{\partial f}{\partial Y}\frac{\partial Y}{\partial y}\right)\\ &= \frac{\partial}{\partial Y}\left(\frac{\partial f}{\partial X} - \frac{\partial f}{\partial Y}\right)\\ &= \frac{\partial^2 f}{\partial Y \partial X} - \frac{\partial^2 f}{\partial Y^2}\end{aligned}$$

which gives

$$\frac{\partial^2 f}{\partial y^2} = \frac{\partial}{\partial y}\left(\frac{\partial f}{\partial X}\right) - \frac{\partial}{\partial y}\left(\frac{\partial f}{\partial Y}\right) = \frac{\partial^2 f}{\partial X^2} - \frac{\partial^2 f}{\partial X \partial Y} - \frac{\partial^2 f}{\partial Y \partial X} + \frac{\partial^2 f}{\partial Y^2}$$

Plugging in to the original equation :

$$\frac{\partial^2 f}{\partial x^2} - \frac{\partial^2 f}{\partial y^2} = \frac{\partial^2 f}{\partial X^2} + \frac{\partial^2 f}{\partial X \partial Y} + \frac{\partial^2 f}{\partial Y \partial X} + \frac{\partial^2 f}{\partial Y^2} - \left(\frac{\partial^2 f}{\partial X^2} - \frac{\partial^2 f}{\partial X \partial Y} - \frac{\partial^2 f}{\partial Y \partial X} + \frac{\partial^2 f}{\partial Y^2}\right)$$

$$= 0 + 2\frac{\partial^2 f}{\partial X \partial Y} + 2\frac{\partial^2 f}{\partial Y \partial X} + 0$$

Assuming mixed partials are equal we get

$$\frac{\partial^2 2f}{\partial X \partial Y} = 0$$

So we are looking for $u \in \mathscr{C}^2$ such that the mixed partials are equal to zero. This gives us the function

$$u = F\left(x+y\right) + G\left(x-y\right) \qquad \text{where } F, G \in \mathscr{C}^2.$$

1.4.3 Fourier Transform

$$\frac{\partial u}{\partial t}(x,t) - \nu \frac{\partial^2 u}{\partial x^2}(x,t) = 0, \qquad x \in \mathbb{R}, t > 0, \nu > 0 \tag{1.3}$$

With $u(x,0) = u_0(x)$
. We want to solve this using the Fourier Transform which we denote using

$$\mathscr{F}\big(f(x)\big) = \widehat{f}(\xi) = \int_{\mathbb{R}} f(x) e^{-2i\pi x\xi}\ dx$$

Using basic properties of the Fourier Transform we have :

$$\frac{\partial u}{\partial t}\widehat{u}(\xi,t) - \nu\left(2\pi i\xi\right)^2 \widehat{u}(\xi,t)$$

$$\frac{\partial u}{\partial t}\widehat{u}(\xi,t) + \nu 4\pi^2\xi^2\widehat{u}(\xi,t)$$

Which gives a seperable equation

$$\int \frac{du}{u} = -\int \nu 4\pi^2 \xi^2\ dt$$

$$\widehat{u} = Ae^{-v4\pi^2\xi^2 t} \qquad \text{where } A = e^{cst}$$

Using initial conditions we have

$$\widehat{u}(\xi,0) = A = \widehat{u}_0(\xi)$$

$$\widehat{u}(\xi,t) = \widehat{u}_0(\xi)e^{-\nu 4\pi^2\xi^2 t}$$

Using the fact that $\widehat{e^{-x^2/a}} = \sqrt{\pi}ae^{-\pi^2 a^2 \xi^2}$, we have :

$$\begin{aligned}
\pi^2 a^2 \xi^2 &= \nu 4\pi^2\xi^2 t \\
a^2 &= \nu 4t \\
a &= 2\sqrt{\nu t} \\
&\text{Then, substituting for a} \\
\mathscr{F}\left(e^{-x^2/2\sqrt{\nu t}}\right) &= 2\sqrt{\pi\nu t}e^{-\nu 4\pi^2\xi^2 t} \\
\mathscr{F}\left(\frac{1}{2\sqrt{\pi\nu t}}e^{-x^2/2\sqrt{\nu t}}\right) &= e^{-\nu 4\pi^2\xi^2 t}
\end{aligned}$$

Finally,

$$\mathscr{F}\left(u_0(x)\frac{1}{2\sqrt{\pi\nu t}}e^{-x^2/2\sqrt{\nu t}}\right) = u_0(x)e^{-\nu 4\pi^2\xi^2 t}$$

$$u(x,t) = \frac{1}{2\sqrt{\pi\nu t}}\int_{-\infty}^{\infty} u_0(y)e^{\frac{-(x-y)^2}{4\nu t}}\ dy$$

1.4.4 Partial Differential Operators

1. Let $\varphi : \mathbb{R}^3 \to \mathbb{R}$. Compute curl $(\nabla\varphi)$
2. Let $\varphi : \mathbb{R}^n \to \mathbb{R}$. Compute div $(\nabla\varphi)$
3. Let $\psi : \Omega \subset \mathbb{R}^2 \to \mathbb{R}$, $(u, v) = \big(\partial\psi/\partial y, -\partial\psi/\partial x\big)$ is the velocitiy field derived from the stream function ψ. Prove that the velocity field is everywhere tangent to the isoline of ψ. Compute the divergence of the velocity field.

Using the fact that, for $\varphi : \mathbb{R}^n \to \mathbb{R}$ we have that

$$\text{grad } \varphi(\boldsymbol{x}) = \nabla\varphi(\boldsymbol{x}) = \begin{pmatrix} \frac{\partial\varphi}{\partial x_1} \\ \vdots \\ \frac{\partial\varphi}{\partial x_n} \end{pmatrix}$$

1.

$$\begin{aligned} \text{curl } \varphi(\boldsymbol{x}) &= \text{curl } \begin{pmatrix} \frac{\partial\varphi}{\partial x_1} \\ \frac{\partial\varphi}{\partial x_2} \\ \frac{\partial\varphi}{\partial x_3} \end{pmatrix} \\ &= \begin{pmatrix} \frac{\partial^2\varphi}{\partial x_2\partial x_3} - \frac{\partial^2\varphi}{\partial x_3\partial x_2} \\ \frac{\partial^2\varphi}{\partial x_3\partial x_1} - \frac{\partial^2\varphi}{\partial x_1\partial x_3} \\ \frac{\partial^2\varphi}{\partial x_1\partial x_2} - \frac{\partial^2\varphi}{\partial x_2\partial x_1} \end{pmatrix} \end{aligned}$$

2.

$$\begin{aligned} \text{div } \varphi(\boldsymbol{x}) &= \text{curl } \begin{pmatrix} \frac{\partial\varphi}{\partial x_1} \\ \vdots \\ \frac{\partial\varphi}{\partial x_n} \end{pmatrix} \\ &= \sum_{i=1}^{n} \frac{\partial^2\varphi_i}{\partial x_i^2} \end{aligned}$$

1.4.5 Proof of the basic Green Formula in the 2D case

We want to prove

$$\int\limits_{\Omega} \frac{\partial u}{\partial x_k} v \; dx = -\int\limits_{\Omega} u \frac{\partial v}{\partial x_k} \; dx + \int\limits_{\partial\Omega} uv \, (e_k \cdot n) \;\; ds \tag{1.4}$$

where e_k is the unit vector in direction x_k, in the 2D-case ($\Omega \subset \mathbb{R}$).

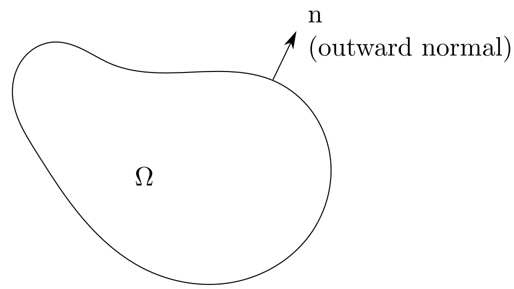

Figure 1.1: greenOnOmega

7.1

Prove this formula for Ω being the reference triangle (i.e, with nodes $(0,0)\,,(1,0)\,,(0,1)$).

The left hand side of 1.4 becomes

$$\int\limits_{\Omega} \frac{\partial u}{\partial x_1} v \; dx_1 dx_2$$

or

$$\begin{aligned}
\int\limits_{T} \frac{\partial u}{\partial x_1} v \; dx_1 dx_2 &= \int\limits_{x_1=0}^{1} \left(\int\limits_{x_2=0}^{x_2=1-x_1} \frac{\partial u}{\partial x_1} v \; dx_2 \right) dx_1 \\
&= \int\limits_{x_2=0}^{1} \left(\int\limits_{x_1=0}^{1-x_2} \frac{\partial u}{\partial x_1} v \; dx_1 \right) dx_2
\end{aligned}$$

The last formulation has a fixed x_2 for the inner part of the equation.

Proposition 1.4.1.

$$\int\limits_{\partial\Omega} f \; d\sigma = \sum_{i=1}^{m} \int\limits_{\partial\Omega_i} f \; d\sigma$$

That is, each side of the boundary can be analyzed independently for simple parametrization, furthermore, the combination of the pieces is that integral of

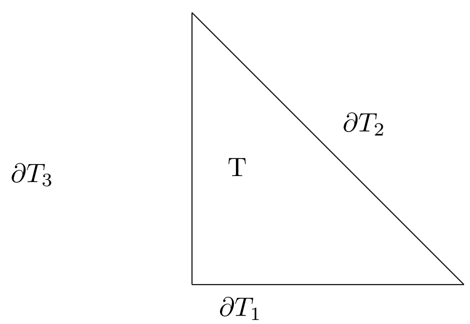

Figure 1.2: green on T

the entire boundary.
We get the following formation due to the defintion of a line integral :

$$\int\limits_{\partial\Omega} f \; d\sigma = \int\limits_{0}^{1} f\left(\gamma_i(t)\right) \|\gamma_i'(t)\| \; dt$$

Furthermore, we calculate the unit normal for each segment of the triangle.

$$\partial T_1 = \begin{pmatrix} 0 \\ 0 \end{pmatrix} - \begin{pmatrix} 1 \\ 0 \end{pmatrix} = \begin{pmatrix} -1 \\ 0 \end{pmatrix} \text{ which has normal } n_1 = \begin{pmatrix} 0 \\ -1 \end{pmatrix}$$

$$\partial T_2 = \begin{pmatrix} 1 \\ 0 \end{pmatrix} - \begin{pmatrix} 0 \\ 1 \end{pmatrix} = \begin{pmatrix} 1 \\ -1 \end{pmatrix} \text{ which has length } \| \cdot \| = \sqrt{2}$$

thus,

$$\begin{pmatrix} 1 \\ -1 \end{pmatrix} \cdot \begin{pmatrix} 1 \\ 1 \end{pmatrix} = 0,$$

and we divide by the length to ensure the normal has length 1

$$\partial T_2 = \begin{pmatrix} \frac{1}{\sqrt{2}} \\ \frac{1}{\sqrt{2}} \end{pmatrix}$$

The last is found simply,

$$\partial T_3 = \begin{pmatrix} -1 \\ 0 \end{pmatrix}$$

We can now solve for each side.

$$\int\limits_{x_2=0}^{1}\left(-\int\limits_{x_1=0}^{1-x_2} u\frac{\partial v}{\partial x_1}\right)\,dx_2 + \int\limits_{x_2=0}^{1} u\left(1-x_2,x_2\right)v\left(1-x_2,x_2\right) - u\left(0,x_2\right)v\left(0,x_2\right)\,dx_2$$

$$\begin{aligned}\int\limits_{\partial T} uvn_1\,d\sigma &= \int\limits_{\partial T_1} uv\overbrace{n_1}^{=0}\,d\sigma + \int\limits_{\partial T_2} uv\overbrace{n_1}^{=1/\sqrt{2}} + \int\limits_{\partial T_3} uv\overbrace{n_1}^{=-1}\,d\sigma\\ &= \int\limits_{\partial T_2} uvn_1\,d\sigma + \int\limits_{\partial T_3} uvn_1\,d\sigma\end{aligned}$$

Now, for ∂T_2 we have the paramaterized line as

$$\gamma_2(t) = \big\{\left(1-t,t\right), t\in[0,1]\big\} \text{ where } \gamma_2'(t) = \begin{pmatrix}-1\\1\end{pmatrix} \text{ and } \|\gamma_2'\| = \sqrt{2}$$

Finally,

$$\int\limits_0^1 u\left(1-t,t\right)v\left(1-t,t\right)\frac{1}{\sqrt{2}}\sqrt{2}\,dt$$

Since $\gamma_3(t) = \big\{\left(0,1-t\right)\big\}$ we have

$$\int\limits_0^1 u\left(0,t\right)v\left(0,t\right)\left(-1\right)\cdot\left(1\right)\,dt$$

and

$$\int\limits_0^1 u\left(1-t,t\right)v\left(1-t,t\right) - u\left(0,t\right)v\left(0,t\right)\,dt$$

1.4.6 Green Formulas

1.

$$\int\limits_\Omega \operatorname{div}\big(\boldsymbol{E}(\boldsymbol{x})\big)\,d\boldsymbol{x} \quad \text{with } \boldsymbol{E}:\Omega\subset\mathbb{R}^n\to\mathbb{R}^n$$

First, it should be noted that the div of a function is a scalar, and we take u = 1. Thus,

$$\int_\Omega u \ \mathrm{div}(\boldsymbol{E}) \ dx = -\int_\Omega \underbrace{\nabla u}_{=0} \cdot \boldsymbol{E} + \int_{\partial\Omega} u \left(\boldsymbol{E}\cdot\boldsymbol{n}\right) \ ds$$
$$= \int_{\partial\Omega} u \left(\boldsymbol{E}\cdot\boldsymbol{n}\right) \ ds$$
$$\text{since } u = 1$$
$$\int_\Omega \mathrm{div}\left(\boldsymbol{E}\right) \ dx = \int_{\partial\Omega} \boldsymbol{E}\cdot\boldsymbol{n} \ ds$$

2.
$$\int_\Omega \mathrm{div}\left(k(\boldsymbol{x})\nabla u(\boldsymbol{x})\right) \ d\boldsymbol{x} \qquad \text{with } u : \Omega \subset \mathbb{R}^n \to \mathbb{R}$$

$$\int_\Omega \mathrm{div}\left(k(\boldsymbol{x})\nabla u(\boldsymbol{x})\right) \ d\boldsymbol{x} =$$

3.
$$\int_\Omega \sum_{i=1}^{n} \alpha_i \frac{\partial u}{\partial x_i}\frac{\partial v}{\partial x_i} \qquad \text{with } u, v : \Omega \subset \mathbb{R}^n \to \mathbb{R} \text{ and } \alpha_i \in \mathbb{R}$$

1.4.7 Boundary conditions and well-posedness

9.1

Let the ODE
$$u''(x) = 0 \text{ in }]a, b[$$

Find its solution considering

(a) Dirichlet Conditions : $u(a) = \alpha,\ u(b) = \beta$

(b) Neumann conditions : $u'(a) = \alpha,\ u'(b) = \beta$

(c) Robin conditions : $u'(a) + \lambda u(a) = \alpha,\ u'(b) + \lambda u(b) = \beta$ with $\lambda \neq 0$

(d) Mixed conditions : $u'(a) = \alpha$, $u(b) = \beta$

We begin with the fact that this ODE has the general form of

$$u(x) = Ax + B$$

(a) This gives us the condition that

$$u(a) = Aa + B = \alpha \qquad u(b) = Ab + B = \beta$$

Intuitively, this is well posed because there exists a unique line between two points. In terms of a solution we get :

$$A = \frac{\beta - \alpha}{b - a} \qquad B = \alpha - \frac{\beta - \alpha}{b - a}(a)$$

(b) Since $u'(x) = A = \alpha = \beta$ which does not guarantee uniqueness.

(c)

$$A + \lambda (Aa + B) = \alpha \qquad A + \lambda (Ab + B) = \beta$$

which gives us

$$A (1 + \lambda a) + \lambda B = \alpha \qquad A (1 + \lambda b) + \lambda B = \beta$$

we can test linear dependence via the determinate, which gives

$$\lambda (1 + \lambda a) - \lambda (1 + \lambda B) = \lambda^2 (a - b) \neq 0$$

(d) The last conditions give :

$$u'(a) = \alpha \implies A = \alpha \qquad \text{then } u(b) = \alpha b + B \implies B = \beta - \alpha b$$

This solution is unique since it depends on both endpoints.

9.2

Consider

$$\triangle u = f \quad \text{ on } \Omega \subset \mathbb{R}^n \tag{1.5}$$

(a) Dirichlet conditions : $u = g$ on $\partial\Omega$

(b) Neumann conditions : $\frac{\partial u}{\partial n} = h$ on $\partial\Omega$

(c) Mixed conditions :

$$u = g \text{ on } \Gamma_0, \quad \frac{\partial u}{\partial n} = h \text{ on } \Gamma_1, \text{ where } \Gamma_0 \cup \Gamma_1 = \partial\Omega \text{ and } \Gamma_0 \cap \Gamma_1 = \emptyset$$

(a) We use the approach of assuming that there can be two solutions which result in a contradiction. Let u_1, u_2 be two solutions of $\triangle u = f$ on Ω. We then have

$$\begin{cases} \triangle u_1 = f \text{ in } \Omega \\ \quad u_1 = g \text{ on } \partial\Omega \end{cases} \qquad \begin{cases} \triangle u_2 = f \text{ in } \Omega \\ \quad u_2 = g \text{ on } \partial\Omega \end{cases}$$

If u_1, u_2 solutions then $u = u_1 - u_2$ is a solution

$$\begin{cases} \triangle u = f - f = 0 & \text{in } \Omega \\ u = g - g = 0 & \text{on } \partial\Omega \end{cases}$$

Using Green's theorem we get :

$$\int_\Omega \triangle uv \ dx = -\int_\Omega \triangle u \triangle v \ dx + \int_{\partial\Omega} \partial_n uv \ d\sigma$$

Where $\partial_n u$ or $\frac{\partial u}{\partial n} = \nabla u \cdot n$ or $\sum \frac{\partial u}{\partial x_k}$

Can be found in the class slides

$$= \int_\Omega \underbrace{\triangle u}_{=0} v \ dx - \int_{\partial\Omega} \underbrace{\nabla u \nabla v}_{=0} \ dx = \int_\Omega \frac{\partial u}{\partial n} \underbrace{u}_{=0} \ d\sigma$$

Assuming smoothnes, this implies that $\nabla u = 0$ in Ω and u is constant on Ω where Ω is simply connected or, for each component of Ω u is constant on it. But this is in contradiction with our assumption that

$$\triangle u = f$$

Therefore $u_1 = u_2$.

b) Neuman

$$\partial_n u = h \qquad \text{on } \partial\Omega \tag{1.6}$$

Let u_1, u_2 be solutions of 1.5 and 1.6 and $u = u_1 - u_2$.

$$\begin{cases} \triangle u & = 0 & \text{in } \Omega \\ \partial_n u & = 0 & \text{on } \partial\Omega \end{cases}$$

Then,

$$\int_{\partial\Omega} u \partial_n u \ d\sigma = 0$$

Thus, $\nabla u = 0$ in Ω and $u = cst$ on each connected component of Ω. which verifies $\partial_n u = 0$ on $\partial\Omega$. No "uniqueness" but "uniqueness up to a constant."

c)

$$\begin{cases} u & = g \text{ on } \Gamma_0 \\ \partial_n u & = h \text{ on } \Gamma_1 \end{cases} \tag{1.7}$$

Let u_1, u_2 be solutions of 1.5 1.7 then $u = u_1 - u_2$ verifies

$$\begin{cases} \nabla u & = 0 \text{ in } \Omega \\ u & = 0 \text{ on } \Gamma_0 \\ \partial_n u & = 0 \text{ on } \Gamma_1 \end{cases}$$

and we have the formula

$$\int\limits_{\partial\Omega} \partial_n u u \, d\sigma = \int\limits_{\Gamma_0} \partial_n u \underbrace{u \, d\sigma}_{=0} + \int\limits_{\Gamma_1} \partial_n u \; u \, d\sigma$$

If Ω is connected, as $u = 0$ on Γ_0, if the measure of Γ_0 is greater than 0 then $u \equiv 0$ in Ω.

Chapter 2

Finite Differences

2.1 Class notes

Chapter 2

Introduction to finite differences

The **finite difference method** provides a numerical approximation of the solutions of ODEs and PDEs. It consists in

- defining a **mesh**, also called a **grid**, approximating the physical domain Ω where the equation is defined. For the finite difference method, contrary to the finite element method, this grid is almost always structured. This means that the **grid points** (or **nodes**) are regularly spaced (i.e. the **space step** is constant), or can be transformed into such a form by a simple function (see Figure 2.1). If one deals with a time-dependent PDE, then a mesh of the time interval is also defined (the time interval is divided into **time steps**, see Figure 2.2)
- looking for an approximation u_i^n of the exact solution at each node i and at each time step n (or more simply for an approximation u_i of the exact solution at each node i if the problem does not depend on time). This is achieved by replacing the exact equation at each node i and at each time step n by an approximate equation involving only the u_j^k, $j = \dots, i-1, i, i+1, \dots$, $k = \dots, n-1, n, n+1, \dots$ The basic tool for building this approximation is the Taylor formula.

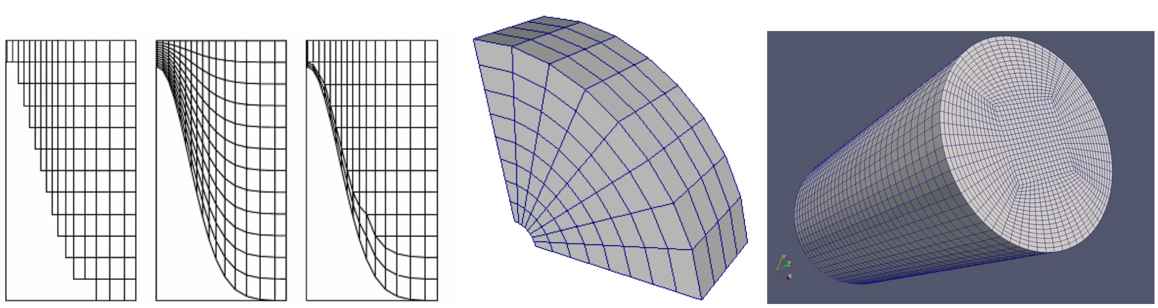

Figure 2.1: some examples of finite difference grids

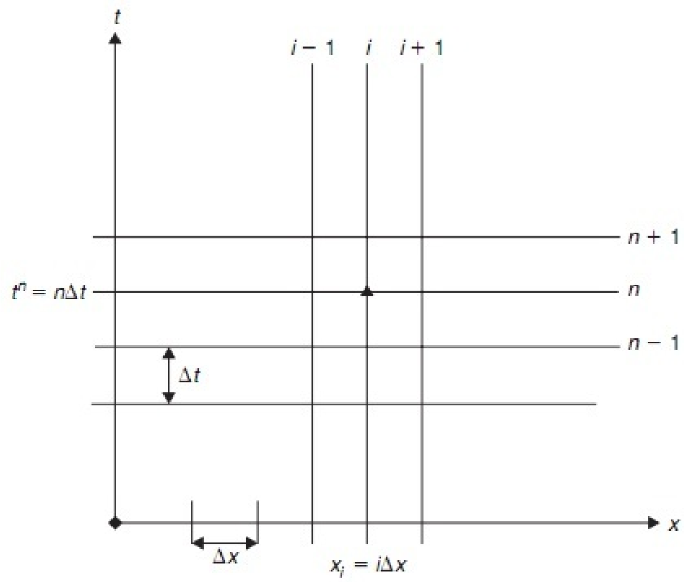

Figure 2.2: Regular space-time discretization

2.1 1-D Taylor formulas

Taylor formulas provide local polynomial approximations of regular functions. Let us recall for instance the Taylor-Lagrange formula for a function of one variable.

Theorem 2.1. Let u with $\mathcal{C}^n$ regularity on $[a,b]$, and with a $(n+1)^{\text{th}}$ derivative on (a,b). Then there exists $\zeta \in (a,b)$ such that

$$u(b) = u(a) + (b-a)u'(a) + \cdots + \frac{(b-a)^n}{n!}\, u^{(n)}(a) + \frac{(b-a)^{n+1}}{(n+1)!}\, u^{(n+1)}(\zeta) \tag{2.1}$$

This can be rewritten in the following way:

Theorem 2.2. Let u with $\mathcal{C}^n$ regularity in a neighborhood of x, and with a $(n+1)^{\text{th}}$ derivative in this neighborhood. Then, for h sufficiently small:

$$u(x+h) = u(x) + h\, u'(x) + \cdots + \frac{h^n}{n!}\, u^{(n)}(x) + \mathcal{O}\left(h^{n+1}\right)$$

This leads to the well-known **Taylor polynomials** approximating common functions. The exact meaning of the notation $\mathcal{O}$ is given in Appendix C.2.

This 1-D formula is sufficient in most cases to derive finite difference schemes, even for multi-dimensional problems. However, for some specific schemes, multidimensional Taylor expansion might be necessary. An example in the 2-D case is given in §2.6.

2.2 Finite difference schemes

In this section, we will explain how finite difference schemes are built, and introduce usual schemes for the approximation of first and second order derivatives. Then we will introduce a way to analyze finite difference schemes.
We will only deal with 1-D functions, and will consider that functions are regular enough, so that their high order derivatives exist and Taylor expansions make sense.

2.2.1 Approximation schemes

Let $x_0, x_1, \dots, x_q$ distinct points and $p \in \mathbb{N}$. If we find real coefficients $\alpha_j\,(j = 0, \dots, q)$ such that

$$u^{(p)}(x_0) \simeq \sum_{j=0}^{q} \alpha_j\, u(x_j)$$

then this linear combination is called an **approximation scheme**, or a **finite difference scheme**, for $u^{(p)}(x_0)$.

This scheme is said to be **consistent** iff $u^{(p)}(x_0) - \sum_{j=0}^{q} \alpha_j u(x_j) \longrightarrow 0$ as $h \longrightarrow 0$.

The scheme is said to be **k^{th}-order accurate** iff $u^{(p)}(x_0) = \sum_{j=0}^{q} \alpha_j\, u(x_j) + \mathcal{O}(h^k)$. k is the **order of accuracy** of the scheme.

The grid points involved in a finite difference scheme form its so-called associated **stencil**.

2.2.2 A general method for deriving a finite difference scheme

Let $x_0, x_1, \dots, x_q$ distinct points, and $h_j = x_j - x_0 \;\; (j = 1, \dots, q)$. We intend to build a consistent approximation scheme for $u^{(p)}(x_0)$, for $p \le q$.

The Taylor-Lagrange formula applied to u at point $x_j \;\; (j = 1, \dots, q)$ at order q reads

$$u(x_j) = u(x_0) + h_j u'(x_0) + \cdots + \frac{h_j^q}{q!}\, u^{(q)}(x_0) + \mathcal{O}(h_j^{q+1})$$

Let build an arbitrary linear combination of these expansions:

$$\sum_{j=1}^{q} \alpha_j u(x_j) = \left(\sum_{j=1}^{q} \alpha_j\right) u(x_0) + \left(\sum_{j=1}^{q} \alpha_j h_j\right) u'(x_0) + \cdots + \frac{1}{q!}\left(\sum_{j=1}^{q} \alpha_j h_j^q\right) u^{(q)}(x_0) + \left(\sum_{j=1}^{q} \alpha_j \mathcal{O}(h_j^{q+1})\right) \tag{2.2}$$

This combination is an approximation scheme for $u^{(p)}(x_0)$ as soon as the coefficients of $u^{(k)}(x_0)$ vanish for $k = 1, \ldots, q,\ k \neq p$:

$$\left\{\begin{array}{lcl} \sum_{j=1}^{q} \alpha_j h_j & = & 0 \\ & \vdots & \\ \sum_{j=1}^{q} \alpha_j h_j^{p-1} & = & 0 \\ \sum_{j=1}^{q} \alpha_j h_j^{p} & = & p! \\ \sum_{j=1}^{q} \alpha_j h_j^{p+1} & = & 0 \\ & \vdots & \\ \sum_{j=1}^{q} \alpha_j h_j^{q} & = & 0 \end{array}\right. \quad \text{i.e.} \quad \begin{pmatrix} h_1 & h_2 & \cdots & h_q \\ \vdots & & & \vdots \\ h_1^{p-1} & h_2^{p-1} & \cdots & h_q^{p-1} \\ h_1^{p} & h_2^{p} & \cdots & h_q^{p} \\ h_1^{p+1} & h_2^{p+1} & \cdots & h_q^{p+1} \\ \vdots & & & \vdots \\ h_1^{q} & h_2^{q} & \cdots & h_q^{q} \end{pmatrix} \begin{pmatrix} \alpha_1 \\ \vdots \\ \alpha_{p-1} \\ \alpha_p \\ \alpha_{p+1} \\ \vdots \\ \alpha_q \end{pmatrix} = \begin{pmatrix} 0 \\ \vdots \\ 0 \\ p! \\ 0 \\ \vdots \\ 0 \end{pmatrix} \quad (2.3)$$

This is a $q \times q$ linear system of Vandermonde type. Thus it has a unique solution $\alpha_1, \ldots, \alpha_q$ iff the h_js are q distinct values, which is obviously the case since the x_js are distinct points. Moreover the only non homogeneous equation in this system implies that $\alpha_j = \mathcal{O}(h^{-p})$, $j = 1, \ldots, q$, where h is a common order of magnitude for the h_js (for instance h can be taken as the minimum, mean, or maximum value of the h_js).
The linear system (2.3) being satisfied, (2.2) becomes

$$\sum_{j=1}^{q} \alpha_j u(x_j) = \left(\sum_{j=1}^{q} \alpha_j\right) u(x_0) + u^{(p)}(x_0) + \mathcal{O}(h^{q+1-p})$$

i.e.

$$u^{(p)}(x_0) = \sum_{j=1}^{q} \alpha_j u(x_j) - \left(\sum_{j=1}^{q} \alpha_j\right) u(x_0) + \mathcal{O}(h^{q+1-p}) \quad (2.4)$$

Theorem 2.3. Using q additional grid points $x_1, \ldots, x_q$, one can build an approximation of $u^{(p)}(x_0)$ at order $q + 1 - p$. [1]

Theorem 2.4. A direct consequence of the preceding result is that a k^{th}-order scheme is exact for any polynomial function u which degree is lower than or equal to k.

This is simply due to the fact that, following (2.1), the error term $\mathcal{O}(h^{q+1-p})$ in (2.4) is a combination of $(q+1)^{\text{th}}$-order derivatives of u. If the scheme is k^{th}-order accurate, then $q+1-p = k$, i.e. $q + 1 = k + p > k$. Given the fact that, for a polynomial of degree k, the derivatives of order greater than k are zero, the error term is thus also zero.

[1] We will actually see later that, if p is even and if the scheme is symmetric, the order of the approximation becomes $q + 2 - p$.

2.2.3 Usual schemes for the first- and second-order derivatives

Using the Taylor-Lagrange formula at points $x+h$ and $x-h$ with a positive increment h leads to the following usual schemes for the first-order derivative:

- $u'(x) = \dfrac{u(x+h)-u(x)}{h} + \mathcal{O}(h)$: first-order **right-sided** (or **downstream**) scheme
- $u'(x) = \dfrac{u(x)-u(x-h)}{h} + \mathcal{O}(h)$: first-order **left-sided** (or **upwind**) scheme
- $u'(x) = \dfrac{u(x+h)-u(x-h)}{2h} + \mathcal{O}(h^2)$: second-order **centered** scheme

The two first-order schemes are said to be **one-sided**, since they involve grid points only on one side of the current grid point of interest x, while the second-order scheme is said to be **two-sided**.

Similarly, the most usual scheme for the second derivative is the second-order centered scheme:

$$u''(x) = \frac{u(x-h)-2u(x)+u(x+h)}{h^2} + \mathcal{O}(h^2) \tag{2.5}$$

We can see that the orders of accuracy of these schemes follow the rule described by Theorem 2.3. The order is indeed equal to $q+1-p$ for the schemes approximating u' ($p=1$, $q=1$ for the one-sided schemes and $q=2$ for the two-sided scheme), and $q+2-p$ for the second-order centered scheme for u'' ($p=q=2$).

2.2.4 Fourier analysis of finite difference schemes

Spectral (or Fourier) analysis is a powerful tool to study the properties and the quality of approximation schemes. It consists in looking at the effect of a numerical scheme in the frequency space.
Since any regular function can be written as an integral or a series of complex exponential functions (see Appendix A), we only need to consider the effect of a finite difference scheme on a generic exponential function $u_\omega(x) = e^{i\omega x}$, $\omega \in \mathbb{R}$. Let then define the **transfer function** T of an operator S as $S(u_\omega) = T(\omega)\, u_\omega$. The transfer function of a finite difference scheme is then obtained taking $h=1$ (for normalization purpose) and $\omega \in [0,\pi]$ (to fulfill the Nyquist-Shannon criterion[2]).

Example *Let consider the derivation operator:*

$$S : u \longrightarrow u'$$

We have obviously $S(u_\omega)(x) = (e^{i\omega x})' = i\omega\, e^{i\omega x}$, *i.e.* $S(u_\omega) = i\omega\, u_\omega$. *The transfer function corresponding to the first order derivation is thus* $T(\omega) = i\omega$. *Moreover, since* $i\omega\, e^{i\omega x} = \omega\, e^{i(\omega x+\pi/2)}$,

[2]The Nyquist-Shannon criterion states that a sufficient condition for a sample to capture all the information from a continuous signal is that the sample rate is larger than, or equal to, twice the maximum frequency contained in the continuous signal. On a regular grid of step h, the sampling rate is equal to $1/h$, i.e. 1 if we take $h=1$ for the sake of normalization. The continuous signal $e^{i\omega x}$ is made of one single frequency $\omega/(2\pi)$. Then the Nyquist-Shannon criterion reads: $1 \geq 2\omega/(2\pi)$, i.e. $\omega \leq \pi$.

the derivation changes the amplitude of u_ω (by a factor of ω) and its phase (by adding a $\pi/2$ delay).
Let now consider the two following finite difference schemes approximating the first derivative:

$$S_h^{(1)} : u \longrightarrow \frac{u(.+h)-u(.)}{h} \quad \text{and} \quad S_h^{(2)} : u \longrightarrow \frac{u(.+h)-u(.-h)}{2h}$$

$S_1^{(1)}(u_\omega) = e^{i\omega(x+1)} - e^{i\omega x}$ *and* $S_1^{(2)}(u_\omega) = \dfrac{1}{2}\left(e^{i\omega(x+1)} - e^{i\omega(x-1)}\right)$*, which implies that their transfer functions are respectively* $T^{(1)}(\omega) = e^{i\omega} - 1$ *and* $T^{(2)}(\omega) = i\sin\omega$*. They are compared with the transfer function* $T(\omega) = i\omega$ *of the exact continuous derivation in Figure 2.3.*

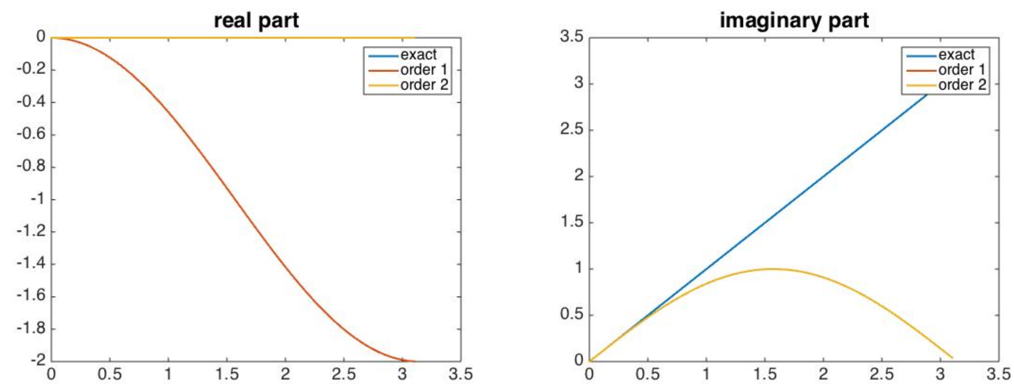

Figure 2.3: Real (left panel) and imaginary (right panel) parts of the transfer function for the exact derivation operator (blue curves), and the $S_h^{(1)}$ (red curves) and $S_h^{(2)}$ (yellow curves) finite difference schemes

An important aspect contributing to the quality of a finite difference scheme is its ability to modify as few as possible the exact transfer function, nor its phase neither its amplitude. In the present example, some simple algebra leads to

$$T^{(1)}(\omega) = \mathrm{sinc}\left(\frac{\omega}{2}\right) e^{i\omega/2}\, T(\omega) \qquad \text{and} \qquad T^{(2)}(\omega) = \mathrm{sinc}(\omega)\; T(\omega)$$

where $\mathrm{sinc}(\omega) = \dfrac{\sin\omega}{\omega}$ *is the cardinal sine function (see Figure A.1 in Appendix A). Under this form, it is clear that* $S^{(1)}$ *modifies both the amplitude and the phase w.r.t.* S*, while* $S^{(2)}$ *modifies the amplitude but not the phase.*

Definition 2.1. A scheme S_h that modifies the amplitude of Fourier components w.r.t. to the exact operator S is said to be **diffusive** or **dissipative**. The modification of this amplitude is called the **diffusion error** or **dissipation error** of the scheme.

Definition 2.2. A scheme S_h that modifies the phase of Fourier components w.r.t. to the exact operator S is said to be **dispersive**. The modification of this phase is called the **dispersion error** of the scheme.

Both errors appear clearly by looking at the ratio T_1/T : there is a dissipation error[3] as soon as the amplitude of this ratio is not equal to 1, and a dispersion error as soon as its phase is non zero (i.e. the ratio is not a real number).
As can be seen in the above example, these errors are not constant, but generally depend on the wavenumber ω. For most schemes, the errors are small for small wavenumbers, and increase for larger ones.

Some generic calculations facilitating the computation of transfer functions are given in Appendix C.1.

2.3 The finite difference method: a simple example

Let now illustrate the principle of the finite difference method on the very simple example of the ODE: $\quad -u''(x) = f(x)$ for $x \in (a,b)$, with boundary conditions $u(a) = 0$ and $u(b) = 0$.

The finite difference method consists in:

- building a mesh of the domain $[a,b]$. Let take here for instance the regular mesh defined by $x_i = a + ih$ $(i = 0, \dots, N+1)$ with $h = (b-a)/(N+1)$.
- considering the ODE on grid points only. The original ODE on (a,b) is replaced by
$$\begin{cases} -u''(x_i) = f(x_i) \quad i = 1, \dots, N \\ u(x_0) = u(x_{N+1}) = 0 \end{cases}$$
- replacing the differential operator by a finite difference scheme. Here, we can use the second order scheme (2.5) seen previously, and the ODE at point x_i reads
$$\begin{cases} -\dfrac{1}{h^2}\left(u(x_{i-1}) - 2u(x_i) + u(x_{i+1})\right) + \varepsilon_i = f(x_i) \quad , i = 1, \dots, N \quad \text{with } \varepsilon_i = \mathcal{O}(h^2) \\ u(x_0) = u(x_{N+1}) = 0 \end{cases} \tag{2.6}$$
- neglecting the error terms ε_i, and then actually solving the remaining system. In the present case, it is thus the simple linear system:
$$\begin{cases} -u_{i-1} + 2u_i - u_{i+1} = h^2 f(x_i) \quad , i = 1, \dots, N \\ u_0 = u_{N+1} = 0 \end{cases} \tag{2.7}$$
where u_i is the approximation of $u(x_i)$.

The preceding problem can of course be written in matrix form. Let

$$A_h = \frac{1}{h^2}\begin{pmatrix} 2 & -1 & & & 0 \\ -1 & 2 & -1 & & \\ & \ddots & \ddots & \ddots & \\ & & -1 & 2 & -1 \\ 0 & & & -1 & 2 \end{pmatrix}, \quad F = \begin{pmatrix} f(x_1) \\ \vdots \\ f(x_N) \end{pmatrix}, \quad E = \begin{pmatrix} \varepsilon_1 \\ \vdots \\ \varepsilon_N \end{pmatrix}$$

[3] Note that one speaks about "dissipation error" even if the amplitude of T_h/T is greater than 1.

$$U = \begin{pmatrix} u(x_1) \\ \vdots \\ u(x_N) \end{pmatrix}, \quad \text{and} \quad U_h = \begin{pmatrix} u_1 \\ \vdots \\ u_N \end{pmatrix}$$

Then (2.6) reads: $A_h U + E = F$, while (2.7) reads:

$$A_h U_h = F \tag{2.8}$$

Before addressing the issues of the existence and uniqueness of U_h and of its convergence towards U, let present some numerical results, for the particular case where the exact solution is $u(x) = e^{-x/8} \sin x$ for $x \in [0, 6\pi]$ (the right-hand side is then $f(x) = \frac{-1}{64} e^{-x/8} (63 \sin x + 16 \cos x)$). Figure 2.4 compares this exact solution u with the numerical approximation u_h for several values of h. It clearly illustrates the convergence of the finite difference solution towards the true solution as h decreases. The rate of this convergence can be quantified by computing the norm of the error $\| U_h - U\|$ for the different values of h. This quantity is displayed in Figure 2.5 in log-log scale. As can be seen, the error decreases almost linearly, with a slope which is very close to 2. This means that the error behaves like $C\,h^2$, which is consistent with the second order discretization of the numerical scheme.

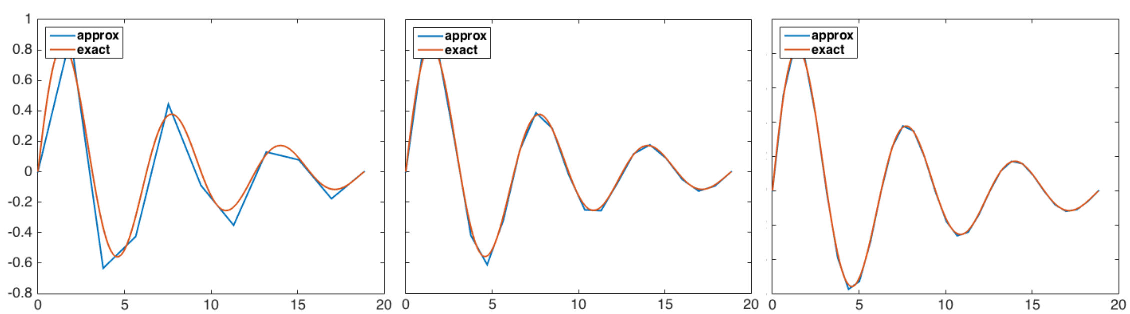

Figure 2.4: $u(x)$ (red curve) and $u_h(x)$ (blue curve) for $N = 10$, $N = 20$ and $N = 30$

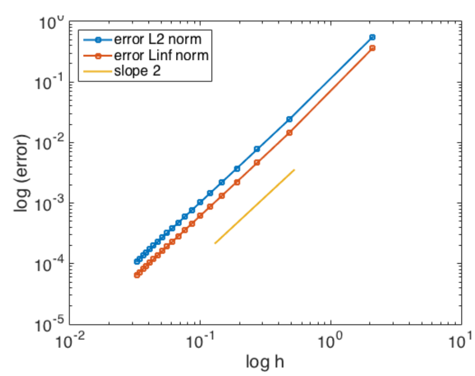

Figure 2.5: $\| U_h - U\|_2$ (blue curve) and $\| U_h - U\|_\infty$ (red curve) compared to the theoretical h^2 slope (yellow line)

2.4 Properties of the scheme and of the numerical solution

2.4.1 Consistence, stability and convergence

As seen before, when applied to an ODE or a PDE, the finite difference method leads (at least for linear equations) to a linear system $A_h U_h = F$, while the exact equations are $A_h U + E_h = F$. At this stage, two questions arise naturally:

- Is the problem well posed, i.e. does the system have a unique solution U_h ?
- If the problem is well posed, does its numerical solution U_h converge to the exact continuous solution U as h tends to 0 ?

Definition 2.3. The scheme is said to be **consistent** iff $E_h \longrightarrow 0$ as $h \longrightarrow 0$.

Definition 2.4. The error of the numerical solution is $\|U_h - U\| = \|A_h^{-1} E_h\| \leq \|A_h^{-1}\| \, \|E_h\|$. The fact that $\|A_h^{-1}\|$ is bounded independently of h is called **stability**.

Theorem 2.5. Stability and consistency lead obviously to **convergence**: $U_h \longrightarrow U$ as $h \longrightarrow 0$. This is even an equivalence for simple linear problems.

Example *In the preceding example, A_h is invertible, since it is a symmetric positive definite matrix. Therefore (2.8) is well posed.*
Given its expression, E_h obviously tends to 0 as h tends to 0: the numerical scheme is consistent. To get the convergence of the approximation method, we have thus to show that $\|A_h^{-1}\|$ is bounded independently of h. Note that this is not obvious at all, since A_h is a $N \times N$ matrix, with N tending to infinity as h tends to 0. In the present case, it can be shown for instance that $\|A_h^{-1}\| \leq \max\left(1, \dfrac{2(b-a)^2}{\pi^2}\right)$ for h sufficiently small.

2.4.2 Equivalent equation

Associated to convergence properties is the notion of **equivalent equation**. As a matter of fact, using Taylor expansion, the numerical scheme can be reformulated as a series (w.r.t. h), the first term of which (i.e. corresponding to h^0) is the original equation (iff the discretization is consistent). This expression is the so-called equivalent equation associated to the numerical scheme. However the most interesting term in the error is the one corresponding to the lowest power of h, also called **dominant error term**, which may give an indication on the way the numerical scheme modifies the true solution. That is why, by extension, the term **equivalent equation** is also frequently employed to indicate the original equation with only the dominant error term in addition.

Example *Coming back to the preceding example, we have:*

$$\frac{u(x+h) - 2u(x) + u(x-h)}{h^2} = u''(x) + \frac{h^2}{12} u^{(4)}(x) + \frac{h^4}{360} u^{(6)}(x) + \dots$$

Therefore the finite difference method actually solves the equivalent equation

$$-u''(x) - \frac{h^2}{12}u^{(4)}(x) - \frac{h^4}{360}u^{(6)}(x) - \ldots = f(x)$$

The dominant error term is: $-\frac{h^2}{12}u^{(4)}(x)$*, and the equation with this additional term only*

$$-u''(x) - \frac{h^2}{12}u^{(4)}(x) = f(x)$$

is also called the equivalent equation.

Some generic calculations facilitating the computation of equivalent PDEs are given in Appendix C.3 and a general result allowing for the interpretation of its dominant error term is given in Appendix C.4.

2.4.3 Other properties

Additional issues may also be of interest. For instance, it might be important that U_h also satisfies some specific mathematical or physical properties satisfied by U (e.g. conservation laws, symmetry, positivity...). Such properties are called **mimetic properties** of the numerical scheme.

Example *Let consider the homogeneous ODE* $-u''(x) = 0$ *on* (a, b)*, with Dirichlet boundary conditions* $u(a) = \alpha$ *and* $u(b) = \beta$*. The exact solution is obviously* $u(x) = \alpha + \frac{x-a}{b-a}(\beta - \alpha)$*. This function satisfies a so-called "maximum principle" (we will come back on this notion in the following chapters) in the sense that the extrema of the function are reached only on the boundary of the domain (for* $x = a$ *and* $x = b$*).*

Following the discretization used previously, the corresponding finite difference solution satisfies:

$$\begin{cases} -u_{i-1} + 2u_i - u_{i+1} = 0 & , i = 1, \ldots, N \\ u_0 = \alpha \ , \ u_{N+1} = \beta \end{cases}$$

Remarking that $u_i = \frac{1}{2}(u_{i-1} + u_{i+1})$*, a simple proof by contradiction shows that the approximate solution also reaches its extrema for* $x = a$ *and* $x = b$*. This is a mimetic property of the numerical scheme.*

2.5 Considering boundary conditions

Until this point, we did not detail the management of boundary conditions in the finite difference method. This aspect was also hidden in the example of §2.3, due to the fact that we had homogeneous Dirichlet conditions $u(a) = u(b) = 0$.

The way boundary conditions must be accounted for depends on each particular case. One must check that the finite difference schemes are still valid in the vicinity of the boundary and, if it is not the case, locally use other schemes. Moreover, boundary conditions must be integrated in the system of discretized equations.

2.5.1 Validity of finite difference schemes near boundaries

Numerical schemes often cannot be used in the vicinity of the boundary. As an example, with the same notations as in section 2.3, if one approximates $u''(x)$ by

$$u''(x_i) = \frac{-u_{i-2} + 16\,u_{i-1} - 30\,u_i + 16\,u_{i+1} - u_{i+2}}{12\,h^2} + \mathcal{O}(h^4)$$

this scheme cannot be used for grid points x_1 and x_N, since x_{-1} and x_{N+2} do not exist. Other schemes must be considered, for instance the usual centered scheme:

$$u''(x_1) \simeq \frac{u_0 - 2u_1 + u_2}{h^2} \qquad \text{and} \qquad u''(x_N) \simeq \frac{u_{N-1} - 2u_N + u_{N+1}}{h^2}$$

However, as seen before, this scheme is only second-order accurate. Discretization errors will then be larger at these two points than elsewhere, which may corrupt the overall quality of the numerical solution. To avoid this, another possibility consists in using one-sided fourth-order schemes, the price to pay being a larger stencil.

2.5.2 Dirichlet conditions

Non homogeneous Dirichlet boundary conditions can be easily integrated within numerical schemes. For instance, if one replaces the homogeneous Dirichlet conditions $u(a) = u(b) = 0$ by nonhomogeneous ones $u(a) = \alpha$ and $u(b) = \beta$ in the example of §2.3, system (2.8) becomes

$$\frac{1}{h^2}\begin{pmatrix} 1 & 0 & & & 0 \\ -1 & 2 & -1 & & \\ & \ddots & \ddots & \ddots & \\ & & -1 & 2 & -1 \\ 0 & & & 0 & 1 \end{pmatrix}\begin{pmatrix} u_0 \\ u_1 \\ \vdots \\ u_N \\ u_{N+1} \end{pmatrix} = \begin{pmatrix} \alpha \\ f(x_1) \\ \vdots \\ f(x_N) \\ \beta \end{pmatrix}$$

or, if directly eliminating u_0 and u_{N+1}:

$$\frac{1}{h^2}\begin{pmatrix} 2 & -1 & & & 0 \\ -1 & 2 & -1 & & \\ & \ddots & \ddots & \ddots & \\ & & -1 & 2 & -1 \\ 0 & & & -1 & 2 \end{pmatrix}\begin{pmatrix} u_1 \\ \vdots \\ \\ \vdots \\ u_N \end{pmatrix} = \begin{pmatrix} f(x_1) + \dfrac{\alpha}{h^2} \\ \vdots \\ \vdots \\ f(x_N) + \dfrac{\beta}{h^2} \end{pmatrix}$$

2.5.3 Neumann conditions

In case of a Neumann boundary condition, the derivative must of course also be approximated by a finite difference scheme. For instance, if one replaces the Dirichlet condition $u(a) = \alpha$ by the Neumann condition $u'(a) = \alpha$ in the previous example, one can use the first-order approximation:

$$\frac{u_1 - u_0}{h} = \alpha$$

which leads to the system

$$\frac{1}{h^2}\begin{pmatrix} -h & h & & & 0 \\ -1 & 2 & -1 & & \\ & \ddots & \ddots & \ddots & \\ & & -1 & 2 & -1 \\ 0 & & & 0 & 1 \end{pmatrix}\begin{pmatrix} u_0 \\ u_1 \\ \vdots \\ u_N \\ u_{N+1} \end{pmatrix} = \begin{pmatrix} \alpha \\ f(x_1) \\ \vdots \\ f(x_N) \\ \beta \end{pmatrix}$$

One could also use the second-order scheme

$$\frac{-3u_0 + 4u_1 - u_2}{2h} = \alpha$$

leading in that case to

$$\frac{1}{h^2}\begin{pmatrix} -3h & 4h & -h & & 0 \\ -1 & 2 & -1 & & \\ & \ddots & \ddots & \ddots & \\ & & -1 & 2 & -1 \\ 0 & & & 0 & 1 \end{pmatrix}\begin{pmatrix} u_0 \\ u_1 \\ \vdots \\ u_N \\ u_{N+1} \end{pmatrix} = \begin{pmatrix} 2\alpha \\ f(x_1) \\ \vdots \\ f(x_N) \\ \beta \end{pmatrix}$$

2.6 The n-D case

Most PDEs involve more than one space variable. However, even in n-D with $n > 1$, the discretization of differential operators very often requires 1-D finite difference schemes only, since it can be done in each direction independently.

Example *Let consider the 2-D Laplacian operator* $\Delta u(x, y) = \dfrac{\partial^2 u}{\partial x^2}(x, y) + \dfrac{\partial^2 u}{\partial y^2}(x, y)$. *Using the usual second-order centered approximation (2.5) for the second derivative, one gets immediately:*

$$\frac{u(x+h, y) - 2u(x, y) + u(x-h, y)}{h^2} + \frac{u(x, y+k) - 2u(x, y) + u(x, y-k)}{k^2} = \Delta u(x, y) + \mathcal{O}(h^2 + k^2)$$

or, taking $h = k$*:*

$$\frac{u(x+h, y) + u(x-h, y) + u(x, y+h) + u(x, y-h) - 4u(x, y)}{h^2} = \Delta u(x, y) + \mathcal{O}(h^2) \quad (2.9)$$

2.2 Building a Finite Difference Scheme

This corresponds to sections 2.2.1 and 2.2.2.
Consider a uniform grid with mesh size h. A generic finite difference scheme can be written as

$$u^{(p)}(x) \approx \sum_{j=1}^{q} \beta_j u(x_{k_j} h) - \frac{1}{h^p}\left(\sum_{j=1}^{q} \beta_j\right) u(x) \tag{2.1}$$

where $k_1, \cdots, k_q$ are non-zero relative integers. The β_js will then be obtained by solving the Vandermonde system

$$\begin{pmatrix} k_1 & k_2 & \cdots & k_q \\ \vdots & & & \vdots \\ k_1^{p-1} & k_2^{p-1} & \cdots & k_q^{p-1} \\ k_1^{p} & k_2^{p} & \cdots & k_q^{p} \\ k_1^{p+1} & k_2^{p+1} & \cdots & k_q^{p+1} \\ \vdots & & & \vdots \\ k_1^{q} & k_2^{q} & \cdots & k_q^{q} \end{pmatrix} \begin{pmatrix} \beta_1 \\ \vdots \\ \beta_{p-1} \\ \beta_p \\ \beta_{p+1} \\ \vdots \\ \beta_q \end{pmatrix} = \begin{pmatrix} 0 \\ \vdots \\ 0 \\ p! \\ 0 \\ \vdots \\ 0 \end{pmatrix}$$

Example 2.2.1 (Finite Difference scheme)**.** *Consider the problem of approximating the 4th order derivative of some function $u(x)$ with 6 points. We then have $p = 4$, stencil $= \{x-3h, x-2h, x-h, x+h, x+2h, x+3h\}$, where p is the order of the function we want to approximate. We let $q = 6$, which is the size of our stencil. In order to create our Vandermonde matrix we first need to look at each stencil.*

$$\begin{aligned}
f(x+3h) &= f(x) - 3hf'(x) + \frac{9h^2 f''(x)}{2} - \frac{27h^3 f'''(x)}{6} + \frac{81h^4 f^4(x)}{24} - \frac{243h^5 f^{(5)}(x)}{120} + \frac{729h^6 f^{(6)}(x)}{720} \\
f(x-2h) &= f(x) - 2hf'(x) + \frac{4h^2 f''(x)}{2} - \frac{8h^3 f'''(x)}{6} + \frac{16h^4 f^4(x)}{24} - \frac{32h^5 f^{(5)}(x)}{120} + \frac{64h^6 f^{(6)}(x)}{720} \\
f(x-h) &= f(x) + hf'(x) + \frac{h^2 f''(x)}{2} + \frac{h^3 f'''(x)}{6} + \frac{h^4 f^4(x)}{24} + \frac{h^5 f^{(5)}(x)}{120} + \frac{h^6 f^{(6)}(x)}{720} \\
f(x+h) &= f(x) - hf'(x) + \frac{h^2 f''(x)}{2} - \frac{h^3 f'''(x)}{6} + \frac{h^4 f^4(x)}{24} - \frac{h^5 f^{(5)}(x)}{120} + \frac{h^6 f^{(6)}(x)}{720} \\
f(x+2h) &= f(x) + 2hf'(x) + \frac{4h^2 f''(x)}{2} + \frac{8h^3 f'''(x)}{6} + \frac{16h^4 f^4(x)}{24} + \frac{32h^5 f^{(5)}(x)}{120} + \frac{64h^6 f^{(6)}(x)}{720} \\
f(x+3h) &= f(x) + 3hf'(x) + \frac{9h^2 f''(x)}{2} + \frac{27h^3 f'''(x)}{6} + \frac{81h^4 f^4(x)}{24} + \frac{243h^5 f^{(5)}(x)}{120} + \frac{729h^6 f^{(6)}(x)}{720}
\end{aligned}$$

Which has the Vandermonde matrix

$$\begin{pmatrix} -3 & -2 & -1 & 1 & 2 & 3 \\ 9 & 4 & 1 & 1 & 4 & 9 \\ -27 & -8 & -1 & 1 & 8 & 27 \\ 81 & 16 & 1 & 1 & 16 & 81 \\ -243 & -32 & -1 & 1 & 32 & 243 \\ 729 & 64 & 1 & 1 & 64 & 729 \end{pmatrix} \begin{pmatrix} \beta_1 \\ \beta_2 \\ \beta_3 \\ \beta_4 \\ \beta_5 \\ \beta_6 \end{pmatrix} = \begin{pmatrix} 0 \\ 0 \\ 0 \\ p! = 24 \\ 0 \\ 0 \end{pmatrix}$$

Solving this (using python) system we get :

$$\beta = \begin{pmatrix} -\frac{1}{6} \\ 2 \\ -\frac{13}{2} \\ -\frac{13}{2} \\ 2 \\ -\frac{1}{6} \end{pmatrix}$$

PDEs and numerical methods - Introduction to finite differences

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Exercise 1 – *1D schemes* See also NoteBook `SchemeBuilding`

1.1 Derive a symmetric scheme for $f''(x)$ with highest possible order using the points $x-2h$, $x-h$, $x+h$ and $x+2h$.

1.2 We want to derive finite difference schemes for $f^{(3)}(x)$ and $f^{(4)}(x)$ using the values of f at points $x-3h$, $x-2h$, $x-h$, x, $x+h$, $x+2h$, $x+3h$. Which approximation order can we expect? (do not derive the approximation schemes).

1.3 Same question with $x, x+h, x+2h, x+3h$.

1.4 Derive left-sided schemes of order 2 and 3 for $f''(x_0)$, assuming that one already knows that $f'(x_0) = 0$.

Exercise 2 – *Transfer functions* See also NoteBook `TransferFunctions`

2.1 Compare the transfer function of the second-order derivative with the transfer function of its usual second-order centered approximation scheme $\dfrac{u(x-h) - 2u(x) + u(x+h)}{h^2}$.

2.2 Same question for the interpolation operator $\dfrac{u(x-h) + u(x+h)}{2}$. Comment on the quality of the approximation for high frequencies.

Exercise 3 – *Equivalent differential equation* See also NoteBook `Sheet2-Exercise3`

Let the ODE : $u''(x) + \mu^2\, u(x) = 0$ for $x \in (a, b)$ discretized on a regular finite difference grid.

3.1 What is the equivalent differential equation if u'' is discretized using a standard two-sided second-order scheme ? What is the effect of the dominant error term?

3.2 We now suppose that u'' is discretized with a fourth-order scheme, but that $u(x)$ is approximated by $\dfrac{1}{2}\left(u(x+h) + u(x-h)\right)$. Same questions.

Exercise 4 – *Compact finite differences*

A drawback of usual finite difference schemes is that it is necessary to use a wide stencil to get a high order of accuracy. In this exercise, we introduce the so-called *compact schemes*, that address this point.

4.1 Let consider the formal relation

$$\alpha u'_{i-1} + u'_i + \alpha u'_{i+1} \simeq a\, \frac{u_{i+1} - u_{i-1}}{2h}$$

4.1.a Find α and a in order for this formula to be as accurate as possible. What is the order of approximation ?

4.1.b How can such a scheme be used in practice ? What about its computation cost ?

4.2 Generalize this approach starting with

$$\beta u'_{i-2} + \alpha u'_{i-1} + u'_i + \alpha u'_{i+1} + \beta u'_{i+2} \simeq a\, \frac{u_{i+1} - u_{i-1}}{2h} + b\, \frac{u_{i+2} - u_{i-2}}{4h}$$

4.3 What are the transfer functions of the preceding schemes ?

4.4 Propose a similar approach for the second-order derivative.

Exercise 5 – *Shooting method*

Let the ODE

$$(P) \quad \left\{ \begin{array}{rcl} y''(x) &=& a(x)y'(x) + b(x)y(x) + c(x) \qquad x \in (\alpha, \beta) \\ y(\alpha) &=& A, \quad y(\beta) = B \end{array} \right.$$

where a, b, c are given regular functions and A, B are given real numbers. Due to the two Dirichlet boundary conditions, a direct one-step method (Euler, Runge-Kutta...) cannot be used. That is why a finite difference scheme is usually implemented. However an alternative method, called *shooting method* can be used, which reduces this boundary value problem to two auxiliary initial value problems.

5.1 Prove that the solution of (P) is given by $\quad y(x) = Z(x) + \dfrac{B - Z(\beta)}{Y(\beta)} Y(x), \quad x \in (\alpha, \beta)$
where $Z(x)$ and $Y(x)$ are the solutions of

$$(P_c) \quad \left\{ \begin{array}{rcl} Z''(x) &=& a(x)Z'(x) + b(x)Z(x) + c(x) \\ Z(\alpha) &=& A, \quad Z'(\alpha) = 0 \end{array} \right.$$

and

$$(P_0) \quad \left\{ \begin{array}{rcl} Y''(x) &=& a(x)Y'(x) + b(x)Y(x) \\ Y(\alpha) &=& 0, \quad Y'(\alpha) = 1 \end{array} \right.$$

5.2 Give a numerical method to solve (P), using the Euler method.

Exercise 6 – *2D Laplacian*

6.1 Let a regular 2-D grid, with space steps h and k in directions x and y.

6.1.a Derive a second-order finite difference scheme for Δf using the five grid points $(x, y), (x \pm h, y), (x, y \pm k)$.

6.1.b Let suppose $h = k$. Simplify the preceding scheme. Derive another five-point scheme using the other set of five grid points $(x, y), (x \pm h, y \pm k)$.

6.1.c Is it possible to get a higher order scheme by combining those two schemes ?

6.2 Derive a scheme for Δu at point (x, y) as a function of the values of u at points $(x + a, y)$, $(x - b, y)$, $(x, y + c)$, $(x, y - d)$.

Exercise 7 – *2D Taylor formula*

7.1 The values of a real function f are given on the four vertices of a rectangle. Build a finite difference interpolation formulation for $f(M)$, for any M within the rectangle.

7.2 The values of a real function f are given on the three vertices A, B and C of a triangle. We seek an approximation of $\dfrac{\partial f}{\partial x} + \dfrac{\partial f}{\partial y}$ at point M within the triangle, under the form $\alpha f(A) + \beta f(B) + \gamma f(C)$. Derive the corresponding linear system for α, β and γ (do not solve it). What is the approximation order ?

2.3 Exercise sheet 2

2.3.1 1D schemes

1.1

Derive a symmetric scheme for $f''(x)$ with the highest possible order using the points, $x-2h, x-h, x+h, x+2h$. We have $p=2, q=4$, using the Taylor formula we have

$$\begin{aligned}
f(x-2h) &= f(x) - 2hf'(x) + \frac{4h^2 f''(x)}{2} - \frac{8h^3 f'''(x)}{6} + \frac{16h^4 f^4(x)}{24}\\
f(x-h) &= f(x) + hf'(x) + \frac{h^2 f''(x)}{2} + \frac{h^3 f'''(x)}{6} + \frac{h^4 f^4(x)}{24}\\
f(x+h) &= f(x) - hf'(x) + \frac{h^2 f''(x)}{2} - \frac{h^3 f'''(x)}{6} + \frac{h^4 f^4(x)}{24}\\
f(x+2h) &= f(x) + 2hf'(x) + \frac{4h^2 f''(x)}{2} + \frac{8h^3 f'''(x)}{6} + \frac{16h^4 f^4(x)}{24}
\end{aligned}$$

which gives us the Vandermonde matrix

$$\begin{pmatrix} -2 & -1 & 1 & 2 \\ 4 & 4 & 1 & 4 \\ -8 & -1 & 1 & 8 \\ 16 & 1 & 1 & 16 \end{pmatrix} \begin{pmatrix} \beta_1 \\ \beta_2 \\ \beta_3 \\ \beta_4 \end{pmatrix} = \begin{pmatrix} 0 \\ 2 \\ 0 \\ 0 \end{pmatrix}$$

We solve it directly using the augmented matrix :

$$\begin{pmatrix} -2 & -1 & 1 & 2 \\ 4 & 4 & 1 & 4 \\ -8 & -1 & 1 & 8 \\ 16 & 1 & 1 & 16 \end{pmatrix} \implies \left(\begin{array}{cccc|c} -1 & -\frac{1}{2} & \frac{1}{2} & 1 & 0 \\ 1 & \frac{1}{4} & \frac{1}{4} & 1 & \frac{1}{2} \\ -1 & -\frac{1}{8} & \frac{1}{8} & 1 & 0 \\ -1 & \frac{1}{16} & \frac{1}{16} & 1 & 0 \end{array}\right)$$

$$R_3 - R_1 \text{ and } R_4 - R_2 \implies$$

$$\left(\begin{array}{cccc|c} -1 & -\frac{1}{2} & \frac{1}{2} & 1 & 0 \\ 1 & \frac{1}{4} & \frac{1}{4} & 1 & \frac{1}{2} \\ 0 & \frac{3}{8} & -\frac{3}{8} & 0 & 0 \\ 0 & -\frac{3}{16} & -\frac{3}{16} & 0 & -\frac{1}{2} \end{array}\right) \implies \left(\begin{array}{cccc|c} -1 & -\frac{1}{2} & \frac{1}{2} & 1 & 0 \\ 1 & \frac{1}{4} & \frac{1}{4} & 1 & \frac{1}{2} \\ 0 & 1 & -1 & 0 & 0 \\ 0 & 1 & 1 & 0 & \frac{8}{3} \end{array}\right)$$

By R_3, R_4 we know that $\beta_2 = \beta_3$ and $2\beta_2 = \frac{4}{3} = \beta_3$. By R_1 we have $\beta_1 = \beta_4$ and by R_2, $2\beta_1 + \frac{4}{12} = \frac{1}{2} \implies \beta_1 = -\frac{1}{12} = \beta_4$ Thus,

$$\beta = \begin{pmatrix} -\frac{1}{12} \\ \frac{4}{3} \\ \frac{4}{3} \\ -\frac{1}{12} \end{pmatrix}$$

applying these coefficients to the equations we have

$$\begin{aligned}
-\frac{1}{12}f(x-2h) &= -\frac{1}{12}f(x) + \frac{1}{6}hf'(x) - \frac{h^2f''(x)}{6} + \frac{h^3f'''(x)}{9} - \frac{h^4f^4(x)}{18} \\
\frac{4}{3}f(x-h) &= \frac{4}{3}f(x) - \frac{4}{3}hf'(x) + \frac{2}{3}h^2f''(x) + \frac{2h^3f'''(x)}{9} + \frac{h^4f^4(x)}{18} \\
\frac{4}{3}f(x+h) &= \frac{4}{3}f(x) + \frac{4}{3}hf'(x) + \frac{2}{3}h^2f''(x) - \frac{2h^3f'''(x)}{9} + \frac{h^4f^4(x)}{18} \\
-\frac{1}{12}f(x-2h) &= -\frac{1}{12}f(x) - \frac{1}{6}hf'(x) - \frac{h^2f''(x)}{6} - \frac{h^3f'''(x)}{9} - \frac{h^4f^4(x)}{18}
\end{aligned}$$

This gives

$$\frac{30}{12}f(x) + h^2f''(x) + \mathcal{O}\left(h^5\right)$$

which results in the scheme

$$u''(x) = \frac{-f(x-2h) + 16f(x-h) + 30f(x) + 16f(x+h) - f(x+2h)}{12h^2}$$

1.2

Since we have symmetric schemes we can use the formula to find the approximation order.

$$p + 2 - q = \text{approx Order}$$

where $p =$ the points of the stencil (not including $f(x)$) and q is the order we want to find. Thus, for $f^{(3)}(x)$ we have

$$6 + 2 - 3 = 5$$

and for $f^{(4)}$ we have

$$6 + 2 - -4 = 4$$

1.3

We no longer have a symmetric scheme. Therefore, we use the formula

$$p + 1 - q = \text{approx Order}$$

Our stencil is $x, x+h, x+2h, x+3h$. Thus, for $f^{(3)}(x)$ we have

$$3 + 1 - 3 = 1$$

and for $f^{(4)}(x)$ we have

$$3 + 1 - 4 = 0$$

which does not converge not matter what h is chosen.

2.3.2 Transfer Functions

2.1

We first find the exact transfer function of $u''(x)$, given by

$$S\left(u_{\omega}\right)(x) = \left(e^{i\omega x}\right)'' = -\omega^2 e^{i\omega x} = -\omega^2 u_{\omega}$$

so we can say that the transfer function is

$$T\left(\omega\right) = -\omega^2$$

The scheme to analyze is

$$\frac{u(x-h) - 2u(x) + u(x_h)}{h^2}$$

and

$$\begin{aligned}
&e^{i\omega(x-1)} - 2e^{i\omega x} + e^{i\omega(x+1)}\\
&e^{i\omega x}\left(e^{-i\omega} - 2 + e^{i\omega}\right)\\
&u_{\omega}\left(2\cos(\omega) - 2\right)\\
&-4\sin^2\left(\frac{\omega}{2}\right)u_{\omega}
\end{aligned}$$

This gives

$$\begin{aligned}
T_1\left(\omega\right) &= 2\left(1 - \frac{\omega^2}{2} + \frac{\omega^4}{4} + \mathcal{O}\left(\omega^5\right)\right) - 2\\
&= -\omega^2 + \frac{\omega}{12} + \mathcal{O}\left(\omega^5\right)
\end{aligned}$$

This scheme is dissipative due to the fact that the amplitude has been altered.

2.2

Consider

$$\frac{u(x-h) + u(x+h)}{2}$$

which is a scheme for finding f'. Thus, the exact spectral analysis gives,

$$S(u_{\omega})(x) = \left(e^{i\omega x}\right)' = i\omega e^{i\omega x} = i\omega u_{\omega}$$

with transfer function :

$$T(\omega) = i\omega$$

$$\frac{e^{i\omega(x-1)}+e^{i\omega(x+1)}}{2}$$
$$\frac{1}{2}e^{i\omega x}\left(e^{-i\omega}+e^{i\omega}\right)$$
$$e^{i\omega x}\frac{1}{2}\left(e^{i\omega}+e^{-i\omega}\right)$$
$$e^{i\omega x}\cos(\omega)$$

which gives

$$T_1(\omega)=\cos\omega$$

Since $\omega\in[0,\pi]$ we can see that, the greater ω, the smaller h must be.

2.3.3 Excercise 3 : Equivalent differential equation

Consider

$$u''(x)+\mu^2u(x)=0 \quad \text{for } x\in[a,b] \tag{2.2}$$

discretized on a regular finite difference grid.

3.1

What is the equivalent ODE?
If we have a standard two-sided second-order scheme then

$$u''(x)\approx\frac{u(x+h)-2u(x)+u(x-h)}{2}+\frac{h^2}{12}u^{(4)}(x)+\mathcal{O}(h^4)$$

substituting into 2.2 we get

$$\frac{u(x+h)-2u+u(x-h)}{h^2}+\mu^2u=0 \tag{S$_h$}$$

and

$$\frac{h^2}{12}u^{(4)}+u''+\mu^2u=0$$

This ODE is close to (S_h) up to a 4th order, while the original equation is up to only a 2nd order. Thus, inspection of analytic solutions will give us some insight to the numerical solution of (S_h).
Solution to the ODE

$$\frac{h^2}{12}X^4+X^2+\mu^2=0$$

Let $Y=X^2$,

$$\frac{h^2}{12}Y^2+Y+\mu^2=0$$

Using quadratic formula,

$$\frac{1\pm\sqrt{1-\frac{h^2\mu^2}{3}}}{\frac{h^2}{6}}$$

which gives

$$R_1 = \frac{6}{h^2}\left(1+\sqrt{1-\frac{h^2\mu^2}{3}}\right) \qquad R_2 = \frac{6}{h^2}\left(1-\sqrt{1-\frac{h^2\mu^2}{3}}\right)$$

Therefore,

$$X = \pm i r_j \qquad r_j = \sqrt{-R_j} \qquad j = 1,2$$

2.3.4 Compact Finite Differences

$$\alpha u'_{i-1} + u'_i + \alpha u'_{i+1} \approx a\frac{u_{i+1}-u_{i-1}}{2h} \tag{2.3}$$

1.a

Find α and a in order for this formula to be as accurate as possible. What is the order of approximation?

We first expand the right hand side of 2.3

$$a\frac{u_{i+1}-u_{i-1}}{2h} = u' + \frac{h^2}{6}u^{(3)} + \mathcal{O}\left(h^5\right)$$

Similarly, we have for the left hand side

$$\begin{aligned}\alpha u'_{i-1} &= u'(x) - hu''(x) + \frac{h^2}{2}u^{(3)}(x) - \frac{h^3}{6}u^{(4)}(x) + \mathcal{O}\left(h^4\right)\\ \alpha u'_{i+1} &= u'(x) + hu''(x) + \frac{h^2}{2}u^{(3)}(x) + \frac{h^3}{6}u^{(4)}(x) + \mathcal{O}\left(h^4\right)\end{aligned}$$

We cancel the 2nd and 4th order terms. Finally,

$$\begin{aligned}\alpha\left(2u'(x) + h^2u^{(3)}(x)\right) + u'_i &\approx au' + a\frac{h^2}{6}u^{(3)}\\ u'(x)\left(2\alpha+1\right) + \alpha u^{(3)}(x) &\approx au' + a\frac{h^2}{6}u^{(3)}\end{aligned}$$

With some simple algebra we have

$$\begin{aligned}2\alpha + 1 &= a \qquad & \alpha &= \frac{a}{6}\\ a &= \frac{3}{2} \qquad & \alpha &= \frac{1}{4}\end{aligned}$$

Plugging into the original equation gives

$$\frac{1}{4}u'_{i-1} + u'_i + \frac{1}{4}u'_{i+1} \approx \frac{3}{2}\frac{u_{i+1}-u_{i-1}}{4h}$$

The left hand side of 2.3 is of of 4th order accuracy and the right is of 5th order accuracy, this results in a final solution having 4th order accuracy.

2.3.5 Shooting method

2.3.6 2D Laplacian

a)

$$f(x+h,y) = f(x,y) + h\partial_x f(x+h,y) + \frac{h^2 \partial_{x^2} f(x+h,y)}{2} + \mathcal{O}(h^2)$$

$$f(x-h,y) = f(x,y) - h\partial_x f'(x+h,y) + \frac{h^2 \partial_{x^2} f(x+h,y)}{2} + \mathcal{O}(h^2)$$

$$f(x,y+k) = f(x,y) + k\partial_y f(x,y+k) + \frac{k^2 \partial_{y^2} f(x,y+k)}{2} + \mathcal{O}(h^2)$$

$$f(x,y-k) = f(x,y) - k\partial_y f(x,y-k) + \frac{k^2 \partial_{y^2} f(x,y-k)}{2} + \mathcal{O}(h^2)$$

which gives us

$$\frac{f(x+h,y) - 2f(x,y) + f(x-h,y)}{h^2} + \mathcal{O}(h^2) + \frac{f(x,y+k) - 2f(x,y) + f(x,y-k)}{k^2} + \mathcal{O}(k^2)$$

b)

We simplify the above scheme to

$$\frac{f(x+h,y) + f(x-h,y) - 4f(x,y) + f(x,y+h) + f(x,y-h)}{h^2} + \mathcal{O}(h^2)$$

We now wish to derive another scheme using the other five gridpoints.

$$f(x+h, y+k) = f(x,y) + h\partial_x f(x+h, y+k) + k\partial_y f(x+h, y+k) + \frac{h^2\partial_{x^2} f(x+h, y+k)}{2}$$
$$+\frac{hk\partial_{xy} f(x+h, y+k)}{2} + \frac{k^2\partial_{y^2} f(x+h, y+k)}{2} + \mathcal{O}(h^2, k^2)$$
$$f(x+h, y-k) = f(x,y) + h\partial_x f(x+h, y+k) - k\partial_y f(x+h, y-k) + \frac{h^2\partial_{x^2} f(x+h, y-k)}{2}$$
$$-\frac{hk\partial_{xy} f(x+h, y-k)}{2} + \frac{k^2\partial_{y^2} f(x+h, y-k)}{2} + \mathcal{O}(h^2, k^2)$$
$$f(x-h, y+k) = f(x,y) - h\partial_x f(x-h, y+k) + k\partial_y f(x-h, y+k) + \frac{h^2\partial_{x^2} f(x-h, y+k)}{2}$$
$$-\frac{hk\partial_{xy} f(x-h, y+k)}{2} + \frac{k^2\partial_{y^2} f(x-h, y+k)}{2} + \mathcal{O}(h^2, k^2)$$
$$f(x-h, y-k) = f(x,y) - h\partial_x f(x-h, y-k) - k\partial_y f(x-h, y-k) + \frac{h^2\partial_{x^2} f(x-h, y-k)}{2}$$
$$+\frac{hk\partial_{xy} f(x-h, y-k)}{2} + \frac{k^2\partial_{y^2} f(x-h, y-k)}{2} + \mathcal{O}(h^2, k^2)$$

Adding these all together we have

$$4f(x,y) + 2h^2\partial_{x^2} f + 2k^2\partial_{y^2} f + \mathcal{O}\left(h^2, k^2\right)$$

Thus,

$$\frac{f(x+h, y+k) + f(x+h, y-k) - 4f(x,y) + f(x-h, y+k) + f(x+h, y-k)}{h^2} + \mathcal{O}\left(h^2, k^2\right)$$

c)

In the 1st scheme, when we try to expand we have $\partial_x^{(4)} f$ and $\partial_y^{(4)} f$ in the error term. In the second scheme we get error terms involving $\partial_{xxyy}^{(4)} f$ which cannot be canceled. Thus we cannot get a higher order scheme using a combination of these two.

2.3.7 Exercise 7 : 2D Taylor Formula

Chapter 3

Laplace and Poisson Equations

3.1 Class notes

However, if one considers a more complex stencil involving other grid points, it may be necessary to use a multi-dimensional Taylor formula to build the finite difference scheme. For instance, in 2-D:

Theorem 2.6. The **Taylor formula in two real variables** reads:

$$\begin{aligned} u(x+h,y+k) = u(x,y) \quad &+ \quad h\,\frac{\partial u}{\partial x}(x,y) + k\,\frac{\partial u}{\partial y}(x,y) \\ &+ \quad \frac{h^2}{2}\,\frac{\partial^2 u}{\partial x^2}(x,y) + hk\,\frac{\partial^2 u}{\partial x \partial y}(x,y) + \frac{k^2}{2}\,\frac{\partial^2 u}{\partial y^2}(x,y) \\ &\vdots \\ &+ \quad \sum_{p=0}^{n} \frac{h^p k^{n-p}}{p!\,(n-p)!}\,\frac{\partial^n u}{\partial x^p \partial y^{n-p}}(x,y) \\ &+ \quad \mathcal{O}(h^{n+1}+k^{n+1}) \end{aligned}$$

Example *Coming back to the 2-D Laplacian operator, the preceding Taylor formula can be used to prove that*

$$\frac{u(x+h,y+h)+u(x-h,y+h)+u(x+h,y-h)+u(x-h,y-h)-4u(x,y)}{2h^2} = \Delta u(x,y) + \mathcal{O}(h^2)$$

More precisely:

$$\frac{u(x+h,y+h)+u(x-h,y+h)+u(x+h,y-h)+u(x-h,y-h)-4u(x,y)}{2h^2} = \\ \Delta u(x,y) + \frac{h^2}{12}\left(\frac{\partial^4 u}{\partial x^4}(x,y) + 6\frac{\partial^4 u}{\partial x^2\,\partial y^2}(x,y) + \frac{\partial^4 u}{\partial y^4}(x,y)\right) + o(h^2)$$

while the more usual scheme (2.9) *satisfies*

$$\frac{u(x+h,y)+u(x-h,y)+u(x,y+h)+u(x,y-h)-4u(x,y)}{h^2} = \\ \Delta u(x,y) + \frac{h^2}{12}\left(\frac{\partial^4 u}{\partial x^4}(x,y) + \frac{\partial^4 u}{\partial y^4}(x,y)\right) + o(h^2)$$

Chapter 3

Laplace and Poisson problems

3.1 Some vocabulary

The steady-state solution of a physical phenomenon governed by diffusion satisfies

$$-\text{div}\,(k(\mathbf{x})\,\nabla u(\mathbf{x})) = f$$

where u is the state variable (temperature, chemical concentration...), k is the diffusion coefficient and f the forcing term (source/sink).

If k is actually a constant, the PDE becomes $-k\,\Delta u = f$, called a **Poisson equation**.

Moreover, if f is equal to zero, the PDE becomes $\Delta u = 0$, called a **Laplace equation**. The solutions of Laplace equation are called **harmonic functions**.

3.2 Some general remarks on harmonic functions

3.2.1 Harmonic functions in $\mathbb{R}^2$

Examples of harmonic functions in $\mathbb{R}^2$ are:

- $u(x, y) = a(x^2 - y^2) + bxy + cx + dy + e$
- $\begin{cases} u^1_\lambda(x, y) = (a\cos\lambda x + b\sin\lambda x)(ce^{\lambda y} + de^{-\lambda y}) \\ u^2_\lambda(x, y) = (ae^{\lambda x} + be^{-\lambda x})(c\cos\lambda y + d\sin\lambda y) \end{cases} \qquad \forall\lambda \in \mathbb{R}, \forall a, b, c, d \in \mathbb{R}$
- In polar coordinates:

$$\begin{cases} u_0(r, \theta) = c_0 \ln r + d_0 \\ u_n(r, \theta) = (a_n \cos n\theta + b_n \sin n\theta)\left(c_n r^n + \dfrac{d_n}{r^n}\right) \qquad \forall n \in \mathbb{N}^* \end{cases} \quad \text{for } r \neq 0,\ \forall a_n, b_n, c_n, d_n \in \mathbb{R}$$

Moreover, Δ being a linear operator, any linear combination of harmonic functions is also an harmonic function.
Therefore there are "many" harmonic functions since Span $\{u^1_\lambda, u^2_\lambda, \lambda \in \mathbb{R}\}$, which is a space of uncountable infinite dimension, is included in the set of harmonic functions in $\mathbb{R}^2$.

3.2.2 Harmonic functions in bounded domains in $\mathbb{R}^2$

PDEs are often defined on bounded domains, rather than on $\mathbb{R}^n$. Analytical solutions can be found in some cases, in particular for domains with simple geometries, like rectangles or disks in $\mathbb{R}^2$. This is the case for the Laplace equation, where preceding elementary harmonic functions can be combined to get solutions on particular domains. For instance:

- The solution to the Laplace equation in $\Omega = (0, L_x) \times (0, L_y)$ with Dirichlet boundary conditions $u(0, y) = h(y), u(L_x, y) = u(x, 0) = u(x, L_y) = 0$ can be obtained by a separation of variables technique. It reads

$$u(x,y) = \sum_{k\geq 1} \alpha_k \left(e^{\lambda_k x} - e^{\lambda_k (2L_x - x)}\right) \sin(\lambda_k y)$$

  where $\lambda_k = \dfrac{k\pi}{L_y}$ and $\alpha_k = \dfrac{2}{L_y\,(1 - e^{2\lambda_k L_x})} \displaystyle\int_0^{L_y} h(y) \sin(\lambda_k y)\, dy.$

- The solution to the Laplace equation on the open disk Ω of center $(0,0)$ and radius R with Dirichlet boundary conditions $u = g(\theta)$ is

$$u(r,\theta) = K(r,\theta)*g(\theta) = \frac{1}{2\pi}\int_0^{2\pi} K(r,\theta-\alpha) g(\alpha)\, d\alpha \quad \text{where } K(r,\theta) = \frac{R^2 - r^2}{R^2 + r^2 - 2rR\cos\theta}$$

3.2.3 Some properties of harmonic functions

The harmonic functions share a number of properties. For an open set $\Omega \subset \mathbb{R}^n$:

- **Global influence of boundary values**: u changes everywhere in Ω as soon as the Dirichlet boundary data changes somewhere on $\partial\Omega$.

- **Regularity**: If the Dirichlet boundary data $g \in \mathcal{C}^0(\partial\Omega)$ then $u \in \mathcal{C}^\infty(\Omega)$.

- **Mean value property**: Let $B(\mathbf{x}, r)$ denote the ball of center $\mathbf{x}$ and radius r. For each closed ball $B(\mathbf{x}, r) \subset \Omega$:

$$u(\mathbf{x}) = \frac{1}{|B(\mathbf{x},r)|}\int_{B(\mathbf{x},r)} u(\mathbf{y})\, d\mathbf{y} = \frac{1}{|\partial B(\mathbf{x},r)|}\int_{\partial B(\mathbf{x},r)} u(\boldsymbol{\sigma})\, d\boldsymbol{\sigma}$$

  This means that the value of an harmonic function at point $\mathbf{x}$ is the average of its values over every ball and every sphere which center is $\mathbf{x}$ and which is contained in the domain. One can even prove that, if u is a $\mathcal{C}^2$ function that satisfies the mean value property, then u is an harmonic function.

- **Maximum principle**: If $u \in \mathcal{C}^2(\Omega)$ and $u \in \mathcal{C}^0(\overline{\Omega})$, then u has no extreme values in Ω.

3.3 Poisson equation in $\mathbb{R}^2$ and $\mathbb{R}^3$

In $\mathbb{R}^2$, the Laplacian operator in polar coordinates reads $\Delta u = \dfrac{\partial^2 u}{\partial r^2} + \dfrac{1}{r}\dfrac{\partial u}{\partial r} + \dfrac{1}{r^2}\dfrac{\partial^2 u}{\partial \theta^2}$.

The corresponding radial harmonic functions, defined on $\mathbb{R}^2 \setminus \{(0,0)\}$, are

$$u(r,\theta) = u(r) = a \ln r + b \qquad \forall a, b \in \mathbb{R}$$

In $\mathbb{R}^3$, the Laplacian operator in spherical coordinates reads

$$\Delta u = \frac{\partial^2 u}{\partial r^2} + \frac{2}{r}\frac{\partial u}{\partial r} + \frac{1}{r^2 \sin\phi}\frac{\partial^2 u}{\partial \theta^2} + \frac{1}{r^2 \sin\phi}\frac{\partial}{\partial \phi}\left(\sin\phi \frac{\partial u}{\partial \phi}\right)$$

The corresponding radial harmonic functions, defined on $\mathbb{R}^3 \setminus \{(0,0,0)\}$, are

$$u(r,\theta,\phi) = u(r) = \frac{a}{r} + b \qquad \forall a, b \in \mathbb{R}$$

The function

$$K(r) = \begin{cases} \dfrac{1}{2\pi} \ln r & \text{in } \mathbb{R}^2 \setminus \{(0,0)\} \\ \dfrac{-1}{4\pi r} & \text{in } \mathbb{R}^3 \setminus \{(0,0,0)\} \end{cases}$$

which corresponds to particular cases of the preceding radial harmonic functions, is called **Poisson kernel** in $\mathbb{R}^2$ or $\mathbb{R}^3$.

Theorem 3.1. Let consider the Poisson problem $\Delta u(\mathbf{x}) = f(\mathbf{x})$ in $\mathbb{R}^n$ ($n = 2$ or 3), with $\|u\| \to 0$ as $\|\mathbf{x}\| \to \infty$. Then $u = K * f$ is a solution to this problem.
Moreover, if $f \in \mathcal{C}^2$ and is zero far away from 0, then $u \in \mathcal{C}^2$.

Theorem 3.2. *(generalization to a bounded domain)*
Let Ω a bounded domain in $\mathbb{R}^n$ ($n = 2$ or 3), and $\mathbf{x} \in \Omega$. Let $K_\mathbf{x}$ the solution of

$$\begin{cases} \Delta K_\mathbf{x} &= 0 & \text{in } \Omega \\ K_\mathbf{x} &= K(. - \mathbf{x}) & \text{on } \partial\Omega \end{cases}$$

Let $G(\mathbf{x},\mathbf{y}) = K(\mathbf{y} - \mathbf{x}) - K_\mathbf{x}(\mathbf{y})$ (G is called a **Green function** associated to the Laplacian operator and to Ω).

Then $u(\mathbf{x}) = \displaystyle\int_\Omega f(\mathbf{y})\, G(\mathbf{x},\mathbf{y})\, d\mathbf{y} - \int_{\partial\Omega} g(\mathbf{s}) \frac{\partial G}{\partial \mathbf{n}}(\mathbf{s})\, ds$ is a solution to the Poisson problem

$$\begin{cases} \Delta u &= f & \text{in } \Omega \\ u &= g & \text{on } \partial\Omega \end{cases}$$

where f and g are given regular functions.

The proofs of these theorems imply the introduction of the so-called distribution theory.

3.4 Companion equations and operators

Several other operators are close to, or derived from, the Laplacian operator. Some well-known ones are:

- the **Helmholtz operator** $\Delta + \lambda^2\,\mathrm{Id}$. $\Delta u + \lambda^2 \ u = 0$ is the Helmholtz equation. It appears for instance in acoustics, seismology, electromagnetic radiation..., and actually for every problem linked to the diffusion equation or to the wave equation. As a matter of fact, as will be discussed later (see §6.2.4, §7.2.1 and Appendix B), solving the Helmholtz equation corresponds to looking for the eigenvalues and eigenfunctions of the Laplacian operator, which are fundamental components of the solutions of these equations.
- the **biharmonic operator** Δ^2: $\Delta^2 u = \Delta(\Delta u)$. It appears for instance in continuum mechanics. A famous example is also the *Chladni figures*, where an experimental device (sand on vibrating plates) highlights the zero isolines of its eigenfunctions.
- and more generally the iterated Laplacian operators Δ^p ($p \in \mathbb{N}$). They appear in particular in the parameterization of dissipation processes in fluid mechanics.

3.5 Finite difference schemes

As seen in Chapter 2, the usual discretization scheme for the second-order derivative is given by (2.5):

$$u''(x) = \frac{u(x+h) - 2u(x) + u(x-h)}{h^2} + \mathcal{O}(h^2)$$

Hence the usual second-order finite difference scheme for the Laplacian:

$$\Delta u_{i_1,i_2,\dots,i_N} = \frac{u_{i_1-1,i_2,\dots,i_N} - 2u_{i_1,i_2,\dots,i_N} + u_{i_1+1,i_2,\dots,i_N}}{h_1^2} + \dots + \frac{u_{i_1,i_2,\dots,i_N-1} - 2u_{i_1,i_2,\dots,i_N} + u_{i_1,i_2,\dots,i_N+1}}{h_N^2} + \mathcal{O}(h^2)$$

with the convention $h^2 = \sum_{i=1}^{N} h_i^2$.

In the particular case $N = 2$, it reads:

$$\Delta u_{i,j} = \frac{u_{i-1,j} - 2u_{i,j} + u_{i+1,j}}{h_x^2} + \frac{u_{i,j-1} - 2u_{ij} + u_{i,j+1}}{h_y^2} + \mathcal{O}(h^2) \ ,$$

which reduces to the well-known five-point scheme if $h_x = h_y$:

$$\Delta u_{i,j} = \frac{u_{i-1,j} + u_{i+1,j} + u_{i,j-1} + u_{i,j+1} - 4u_{ij}}{h^2} + \mathcal{O}(h^2)$$

The discretization of the Laplace equation with these second-order schemes leads to a numerical solution that obviously satisfies the maximum principle, since $u_{i_1,i_2,\dots,i_N}$ appears as a weighted average, with positive weights, of neighboring points.

Some properties of this scheme, and of an alternative 9-point scheme, are given in the exercise sheet.

3.2 Exercises

PDEs and numerical methods - Laplace and Poisson problems

Exercise 1 *A property of harmonic functions*

Let Ω an open set in $\mathbb{R}^n$, and a function $u : \Omega \to \mathbb{R}$.
u is an harmonic function iff $u \in \mathcal{C}^2(\Omega)$ and $\Delta u = 0$ on Ω.

1.1 Let u a quadratic form: $u(x_1, \dots, x_n) = \sum_{i=1}^{n} a_i\, x_i^2 + \sum_{i<j} b_{ij}\, x_i x_j$. What is the condition for u to be harmonic?
1.2 Prove that, if u is harmonic and if $u \in \mathcal{C}^3(\Omega)$, then $\dfrac{\partial u}{\partial x_i}$ is also harmonic ($i = 1, \dots, n$).
1.3 Prove that, if u is harmonic and if $u \in \mathcal{C}^{m+2}(\Omega)$, then its partial derivatives up to order m are also harmonic functions.

Exercise 2 *Laplace equation on a rectangle*

Let consider the problem:

$$\begin{cases} \Delta u = 0 \quad \text{in } (0, L_x) \times (0, L_y) \\ u(0,y) = h(y), u(L_x, y) = u(x,0) = u(x, L_y) = 0 \end{cases}$$

Using separation of variables, prove that $u(x,y) = \sum_{k \geq 1} \alpha_k \left(e^{\lambda_k x} - e^{\lambda_k (2L_x - x)} \right) \sin(\lambda_k y)$

where $\lambda_k = \dfrac{k\pi}{L_y}$ and $\alpha_k = \dfrac{2}{L_y\,(1 - e^{2\lambda_k L_x})} \displaystyle\int_0^{L_y} h(y)\, \sin(\lambda_k y)\, dy$

Exercise 3 *Laplace equation on a disk*

Let Ω the open disk of center $(0,0)$ and radius R. Let consider the problem:

$$\begin{cases} \Delta u &= 0 \qquad \text{in } \Omega \\ \quad u &= g(\theta) \qquad \text{on } \partial\Omega \end{cases} \tag{1}$$

The Laplacian operator in polar coordinates reads $\Delta u = \dfrac{\partial^2 u}{\partial r^2} + \dfrac{1}{r}\dfrac{\partial u}{\partial r} + \dfrac{1}{r^2}\dfrac{\partial^2 u}{\partial \theta^2}$.

3.1 Let first solve $\Delta u = 0$ without wondering about boundary conditions, looking for solutions of the form $u(r, \theta) = v(r) w(\theta)$ (separation of variables technique). Prove that this leads to two ODEs, one for v and one for w. Solve first the equation for w, noting that w must be 2π-periodic (since u is $\mathcal{C}^0$ and Ω is a disk). Then solve the equation for v.

The solution at the end should be:

$$u(r,\theta) = \sum_{n\geq 0} (\alpha_n \cos n\theta + \beta_n \sin n\theta)\ r^n \tag{2}$$

3.2 Assuming that $g \in \mathcal{C}^1$, its Fourier series reads $g(\theta) = a_0 + \sum_{n\geq 1} (a_n \cos n\theta + b_n \sin n\theta)$ with $a_0 = \dfrac{1}{2\pi}\displaystyle\int_0^{2\pi} g(\alpha)\, d\alpha$, $a_n = \dfrac{1}{\pi}\displaystyle\int_0^{2\pi} g(\alpha)\ \cos n\alpha\ \ d\alpha$, $b_n = \dfrac{1}{\pi}\displaystyle\int_0^{2\pi} g(\alpha)\ \sin n\alpha\ \ d\alpha$.

Using (2), prove that the solution of (1) is $u(r,\theta) = a_0 + \sum_{n\geq 1} (a_n \cos n\theta + b_n \sin n\theta) \left(\dfrac{r}{R}\right)^n$

3.3 Prove that the preceding expression can be transformed into

$$u(r,\theta) = \frac{1}{\pi}\left[\frac{1}{2}\int_0^{2\pi} g(\alpha)\ \ d\alpha + \sum_{n\geq 1} \frac{r^n}{R^n} \int_0^{2\pi} g(\alpha)\ \cos n(\theta-\alpha)\ \ d\alpha\right]$$

3.4 Prove that the preceding expression can be transformed into

$$u(r,\theta) = K(r,\theta) * g(\theta) = \frac{1}{2\pi}\int_0^{2\pi} K(r,\theta-\alpha) g(\alpha)\, d\alpha \quad \text{ where } K(r,\theta) = \frac{R^2 - r^2}{R^2 + r^2 - 2rR\cos\theta}$$

3.5 Admitting that $\dfrac{1}{2\pi}\displaystyle\int_0^{2\pi} K(r,\theta-\alpha)\, d\alpha = 1 \quad \forall r < R$ (you can actually prove it if you have 15 minutes left), prove that $u(r,\theta)$ satisfies the maximum principle.

Exercise 4 *1D and 2D Laplacian matrices*

4.1 Let first consider the ODE: $-u''(x) = f(x)$, $x \in (0, L)$, with $u(0) = u(L) = 0$.
What are the eigenvalues and eigenvectors of the second order derivative operator defined on the space $\{u \in \mathcal{C}^2(0,L), u(0) = u(L) = 0\}$?

4.2 Let now a standard second order finite difference discretization of this problem, with mesh step $h = L/(N+1)$. It reads

$$\frac{1}{h^2}\mathbf{A}_N\,\mathbf{U} = \mathbf{F} \quad \text{ with } \mathbf{A}_N = \begin{bmatrix} 2 & -1 & 0 & \cdots & 0 \\ -1 & 2 & -1 & & \vdots \\ 0 & \ddots & \ddots & \ddots & 0 \\ \vdots & & \ddots & \ddots & -1 \\ 0 & \cdots & 0 & -1 & 2 \end{bmatrix}$$

By analogy with the continuous case (or by a direct calculation), find the eigenvectors and eigenvalues of $\mathbf{A}_N$ (and make sure that it is consistent with the continuous case).
What is the condition number of $\mathbf{A}_N$?

4.3 Let consider now the 2D Poisson problem $-\Delta u = f$ on $\Omega = (0, L_x) \times (0, L_y)$, with zero Dirichlet boundary condition. We consider a regular discretization grid, with mesh steps $h_x = L_x/(N_x + 1)$ and $h_y = L_y/(N_y + 1)$ in the x and y directions respectively (N_x and N_y are integers).

4.3.1 Write the linear system $\mathbf{A}_{2D}\,\mathbf{U} = \mathbf{F}$ corresponding to the usual 5-point second order finite difference scheme for the Laplacian (with the unknowns ordered as $\mathbf{U}_{i+(j-1)N_x} = u_{ij}$).

The tensor product (also called Kronecker product) of 2 matrices $\mathbf{A}$ and $\mathbf{B}$ being defined, with obvious notations, as the block matrix

$$\mathbf{A} \otimes \mathbf{B} = \begin{bmatrix} a_{11}\mathbf{B} & a_{12}\mathbf{B} & \cdots & a_{1p}\mathbf{B} \\ \vdots & \vdots & \vdots & \vdots \\ a_{n1}\mathbf{B} & a_{n2}\mathbf{B} & \cdots & a_{np}\mathbf{B} \end{bmatrix},$$

prove that $\mathbf{A}_{2D} = \dfrac{1}{h_x^2}\,\mathbf{I}_{N_y} \otimes \mathbf{A}_{N_x} + \dfrac{1}{h_y^2}\,\mathbf{A}_{N_y} \otimes \mathbf{I}_{N_x}$ where $\mathbf{I}_n$ is the identity matrix of size n.

4.3.2 Prove that the eigenvalues and eigenvectors of $\mathbf{A}_{2D}$ are

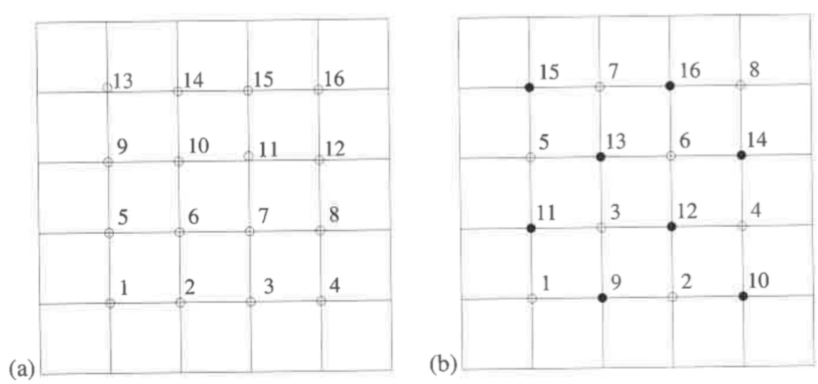
$$\lambda_{k,l} = \frac{4}{h_x^2}\sin^2\left(\frac{k\pi}{2(N_x+1)}\right) + \frac{4}{h_y^2}\sin^2\left(\frac{l\pi}{2(N_y+1)}\right) \qquad (1 \le k \le N_x, 1 \le l \le N_y)$$

and

$$X_{k,l}(i,j) = \sin\frac{k\pi i}{N_x+1}\ \sin\frac{l\pi j}{N_y+1} \qquad (1 \le k \le N_x, 1 \le l \le N_y)$$

4.3.3 What is the condition number of $\mathbf{A}_{2D}$?

4.3.4 Let consider the alternative so called "red-black" order of unknowns, as illustrated below for a 4×4 grid:



Left: natural rowwise ordering; Right: red-black ordering

What about the corresponding new form for $\mathbf{A}_{2D}$?

Exercise 5 *9-point 2D Laplacian - Fourth order scheme*

Let consider the Poisson problem $\Delta u = f$ in $\Omega \subset \mathbb{R}^2$. On a regular 2D grid, let consider the usual 5-point scheme for the Laplacian

$$\Delta_5 u_{ij} = \frac{1}{h^2}\left[u_{i-1,j} + u_{i+1,j} + u_{i,j-1} + u_{i,j+1} - 4u_{i,j}\right]$$

and the alternative 9-point scheme

$$\Delta_9 u_{ij} = \frac{1}{6h^2}\left[4u_{i-1,j} + 4u_{i+1,j} + 4u_{i,j-1} + 4u_{i,j+1} + u_{i-1,j-1} + u_{i+1,j-1} + u_{i-1,j+1} + u_{i+1,j+1} - 20u_{i,j}\right]$$

5.1 What is the dominant error term for each scheme ? Is the 9-point scheme more accurate than the 5-point one ?

Some results from Taylor expansions, to spare time:

$$u_{i-1,j} + u_{i+1,j} + u_{i,j-1} + u_{i,j+1} = 4u_{ij} + h^2\left(\frac{\partial^2 u}{\partial x^2} + \frac{\partial^2 u}{\partial y^2}\right) + \frac{h^4}{12}\left(\frac{\partial^4 u}{\partial x^4} + \frac{\partial^4 u}{\partial y^4}\right) + \mathcal{O}(h^4)$$

$$u_{i-1,j-1} + u_{i+1,j-1} + u_{i-1,j+1} + u_{i+1,j+1} = 4u_{ij} + 2h^2\left(\frac{\partial^2 u}{\partial x^2} + \frac{\partial^2 u}{\partial y^2}\right) + 2\frac{h^4}{12}\left(\frac{\partial^4 u}{\partial x^4} + 6\frac{\partial^4 u}{\partial x^2 \partial y^2} + \frac{\partial^4 u}{\partial y^4}\right) + \mathcal{O}(h^4)$$

5.2 Using the expression of $\Delta(\Delta u)$, prove that the 9-point scheme is actually fourth order accurate if f is an harmonic function (i.e. satisfies $\Delta f = 0$).

5.3 More generally, prove that solving $\Delta_9 u_{ij} = f_{ij}$ and defining

$$f_{ij} = f(x_i, y_j) + \frac{h^2}{12}\Delta f(x_i, y_j)$$

(if f is sufficiently smooth) instead of $f_{ij} = f(x_i, y_j)$ leads to a fourth order accurate method.

This method corresponds to deliberately introducing a $\mathcal{O}(h^2)$ error into the right-hand side of the equation that is chosen to exactly cancel the $\mathcal{O}(h^2)$ part of the local truncation error.

5.4 If f is known only at the grid points (but is known to be sufficiently smooth), prove that we can achieve the same fourth order accuracy by using

$$f_{ij} = f(x_i, y_j) + \frac{h^2}{12}\Delta_5 f(x_i, y_j)$$

3.3 Solutions

E1 : A property of harmonic functions

1.

$$\begin{aligned} u &= \sum_{i=1}^{n} a_i x_i^2 + \sum_{i<j} b_{ij} x_i x_j \\ \Delta u &= \sum_{i=1}^{n} 2a_i + 0 \\ 0 &= \sum_{i=1}^{n} 2a_i \end{aligned}$$

2. Since $u \in \mathscr{C}^3$, $\frac{\partial^3 u}{\partial x_i^3}$ exists

$$\begin{aligned} \sum_{i=1}^{n} \frac{\partial^3 u}{\partial x_i^3} u &= \sum_{i=1}^{n} \left(\frac{\partial u}{\partial x_i} \left(\frac{\partial^2 u}{\partial x_i^2} \right) \right) \\ &\forall j \in \{1, \cdots, n\} \text{ we have} \\ &= \frac{\partial u}{x_j} \sum_{i=1}^{n} \frac{\partial^2 u}{\partial x_i^2} \\ &= \frac{\partial u}{\partial x_j} (\Delta u) = 0 \end{aligned}$$

3. Since $u \in \mathscr{C}^{m+2}$, $\frac{\partial^{m+2} u}{\partial x_i^{m+2}}$ exists and

$$\begin{aligned} \sum_{i=1}^{n} \frac{\partial^{m+2} u}{\partial x_i^{m+2}} u &= \sum_{i=1}^{n} \left(\frac{\partial^m u}{\partial x_i^{m+2}} \left(\frac{\partial^2 u}{\partial x_i^2} \right) \right) \\ &\forall j \in \{1, \cdots, n\} \text{ we have} \\ &= \frac{\partial u^m}{x_j^m} \sum_{i=1}^{n} \frac{\partial^2 u}{\partial x_i^2} \\ &= \frac{\partial^m u}{\partial x_j^m} (\Delta u) = 0 \end{aligned}$$

3.3.1 E2 : Laplace equation on a rectangle

3.3.2 E3 : Laplace equation on a disk

3.3.3 E4 : 1D and 2D Laplacian matrices

3.3.4 E5 : 9-point 2D laplacian - Fourth order scheme

Chapter 4

Class notes

Appendix A

Reminder on Fourier series and Fourier transforms

A.1 Fourier series expansion

Let f a integrable and periodic function, with period L. One can then define:

$$F(x) = a_0 + \sum_{n\geq 1}\left(a_n \cos\frac{2\pi n x}{L} + b_n \sin\frac{2\pi n x}{L}\right)$$

with $a_0 = \frac{1}{L}\int_0^L f(x)\,dx$, $\quad a_n = \frac{2}{L}\int_0^L f(x)\,\cos\frac{2\pi n x}{L}\,dx$, $\quad b_n = \frac{2}{L}\int_0^L f(x)\,\sin\frac{2\pi n x}{L}\,dx$

F is the so-called **Fourier series expansion** of f.

This expansion also reads

$$F(x) = \sum_{n=-\infty}^{+\infty} c_n\, e^{\frac{2i\pi n x}{L}} \qquad \text{with } c_n = \frac{1}{L}\int_0^L f(x)\, e^{-\frac{2i\pi n x}{L}}\,dx$$

- If f is an even function, $b_n = 0 \quad \forall n \geq 1$ (i.e. $c_n = c_{-n} \quad \forall n$)
- If f is an odd function, $a_n = 0 \quad \forall n \geq 0$ (i.e. $c_n = -c_{-n} \quad \forall n$)

Theorem A.1. (**Pointwise convergence**)
If f is $\mathcal{C}^1(0, L)$, then $F = f$ (note that some similar results exist which require less regularity for f)

Theorem A.2. (**Parseval's equality**, or conservation of energy)
If $f \in \mathcal{L}^2(0, L)$, then

$$\frac{1}{L}\int_0^L |f(x)|^2\,dx = a_0^2 + \frac{1}{2}\sum_{n=1}^{+\infty}(a_n^2 + b_n^2) = \sum_{n=-\infty}^{+\infty} |c_n|^2$$

A.2 Fourier transform

Let f integrable on $\mathbb{R}$. The **Fourier transform** of f is

$$FT[f](\xi) = \widehat{f}(\xi) = \int_{\mathbb{R}} f(x)\, e^{-2i\pi\xi x}\, dx$$

and the **inverse Fourier transform** of $\widehat{f}$ is

$$FT^{-1}[\widehat{f}](x) = \int_{\mathbb{R}} \widehat{f}(\xi)\, e^{2i\pi\xi x}\, d\xi$$

Some properties of the Fourier transform

- If $f \in \mathcal{C}^1(\mathbb{R})$ and if $\widehat{f}$ is $L^1(\mathbb{R})$, then $FT^{-1}[\widehat{f}] = f$ (reciprocity of the Fourier transform)
- $\widehat{f}\,\widehat{g} = \widehat{f * g}$ Reminder: convolution product $(a * b)(x) = \displaystyle\int_{\mathbb{R}} a(y)\, b(x-y)\, dy$
- $\widehat{f} * \widehat{g} = \widehat{fg}$
- $\widehat{f'}(\xi) = 2i\pi\xi\, \widehat{f}(\xi)$
- If $g(x) = f(x - x_0)$, then $\widehat{g}(\xi) = e^{-2i\pi x_0 \xi}\, \widehat{f}(\xi)$
- The Fourier transform of the **Gaussian function** $\exp(-\pi\alpha x^2)$ is the Gaussian function $\dfrac{1}{\sqrt{\alpha}} \exp\left(-\dfrac{\pi}{\alpha}\,\xi^2\right)$
- The Fourier transform of the **gate function** $\Pi(x) = 1$ for $x \in (-1/2; 1/2)$ and 0 elsewhere is $\operatorname{sinc}(\pi\xi)$ where sinc is the **cardinal sine function** defined by $\operatorname{sinc} a = (\sin a)/a$.

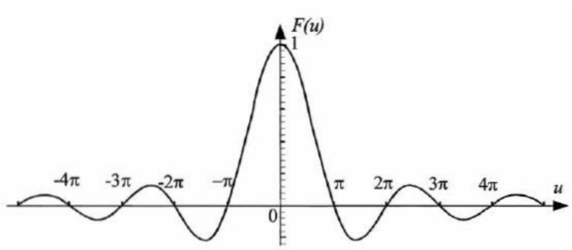


Figure A.1: Plot of the cardinal sine function $\operatorname{sinc} u = \dfrac{\sin u}{u}$

Theorem A.3. (**Parseval's equality**, or conservation of energy)
If $f \in \mathcal{L}^2(\mathbb{R})$, then

$$\int_{\mathbb{R}} |f(x)|^2\, dx = \int_{\mathbb{R}} \left|\widehat{f}(\xi)\right|^2\, d\xi$$

These definitions and properties of the Fourier transform in $\mathbb{R}$ can be directly generalized to $\mathbb{R}^n$.

Appendix B

The Laplacian operator and its spectrum

B.1 General results

Let $\Omega \subset \mathbb{R}^n$ a bounded domain, and consider the following eigenvalue problem:

$$\begin{cases} \Delta X(\mathbf{x}) = \displaystyle\sum_{i=1}^{n} \frac{\partial^2 X}{\partial x_i^2}(x_1, \ldots, x_n) = \lambda\, X(x_1, \ldots, x_n) & \mathbf{x} \in \Omega \\ X(\mathbf{x}) = 0 \quad \text{on } \partial\Omega & \end{cases}$$

Theorem B.1. There is a countable set of eigenvalues, all of them being negative: $\lambda_k = -\omega_k^2$. The corresponding eigenfunctions $X_k(\mathbf{x})$ form an orthonormal basis of $\mathcal{L}^2(\Omega)$.

The proof of this theorem can be found for instance in Evans (1998). It is quite long and technical, and is out of the scope of these notes, but note that two aspects at least are obvious:

- All eigenvalues are negative:

  $$(\Delta X - \lambda X = 0) \Longrightarrow \int_\Omega X \Delta X = -\int_\Omega \|\nabla X\|^2 = \lambda \int_\Omega X^2$$

  Hence

  $$\lambda = -\frac{\int_\Omega \|\nabla X\|^2}{\int_\Omega X^2} \leq 0$$

- Eigenfunctions associated to different eigenvalues are orthogonal:

  Let X_k and X_l two eigenfunctions associated to two different eigenvalues $-\omega_k^2$ and $-\omega_l^2$.

  $$\begin{cases} \Delta X_k + \omega_k^2 X_k = 0 & \Longrightarrow \int_\Omega \Delta X_k\, X_l + \omega_k^2 \int_\Omega X_k\, X_l = -\int_\Omega \nabla X_k\, \nabla X_l + \omega_k^2 \int_\Omega X_k\, X_l = 0 \\ \Delta X_l + \omega_l^2 X_l = 0 & \Longrightarrow \int_\Omega \Delta X_l\, X_k + \omega_l^2 \int_\Omega X_l\, X_k = -\int_\Omega \nabla X_l\, \nabla X_k + \omega_l^2 \int_\Omega X_l\, X_k = 0 \end{cases}$$

  Making the difference between those two equations yields $(\omega_k^2 - \omega_l^2) \displaystyle\int_\Omega X_l\, X_k = 0$, hence $\displaystyle\int_\Omega X_l\, X_k = 0$. Note that this also implies $\displaystyle\int_\Omega \nabla X_l\, \nabla X_k = 0$. X_k and X_l are orthogonal both in $L^2(\Omega)$ and in $H^1(\Omega)$.

B.2 The 1-D case

In the 1-D case, let consider $\Omega = (0, L)$. The eigenvalue problem reads

$$\begin{cases} X''(x) = \lambda\, X(x) & x \in (0, L) \\ X(0) = X(L) = 0 \end{cases}$$

As previously, λ is negative and can be written $\lambda = -\omega^2$. Hence $X''(x) + \omega^2 X(x) = 0$, which yields $X(x) = \alpha \sin \omega x + \beta \cos \omega x$. $X(0) = 0$ implies $\beta = 0$, while $X(L) = 0$ implies $\alpha \sin \omega L = 0$. Non zero solutions are then obtained for

$$\omega_k = \frac{k\pi}{L} \quad \text{and} \quad X_k(x) = \sin \frac{k\pi x}{L} \quad , k \in \mathbb{N}$$

Appendix C

Some generic calculations related to finite difference schemes

C.1 Fourier analysis: computation of transfer functions and stability studies

Computing both transfer functions (§2.2.4) and stability criteria (§4.3.2) requires some repetitive calculations involving complex exponentials. Some generic formula are given below, in order to facilitate these computations.

Transfer functions With the same notations as in §2.2.4:

Scheme	Transfer function	
$\dfrac{u(x-h)+u(x+h)}{2}$	$\cos\omega$	
$\dfrac{u(x+h)-u(x)}{h}$	$e^{i\omega}-1$	$= e^{i\omega/2}\,2i\,\sin(\omega/2)$
$\dfrac{u(x)-u(x-h)}{h}$	$1-e^{-i\omega}$	$= e^{-i\omega/2}\,2i\,\sin(\omega/2)$
$\dfrac{u(x+h)-u(x-h)}{2h}$	$i\,\sin\omega$	
$\dfrac{u(x+h)-2u(x)+u(x-h)}{h^2}$	$2\,(\cos\omega-1)$	

Note that these results can be easily adapted to slightly different schemes. For instance, if the scheme $S_h = \frac{\cdots}{h^p}$ has a transfer function $T(\omega)$, then the transfer function of $S_{\lambda h}$ is $\dfrac{1}{\lambda^p}\,T(\lambda\omega)$. This is useful typically for $\lambda = 2$ or $\lambda = 1/2$.

Amplification factors With usual notations, replacing u_j^n by $\xi^n e^{ipj\delta x}$ in a numerical scheme, one will obtain this term $\xi^n e^{ipj\delta x}$ multiplied by an amplification factor.

Scheme	Amplification factor	
$\dfrac{u_j^{n-1}+u_j^{n+1}}{2}$	$\dfrac{1/\xi+\xi}{2}$	$=\dfrac{\xi^2+1}{2\,\xi}$
$\dfrac{u_j^{n+1}-u_j^{n}}{\delta t}$	$\dfrac{\xi-1}{\delta t}$	
$\dfrac{u_j^{n+1}-u_j^{n-1}}{2\,\delta t}$	$\dfrac{\xi-1/\xi}{2\,\delta t}$	$=\dfrac{\xi^2-1}{2\,\xi\,\delta t}$
$\dfrac{u_j^{n+1}-2u_j^n+u_j^{n-1}}{\delta t^2}$	$\dfrac{\xi-2+1/\xi}{\delta t^2}$	$=\dfrac{(\xi-1)^2}{\xi\,\delta t^2}$
$\dfrac{u_{j-1}^n+u_{j+1}^n}{2}$	$\cos(p\,\delta x)$	
$\dfrac{u_{j+1}^n-u_j^n}{\delta x}$	$\dfrac{e^{ip\,\delta x}-1}{\delta x}$	$=e^{ip\,\delta x/2}\,\dfrac{2i\,\sin(p\delta x/2)}{\delta x}$
$\dfrac{u_j^n-u_{j-1}^n}{\delta x}$	$\dfrac{1-e^{-ip\,\delta x}}{\delta x}$	$=e^{-ip\,\delta x/2}\,\dfrac{2i\,\sin(p\delta x/2)}{\delta x}$
$\dfrac{u_{j+1}^n-u_{j-1}^n}{2\,\delta x}$	$\dfrac{i\,\sin(p\,\delta x)}{\delta x}$	
$\dfrac{u_{j+1}^n-2u_j^n+u_{j-1}^n}{\delta x^2}$	$2\;\dfrac{\cos(p\,\delta x)-1}{\delta x^2}$	

Note that these results can be easily adapted to slightly different schemes, for instance by multiplying the amplification factor by ξ if the scheme is at time $n+1$ instead of n, or by replacing δx by $2\delta x$ if the scheme involves $j-2$ and $j+2$ instead of $j-1$ and $j+1$.

Examples *Below are two applications of the previous tables.*

- *Let consider the Dufort-Frankel scheme for the 1-D diffusion equation:*

$$\frac{u_j^{n+1}-u_j^{n-1}}{2\delta t}-\nu\,\frac{u_{j+1}^n-2\,\dfrac{u_j^{n-1}+u_j^{n+1}}{2}+u_{j-1}^n}{\delta x^2}=0$$

Using the tables, replacing u_j^n by $\xi^n e^{ipj\delta x}$ immediatly leads to:

$$\frac{\xi^2-1}{2\,\xi\,\delta t}-\frac{\nu}{\delta x^2}\left(2\cos(p\,\delta x)-2\;\frac{\xi^2+1}{2\,\xi}\right)=0$$

i.e.

$$(2\lambda+1)\xi^2 - 4\lambda\cos(p\,\delta x)\,\xi + (2\lambda-1) = 0 \qquad \textit{with } \lambda = \frac{\nu\,\delta t}{\delta x^2}$$

One has then to study the modulus of ξ to prove the stability of the scheme.

- *Let consider the following scheme for the 1-D transport equation:*

$$\frac{u_j^{n+1}-u_j^{n-1}}{2\delta t} + c\left(\frac{4}{3}\,\frac{u_{j+1}^{n+1}-u_{j-1}^{n+1}}{2\,\delta x} - \frac{1}{3}\,\frac{u_{j+2}^{n}-u_{j-2}^{n}}{4\,\delta x}\right) = 0$$

Using the tables, replacing u_j^n by $\xi^n e^{ipj\delta x}$ directly leads to:

$$\frac{\xi^2-1}{2\,\xi\,\delta t} + c\,\xi\left(\frac{4}{3}\,\frac{i\,\sin(p\,\delta x)}{\delta x} - \frac{1}{3}\,\frac{i\,\sin(2p\,\delta x)}{2\delta x}\right) = 0$$

Hence
$$\xi^2 = \left[1 + i\,\frac{2c\,\delta t}{3\,\delta x}\left(4\sin(p\,\delta x) - \frac{1}{2}\sin(2p\,\delta x)\right)\right]^{-1}$$

which implies that $|\xi| \leq 1$.

C.2 Small o and big O

Definition C.1. $f(x) = o(x^p)$ (pronounce *small o*) in the vicinity of 0 iff $f(x) = x^p\,\varepsilon(x)$ with $\varepsilon(x) \to 0$ as $x \to 0$. In other words, $f(x)$ is negligible w.r.t. x^p in the vicinity of 0.

Definition C.2. $f(x) = \mathcal{O}(x^p)$ (pronounce *big o*) in the vicinity of 0 iff there exists two positive constants α and β such that $\alpha|x|^p \leq |f(x)| \leq \beta|x|^p$ in a neighborhood of 0. In other words, $f(x)$ is of the same order as x^p in the vicinity of 0.

C.3 Computation of equivalent PDEs

Computing equivalent PDEs requires linear combinations of Taylor expansions. Some formulas corresponding to frequently used schemes are given below, in order to facilitate these computations.

$$\frac{u(x,t+\delta t)+u(x,t-\delta t)}{2} = u(x,t) + \frac{\delta t^2}{2}\frac{\partial^2 u}{\partial t^2}(x,t) + \frac{\delta t^4}{24}\frac{\partial^4 u}{\partial t^4}(x,t) + \mathcal{O}(\delta t^6)$$

$$\frac{u(x,t+\delta t)-u(x,t)}{\delta t} = \frac{\partial u}{\partial t}(x,t) + \frac{\delta t}{2}\frac{\partial^2 u}{\partial t^2}(x,t) + \frac{\delta t^2}{6}\frac{\partial^3 u}{\partial t^3}(x,t) + \mathcal{O}(\delta t^3)$$

$$\frac{u(x,t)-u(x,t-\delta t)}{\delta t} = \frac{\partial u}{\partial t}(x,t) - \frac{\delta t}{2}\frac{\partial^2 u}{\partial t^2}(x,t) + \frac{\delta t^2}{6}\frac{\partial^3 u}{\partial t^3}(x,t) + \mathcal{O}(\delta t^3)$$

$$\frac{u(x,t+\delta t)-u(x,t-\delta t)}{2\,\delta t} = \frac{\partial u}{\partial t}(x,t) + \frac{\delta t^2}{6}\frac{\partial^3 u}{\partial t^3}(x,t) + \frac{\delta t^4}{120}\frac{\partial^5 u}{\partial t^5}(x,t) + \mathcal{O}(\delta t^6)$$

$$\frac{u(x,t+\delta t)-2u(x,t)+u(x,t-\delta t)}{\delta t^2} = \frac{\partial^2 u}{\partial t^2}(x,t) + \frac{\delta t^2}{12}\frac{\partial^4 u}{\partial t^4}(x,t) + \frac{\delta t^4}{360}\frac{\partial^6 u}{\partial t^6}(x,t) + \mathcal{O}(\delta t^6)$$

$$\frac{u(x+\delta x,t)+u(x-\delta x,t)}{2} = u(x,t) + \frac{\delta x^2}{2}\frac{\partial^2 u}{\partial x^2}(x,t) + \frac{\delta x^4}{24}\frac{\partial^4 u}{\partial x^4}(x,t) + \mathcal{O}(\delta x^6)$$

$$\frac{u(x+\delta x,t)-u(x,t)}{\delta x} = \frac{\partial u}{\partial x}(x,t) + \frac{\delta x}{2}\frac{\partial^2 u}{\partial x^2}(x,t) + \frac{\delta x^2}{6}\frac{\partial^3 u}{\partial x^3}(x,t) + \mathcal{O}(\delta x^3)$$

$$\frac{u(x,t)-u(x-\delta x,t)}{\delta x} = \frac{\partial u}{\partial x}(x,t) - \frac{\delta x}{2}\frac{\partial^2 u}{\partial x^2}(x,t) + \frac{\delta x^2}{6}\frac{\partial^3 u}{\partial x^3}(x,t) + \mathcal{O}(\delta x^3)$$

$$\frac{u(x+\delta x,t)-u(x-\delta x,t)}{2\,\delta x} = \frac{\partial u}{\partial x}(x,t) + \frac{\delta x^2}{6}\frac{\partial^3 u}{\partial x^3}(x,t) + \frac{\delta x^4}{120}\frac{\partial^5 u}{\partial x^5}(x,t) + \mathcal{O}(\delta x^6)$$

$$\frac{u(x+\delta x,t)-2u(x,t)+u(x-\delta x,t)}{\delta x^2} = \frac{\partial^2 u}{\partial x^2}(x,t) + \frac{\delta x^2}{12}\frac{\partial^4 u}{\partial x^4}(x,t) + \frac{\delta x^4}{360}\frac{\partial^6 u}{\partial x^6}(x,t) + \mathcal{O}(\delta x^6)$$

Example *Let consider the following explicit scheme for the 1-D diffusion equation:*

$$\frac{u_j^{n+1}-u_j^n}{\delta t} - \nu\,\frac{u_{j+1}^n - 2\,u_j^n + +u_{j-1}^n}{\delta x^2} = 0$$

Using the previous table, its equivalent PDE follows:

$$\frac{\partial u}{\partial t}(x,t) + \frac{\delta t}{2}\frac{\partial^2 u}{\partial t^2}(x,t) + \mathcal{O}(\delta t^2) - \nu\left(\frac{\partial^2 u}{\partial x^2}(x,t) + \frac{\delta x^2}{12}\frac{\partial^4 u}{\partial x^4}(x,t) + \mathcal{O}(\delta x^4)\right) = 0$$

Since $\frac{\partial^2 u}{\partial t^2} = \frac{\partial}{\partial t}\left(\frac{\partial u}{\partial t}\right) = \frac{\partial}{\partial t}\left(\nu\frac{\partial^2 u}{\partial x^2}\right) = \nu\,\frac{\partial^2}{\partial x^2}\left(\frac{\partial u}{\partial t}\right) = \nu^2\,\frac{\partial^4 u}{\partial x^4}$*, it becomes:*

$$\frac{\partial u}{\partial t}(x,t) - \nu\,\frac{\partial^2 u}{\partial x^2}(x,t) + \left(\nu^2\frac{\delta t}{2} - \nu\,\frac{\delta x^2}{12}\right)\frac{\partial^4 u}{\partial x^4}(x,t) + \mathcal{O}(\delta t^2) + \mathcal{O}(\delta x^4) = 0 \qquad \text{(C.1)}$$

Once an equivalent PDE has been computed, its dominant error term can be interpreted thanks to the following section.

C.4 Interpretation of the effect of the dominant error term

Let consider the generic 1-D PDE

$$\begin{cases} \dfrac{\partial u}{\partial t} + c\,\dfrac{\partial u}{\partial x} - \nu\dfrac{\partial^2 u}{\partial x^2} + \mu\,\dfrac{\partial^3 u}{\partial x^3} + \eta\,\dfrac{\partial^4 u}{\partial x^4} = 0 \qquad x \in \mathbb{R}, t > 0 \\ u_0(x) = e^{ikx} \qquad x \in \mathbb{R} \end{cases} \tag{C.2}$$

Looking for a plane wave solution $u(x,t) = e^{i(kx+\omega t)}$ leads almost directly to

$$u(x,t) = \exp\left(ik\left[x - (c - k^2\mu)t\right]\right)\ \exp\left(\left[-\nu - \eta k^2\right]k^2 t\right) \tag{C.3}$$

This general expression can then be used to interpret the effect of the dominant error term of equivalent PDEs of finite difference schemes. As indicated in §2.2.4, a scheme will be said

- **dissipative** if it modifies the amplitude of the wave
- **dispersive** if it modifies the phase (i.e. the velocity) of the wave

Example *Coming back to the preceding example, the equivalent PDE is given by* (C.1)*. It thus corresponds to* $c = \mu = 0$ *and* $\eta = \nu^2\dfrac{\delta t}{2} - \nu\,\dfrac{\delta x^2}{12}$ *in* (C.2)*. Looking now to* (C.3)*, it appears that the dominant error term creates the artificial multiplicative factor* $\exp(-\eta k^4 t)$ *with regard to the exact solution. It will thus result in an artificial damping or amplification of the solution, depending on the sign of* η*, i.e. depending on whether* $\nu\delta t/\delta x^2$ *is greater or larger than* $1/6$*.*

If we consider similarly the second-order in time equation

$$\begin{cases} \dfrac{\partial^2 u}{\partial t^2} - c^2\dfrac{\partial^2 u}{\partial x^2} + \eta\,\dfrac{\partial^4 u}{\partial x^4} = 0 \qquad x \in \mathbb{R}, t > 0 \\ u_0(x) = e^{ikx} \qquad x \in \mathbb{R} \end{cases} \tag{C.4}$$

its plane wave solutions are

$$u(x,t) = A\exp\left(ik\left[x - (c^2 + \eta k^2)^{1/2}t\right]\right) + B\exp\left(ik\left[x + (c^2 + \eta k^2)^{1/2}t\right]\right) \tag{C.5}$$

Chapter 5

Ordinary Differential Equations

5.1 Elementary Integration Methods

5.1.1 First Order Equations

Seperable Variables

Consider

$$y' = f(x)g(y) \tag{5.1}$$

can be serperated and divided such that

$$\int \frac{dy}{g(y)} = \int f(x)\ dx + C$$

A special case of this is $y' = f(x)y$, which has solution

$$y(x) = CR(x), \qquad R(x) = exp\left(\int f(x)\ dx\right)$$

Inhomogeneous Linear Equation

$$y' = f(x)y + g(x) \tag{5.2}$$

Then the solution is given by

$$y = e^{-\int f(x)\ dx}\left(C + \int g(x)e^{\int f(x)\ dx}\ dx\right)$$

5.1.2 Linear Differential Equations

Equations with Constant Coefficients

$$y^{(n)}(x) = 0 \tag{5.3}$$

Integrating n times gives

$$y(x) = C_1 x^{n-1} + C_2 x^{n-2} + \cdots + C_n$$

The general equation with constant coefficients is

$$y^{(n)} + A_{n-1} y^{(n-1)} + \cdots + A_0 y = 0$$