Models with Partial Differential Equations (Introduction)

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1 Introduction

Some of the most useful models in classic physical phenomena are based on partial differential equations (PDEs). Here we will introduce three fundamental equations:

- Laplace equation, that models a simple equilibrium - elliptic PDE.
- Heat equation, that models simple diffusion processes - parabolic PDE.
- Transport and Wave equation, that model translations and oscillations - hyperbolic PDE.

These are some of the basic equations in physical mathematics, and here we will also mention some other PDEs related to many different applications. For instance, Advection-Diffusion equation is related to pollution problems, Black-Scholes equation was used in Finantial Mathematics.

Models arise from simple physical notions, such as velocity and acceleration, assuming continuity of space and time. This continuity of space and time allows us to consider a physical property P in some point (x, t), where x is the spatial location and t refers to the time instant.

If P stands for the temperature, then we may assume that we can measure the temperature

$$P(x, t)$$

for some (x, t) in a continuous space-time domain, but it is clear that we will only be able to do it in a finite number of events (x_n, t_m). For instance, if we use thermography camera, this x_n will be related at most to the pixel resolution of the camera, and t_m to the time when the pictures were taken. Moreover, the temperature notion is macroscopic, and refers to the vibration of a set of particles. It is not exactly a point-by-point notion, but at our macroscopic level of measurement it can be treated in that sense.

We should take into account the displacement in time and in space. The displacement in time is taking into account if we assume that the same particle changed its property P, from time t to time $t + \epsilon$

$$\frac{P(x, t+\epsilon) - P(x, t)}{\epsilon} \underset{\epsilon \to 0}{\longrightarrow} \frac{\partial P}{\partial t}(x, t).$$

On the other hand, the displacement in space in some direction h is considered at a fixed time t,

$$\frac{P(x, t+\epsilon h) - P(x,t)}{\epsilon} \underset{\epsilon \to 0}{\longrightarrow} h \cdot \nabla P(x,t).$$

(the gradient ∇P is the vector with components $\frac{\partial P}{\partial x_k}(x,t)$, given by taking $h = e_k$ for each canonical direction).

We can see two sources for displacements. A displacement in time, that is given by the time derivatives, and a displacement in space, given by the space derivatives.

Unlike time derivatives, space derivatives can be vectorial, with the vector dimension related to the space dimension. The units are different. When dealing with time, the displacement is divided by time units and refers to the notion of velocity. When dealing with space, the displacement is divided by space units and may be seen as a transfer (or displacement).

In an equilibrium state, no changes occur in time, differences occur only in space.

On the other hand, if there are no changes with respect to space, only in time, the problem can be reduced to a single time dimension, modelled by ordinary differential equations (ODEs).

Remark 1.1. The movement of individual particles does not depend on space, because the space position $P(t)$ can be understood as the property P that changes in time. The interaction between the particles may be considered individually in a nonlinear system of ODEs, but a continuous interaction is only considered when space is also a variable, and space derivatives appear.

Laplacian. We already saw the Gradient operator

$$\nabla P = \left(\frac{\partial P}{\partial x_1}, \frac{\partial P}{\partial x_2}, \frac{\partial P}{\partial x_3}\right) \tag{1}$$

that reflects the transfer in terms of space.

The transfer with respect to time includes not only the notion of velocity, in the first derivative $\frac{\partial P}{\partial t}$, but also the notion of acceleration, with respect to the second derivative in time, $\frac{\partial^2 P}{\partial t^2}$.

The second derivatives also occur in space, usually in the form of the Laplacian, which is the divergence of gradient:

$$\begin{aligned}
\Delta P &= \nabla \cdot \nabla P = (\frac{\partial}{\partial x_1}, \frac{\partial}{\partial x_2}, \frac{\partial}{\partial x_3}) \cdot (\frac{\partial P}{\partial x_1}, \frac{\partial P}{\partial x_2}, \frac{\partial P}{\partial x_3}) \\
\Delta P &= \frac{\partial^2 P}{\partial x_1^2} + \frac{\partial^2 P}{\partial x_2^2} + \frac{\partial^2 P}{\partial x_3^2}.
\end{aligned}$$

Heat Equation

This models standard diffusion processes, where the change of P in time is directly related to the Laplacian in space, through a coefficient $\alpha > 0$:

$$\frac{\partial P}{\partial t} = \alpha \Delta P. \tag{2}$$

The coefficient α is called *diffusivity* or *diffusion coefficient.* In terms of units we can see that the equation leads to $P/time \sim \alpha P/space^2$, and therefore this diffusivity expresses it self as

$$\alpha \sim space^2/time$$

in the SI system in m^2/s.

Laplace Equation

It is also clear that when P does not change in time $\frac{\partial P}{\partial t} = 0$, and we arrive at an equilibrium state, given by the Laplace equation

$$\Delta P = 0. \tag{3}$$

Wave Equation

Wave phenomena occur when the relation between the changes in space and time are connected through the second derivative in time

$$\frac{\partial^2 P}{\partial t^2} = c^2 \Delta P. \tag{4}$$

The constant c is the wave speed, and in unit terms, it can be seen that $P/time^2 \sim c^2 P/space^2$ leads to

$$c^2 \sim space^2/time^2 = velocity^2.$$

We saw the Laplacian in space related to 0, $\frac{\partial P}{\partial t}$, $\frac{\partial^2 P}{\partial t^2}$, (elliptic, parabolic, hyperbolic PDE) and further derivatives in time usually do not appear, as they would be beyond the acceleration notion. This surveys the simplest possibilities with second derivatives, and we will just finish with the simplest first order equation, which is also a hyperbolic equation.

Transport Equation

The transport equation relates the first derivatives in space and time

$$\frac{\partial P}{\partial t} = V \cdot \nabla P \tag{5}$$

where $-V$ is a velocity vector (in unit terms $P/time \sim VP/space$ gives $V \sim space/time$).

This equation in 1D, with scalar velocity V, resumes to

$$\frac{\partial P}{\partial t} = V \frac{\partial P}{\partial x}$$

and it is easy to see that $P(x, t) = u(x+Vt)$ is a solution for any differentiable function u, because

$$\frac{\partial P}{\partial t} = V u'(x + V t) = V \frac{\partial P}{\partial x}.$$

Now, notice that we start with $P(x, 0) = u(x)$, and the solution $u(x + V t)$ tells us that at instant t the value in x will be given by the value held in $x + V t$.

2 Laplace and Poisson Equations

2.1 Laplace Equation

The Laplace differential equation on an interior domain Ω (a bounded open set), imposes that a solution should verify

$$\Delta u(x) = 0, \quad \forall x \in \Omega. \tag{6}$$

The functions u that verify the Laplace equation are called *harmonic functions*.

In 1D this equation resumes to the simple linear case

$$\frac{\partial^2 u}{\partial x^2} = u''(x) = 0 \Leftrightarrow u(x) = A + Bx$$

and we see that the solutions are only first degree polynomials. This is no longer the case in higher dimensions.

2.1.1 Complex analysis solutions in 2D

In 2D we have a huge amount of possibilities that can be derived from complex analysis, since the Cauchy-Riemann conditions for analytic functions

$$\frac{\partial u}{\partial x} = \frac{\partial v}{\partial y}, \quad \frac{\partial u}{\partial y} = -\frac{\partial v}{\partial x} \tag{7}$$

imply for u (and analogous for v)

$$\Delta u = \frac{\partial^2 u}{\partial x^2} + \frac{\partial^2 u}{\partial y^2} = \frac{\partial}{\partial x}\frac{\partial v}{\partial y} + \frac{\partial}{\partial y}(-\frac{\partial v}{\partial x}) = \frac{\partial}{\partial x}\frac{\partial v}{\partial y} - \frac{\partial}{\partial y}\frac{\partial v}{\partial x} = 0.$$

This implies that any analytic function in its complex form with $z = x+iy$ will be harmonic, either by taking its real or complex parts.

Example 2.1. Any complex polynomial is harmonic, in particular, for any $p \in \mathbb{N}_0$,

$$z^p = (x + yi)^p$$

lead to harmonic functions. The case $p = 0$ leads to $z^0=1$, which is clearly harmonic. The case $p = 1$ leads to $z^1 = x + iy$, and either $u(x, y) = x$ or

$v(x,y) = y$ are harmonic. Just from these two trivial examples, we conclude that first degree polynomials

$$u(x,y) = A + Bx + Cy$$

will be harmonic functions. This part is similar to the 1D case, but now in 2D we have much more. Taking the real and complex parts of

$$z^2 = \underbrace{x^2 - y^2}_{u(x,y)} + \underbrace{2xy}_{v(x,y)}\, i$$

and joining to the previous, we conclude that

$$u(x,y) = A + Bx + Cy + D(x^2 - y^2) + Exy$$

are 2D polynomials of second degree that are also harmonic. We may proceed with polynomials of higher order,

$$z^3 = \underbrace{x^3 - 3xy^2}_{u(x,y)} + \underbrace{3x^2y - y^3}_{v(x,y)}\, i \ \ldots$$

Not all 2D polynomials in (x,y) variables are harmonic, but the complex polynomials in $z = x + yi$ variable, are harmonic.

Example 2.2. Since each complex polynomial is harmonic, the analytic functions which can be expressed by the Taylor polynomial are also harmonic (where the expansion is valid). For instance the entire functions, which are analytic in the whole $\mathbb{C}$ are harmonic everywhere in 2D. One simple case is the exponencial function

$$e^z = e^{x+yi} = \underbrace{e^x \cos(y)}_{u(x,y)} + \underbrace{e^x \sin(y)}_{v(x,y)}\, i$$

It also applies for $e^{\mu z} = e^{\mu x}\cos(\mu y) + e^{\mu x}\sin(\mu y) i$, for any constant$\mu$. As an exercise, we can verify by definition that $\Delta u = 0, \Delta v = 0$. Other examples, include for instance

$$\begin{aligned}
\cos(z) &= \frac{1}{2}(e^{iz} + e^{-iz}) = \frac{1}{2}(e^{-y}\cos(x) + e^{-y}\sin(x)i + e^{y}\cos(x) - e^{y}\sin(x)i) \\
&= \cosh(y)\cos(x) + \sinh(y)\sin(x)i \\
\cosh(z) &= \frac{1}{2}(e^{z} + e^{-z}) = \frac{1}{2}(e^{x}\cos(y) + e^{x}\sin(y)i + e^{-x}\cos(y) + e^{-x}\sin(y)i) \\
&= \cosh(x)\cos(y) + \sinh(x)\sin(y)i
\end{aligned}$$

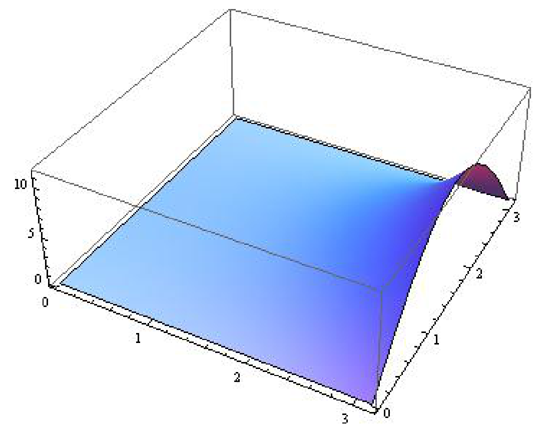

Figure 1: The function $u(x, y) = \sinh(x)\sin(y)$ is harmonic

and again, as an exercise, we can also verify that the real and imaginary part are harmonic, through the definition.

2.1.2 Separation of variables

This case of Laplace equation in 2D is an exception in PDEs, due to its connection to the complex analysis. In other cases, we must take other ways to find particular solutions. For instance in 3D, one possibility is to consider (a separation of variables)

$$u(x_1, x_2, x_3) = v(x_1, x_2)w(x_3)$$

now the laplacian gives

$$\Delta u(x, y, z) = w(x_3)(\frac{\partial^2 v}{\partial x_1^2} + \frac{\partial^2 v}{\partial x_2^2})(x_1, x_2) + v(x_1, x_2)w''(x_3)$$

and this is null, if v is harmonic in 2D and $w(x_3) = A + Bx_3$. One example of 3D solution:

$$u(x_1, x_2, x_3) = e^{x_1}\cos(x_2)x_3.$$

Remark 2.3. A usual way to get particular solutions of a partial differential equation is to consider a separation of variables. Again, in the 2D case, we assume

$$u(x, y) = v(x)w(y)$$

From$\Delta u(x,y) = v''(x)w(y) + v(x)w''(y) = 0$ we may divide by $v(x)w(y)$ to obtain

$$\frac{v''(x)}{v(x)} + \frac{w''(y)}{w(y)} = 0 \Longrightarrow \frac{v''}{v}(x) = -\frac{w''}{w}(y) = C$$

this is equal to a constant C, because $\frac{v''}{v}$ and $\frac{w''}{w}$ are equal, but depend on different variables. Now this leads to two different ODEs

$$v'' = Cv, \quad w'' = -Cw,$$

and the solution of ODEs of the form $p'' + ap' + bp = 0$ is given through the solutions of the characteristic equation

$$r^2 + ar + b = 0 \text{ with roots } r_1, r_2$$

that will be in the general form $p(t) = A\exp(r_1 t) + B\exp(r_2 t)$, when the roots are different. In our case we then have for v the characteristic equation $r^2 = C$ with solutions $r_1 = \sqrt{C}$ and $r_2 = -\sqrt{C}$, giving

$$v(x) = A_v \exp(\sqrt{C}x) + B_v \exp(-\sqrt{C}x).$$

Likewise, for w we get

$$w(y) = A_w \exp(\sqrt{-C}y) + B_w \exp(-\sqrt{-C}y).$$

Now, suppose that $C = \mu^2 > 0$, then we have

$$v(x) = A_v e^{\mu x} + B_v e^{-\mu x}, \; w(y) = A_w e^{i\mu y} + B_w e^{-i\mu y}.$$

The multiplication of both gives the solution, for instance

$$u(x,y) = v(x)w(y) = e^{\mu x} e^{i\mu y} = e^{\mu(x+yi)}$$

and we recover the previous complex solution $e^{\mu z}$ that we found before.

2.1.3 Polar representation with Fourier Series

We notice that, if instead of taking $z = x + yi$ we consider the polar form in complex variables

$$z = re^{i\theta} = r(\cos\theta + i\,\sin\theta)$$

being $r = |z|, \; \theta = \arg(z)$, the polynomials are combinations of

$$z^m = r^m e^{im\theta} = r^m(\cos(m\theta) + i\,\sin(m\theta))$$

meaning that an analytic function can be written with

$$f(z) = \sum_{m\geq 0} a_m z^m = \sum_{m\geq 0} a_m r^m e^{im\theta} = \sum_{m\geq 0} a_m r^m (\cos(m\theta) + i\ \sin(m\theta))$$

and this is a Fourier series expansion that verifies the Laplace equation.

Example 2.4. Assume that the domain is a ball with radius R, say$\Omega = B(0, R)$. Its boundary is defined by the points $\partial\Omega = \{z \in \mathbb{C} :\ r = |z| = R\}$ and in those boundary points

$$f(z) = \sum_{m\geq 0} a_m R^m e^{im\theta}$$

On the other hand, if we have a Fourier series expansion of the boundary function

$$g(\theta) = \sum_{m\geq 0} b_m e^{im\theta},\ \text{with } 2\pi b_m = \left\langle g, e^{im\theta} \right\rangle = \int_0^{2\pi} g(\theta) e^{-im\theta} d\theta$$

this gives an identification of the coefficients $a_m R^m = b_m$ and we can take $u(z) = f(z)$ as the solution for the points in $\Omega = \{z \in \mathbb{C} :\ |z| < R\}$,

$$u(z) = \sum_{m\geq 0} a_m r^m e^{im\theta} = \sum_{m\geq 0} b_m \frac{r^m}{R^m} e^{im\theta}$$

2.2 Poisson Equation

Poisson equation is the name used for the non-homogeneous Laplace equation, meaning that we now consider a non null right-hand side on the equation,

$$\Delta u = f. \tag{8}$$

This $f(x)$ reflects a perturbation of the equilibrium that exists in the harmonic case. The harmonic case, in the Laplace equation, resumes to consider no perturbation, $f = 0$.

In terms of the heat equation it can be seen as a temperature source in the domain that does not change in time. The equilibrium now has to equalize with that external source of temperature.

It is enough to find a single particular solution that verifies

$$\Delta v = f$$

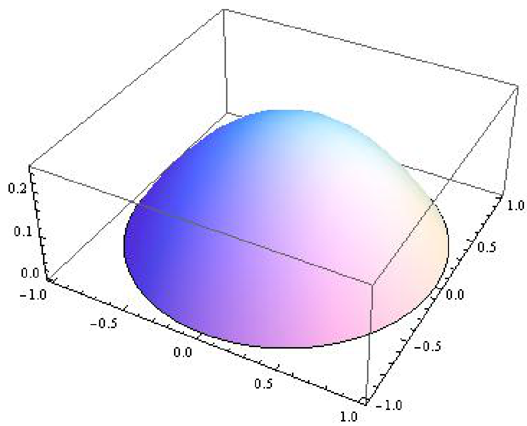

Figure 2: The function $v(x, y) = \frac{1}{4}(1 - x^2 - y^2)$, verifies $\Delta v = -1$ (and null boundary conditions in the unitary circle).

because any other solution will verify $\Delta(u - v) = f - f = 0$.

This means that all solutions to $\Delta u = f$ are given by $u = v + h$, the sum of the particular solution v with any h harmonic.

Example 2.5. We can use $\Delta u = 1$ as an example in 2D. A particular solution can be obtained from a non harmonic polynomial $v(x, y) = \frac{1}{4}(x^2 + y^2)$, that verifies $\Delta v = 1$, and all other solutions are of the form $u = v + h$, with h harmonic. For instance, $u(x, y) = \frac{1}{4}(x^2 + y^2) + e^{\mu x} \cos(\mu y)$ will verify $\Delta u = 1$, for any μ.

2.3 Boundary conditions

As we saw there are infinite solutions to the differential equation alone in any domain Ω. A single solution will be obtained if we impose boundary conditions on $\partial\Omega$.

2.3.1 Dirichlet problem

The Dirichlet boundary conditions, resume to impose a value of u on each point of the boundary $\partial\Omega$, for instance, we may assume that the values $x \in \partial\Omega$ are given by $u(x) = g(x)$, where g is a given function.

The differential equation together with this boundary condition lead to the *Dirichlet Problem* (for the Poisson equation)

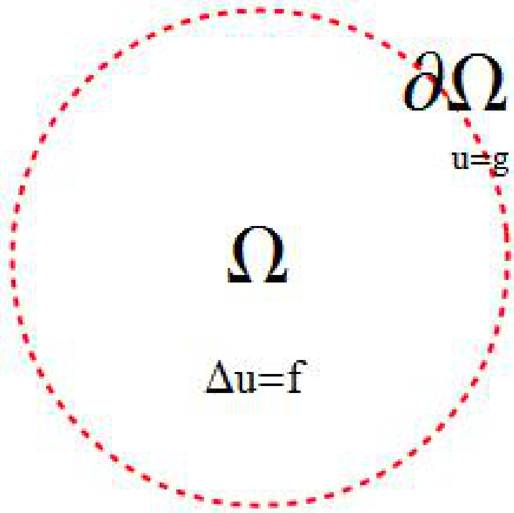

Figure 3: Scheme for the Dirichlet boundary value problem - Poisson equation.

$$(DP)\begin{cases} \Delta u = f, & \text{in } \Omega \\ u = g, & \text{on } \partial\Omega \end{cases} \tag{9}$$

Remark 2.6. If the physical context is the temperature, then f is the invariant temperature source inside the domain, and g reflects the temperature imposed on the boundary of the domain. When $f = 0$, the internal temperature only depends on the values of the temperature fixed on the boundaries of the domain.

Analogous interpretations can be derived for other phenomena. For instance, when u models the electrical field, then f is an internal electric source, and g, the value at the boundary, is the imposed electric current.

2.3.2 Neumann problem

On the other hand, we consider a Neumann boundary condition if the condition is prescribed on the normal derivate, meaning for $x \in \partial\Omega$,

$$\frac{\partial u}{\partial n}(x) = n(x) \cdot \nabla u(x) = g(x), \tag{10}$$

where $n(x)$ is the normal vector, pointing outwards the domain Ω.

This corresponds to measure the boundary heat, which can be regarded as the change rate of temperature through the boundary. The notion of heat is also intuitive, if something is touching the boundary, it is not the temperature that we fix, but the increase or decrease of temperature. A typical situation in thermal equilibrium is that there is no increase or decrease of temperature, through the boundary, and in that case $\frac{\partial u}{\partial n} = 0$.

The *Neumann Problem* (for the Poisson equation) is

$$(NP) \begin{cases} \Delta u = f, & \text{in } \Omega \\ \frac{\partial u}{\partial n} = g, & \text{on } \partial\Omega \end{cases} \tag{11}$$

2.3.3 Mixed problems

We can also assume that the conditions through the boundary are not the same. For instance we may split the domain boundary in two parts $\partial\Omega = \Gamma_D \cup \Gamma_N$ such that in Γ_D a Dirichlet boundary condition is imposed, and in Γ_N a Neumann one. Thus, a *mixed problem* is of the form

$$(MP) \begin{cases} \Delta u = f, & \text{in } \Omega \\ u = g_D, & \text{on } \Gamma_D \\ \frac{\partial u}{\partial n} = g_N, & \text{on } \Gamma_N \end{cases} \tag{12}$$

Sometimes it is also consider a combination of the two boundary conditions in a single condition, which is called Robin condition

$$\alpha \frac{\partial u}{\partial n} + \beta u = g_R \tag{13}$$

and we notice that if $\alpha = 0, \beta = 1$, we have the Dirichlet condition, and if $\alpha = 1, \beta = 0$, we have the Neumann condition. If these α, β are functions on the boundary, they may define the type of boundary condition at each point. The *Robin problem* can be resumed as

$$(RP) \begin{cases} \Delta u = f, & \text{in } \Omega \\ \alpha \frac{\partial u}{\partial n} + \beta u = g_R & \text{on } \partial\Omega \end{cases} \tag{14}$$

and incorporates all previous cases.

2.4 Uniqueness

To prove uniqueness for the boundary value problems we will make use of the Green formulas, which are consequence of the Divergence-Gauss theorem:

Theorem 2.7. *Given any bounded domain* Ω *with piecewise* C^1 *boundary* $\partial\Omega$ *and* $u \in C^1(\bar{\Omega})$, *we have (Gauss version)*

$$\int_\Omega \nabla u(x)\, dx = \int_{\partial\Omega} \mathbf{n}(x) u(x)\, ds_x \tag{15}$$

where $\mathbf{n}(x)$ *is the normal vector to* $x \in \partial\Omega$, *that exists almost everywhere. The Divergence version gives*

$$\int_\Omega \nabla \cdot \mathbf{u}\, dx = \int_{\partial\Omega} \mathbf{n} \cdot \mathbf{u}\, ds. \tag{16}$$

Remark 2.8. The condition $u \in C^1(\bar{\Omega})$ imposes a regularity that is no longer needed when we consider Lebesgue integrable functions, Sobolev spaces - for instance, $u \in H^1(\Omega)$, with $u, \nabla u \in L^2(\Omega)$.

2.4.1 Green formulas

From the Divergence theorem, and

$$\nabla(uv) = u\nabla v + v\nabla u, \text{ or } \nabla \cdot (u\mathbf{v}) = u\nabla \cdot \mathbf{v} + \mathbf{v} \cdot \nabla u$$

we obtain an integration-by-parts type of formula

Theorem 2.9. *The integration-by-parts formula*

$$\int_\Omega \nabla \cdot (u\mathbf{v})\, dx = \int_\Omega (u\nabla \cdot \mathbf{v} + \mathbf{v} \cdot \nabla u)\, dx = \int_{\partial\Omega} u\ \mathbf{n} \cdot \mathbf{v}\, ds,$$

using $\mathbf{v} = \nabla v$, *gives the First Green Formula*

$$\int_\Omega (u\Delta v + \nabla u \cdot \nabla v)\, dx = \int_{\partial\Omega} u \frac{\partial v}{\partial n}\, ds, \tag{17}$$

and, changing the roles of u, v, *and subtracting we get the Second Green Formula:*

$$\int_\Omega (u\Delta v - u\Delta v)\, dx = \int_{\partial\Omega} \left(u\frac{\partial v}{\partial n} - v\frac{\partial u}{\partial n} \right) ds. \tag{18}$$

2.4.2 Uniqueness - Dirichlet Problem

Assume that u_1, u_2 both verify

$$(DP)\begin{cases} \Delta u_k = f, & \text{in } \Omega \\ u_k = g, & \text{on } \partial\Omega \end{cases} \quad (k = 1, 2) \tag{19}$$

this implies that $u = u_1 - u_2$ verifies the homogeneous problem

$$\begin{cases} \Delta u = 0, & \text{in } \Omega \\ u = 0, & \text{on } \partial\Omega \end{cases} \tag{20}$$

Now, using the first Green formula, we have (taking $u = v$)

$$\begin{aligned} \int_\Omega (u\Delta u + \nabla u \cdot \nabla u)\, dx &= \int_{\partial\Omega} u \frac{\partial u}{\partial n}\, ds \\ &\Leftrightarrow \\ \int_\Omega \|\nabla u\|^2\, dx &= 0 \end{aligned}$$

(because $u = 0$ on $\partial\Omega$ and $\Delta u = 0$ in Ω).

This implies $\nabla u = 0$ in Ω and therefore u is constant in Ω, but since $u = 0$ on the boundary, by continuity the constant is null. Thus, $u = 0$, and $u_1 = u_2$ in all $\bar{\Omega}$.

Theorem 2.10. *Uniqueness is proven, for the Dirichlet problem.*

The prove does not change much for other boundary conditions. We will consider the general Robin case.

Theorem 2.11. *Uniqueness holds for the Robin problem with constants $\alpha, \beta > 0$. The uniqueness is up to a constant in the Neumann problem.*

Proof. Again we are led to the homogeneous

$$(RP)\begin{cases} \Delta u = 0, & \text{in } \Omega \\ \alpha \frac{\partial u}{\partial n} + \beta u = 0 & \text{on } \partial\Omega \end{cases}$$

and the Green formula gives with $\alpha \neq 0$,

$$\begin{aligned} \alpha \int_\Omega (u\Delta u + \nabla u \cdot \nabla u)\, dx &= \int_{\partial\Omega} u\alpha \frac{\partial u}{\partial n}\, ds = -\int_{\partial\Omega} \beta u^2\, ds \\ &\Leftrightarrow \\ \int_\Omega \|\nabla u\|^2\, dx &+ \frac{\beta}{\alpha} \int_{\partial\Omega} u^2\, ds \geq 0 \end{aligned}$$

When $\beta/\alpha > 0$ this implies directly $\nabla u = 0$ in Ω and $u = 0$ on $\partial\Omega$. Thus, u is constant and null at the boundary, implies u null everywhere. If $\beta = 0$ (Neumann problem) then we can only conclude that $\nabla u = 0$ in Ω and u is constant, meaning that $u = u_1 - u_2 = C$ and the solutions u_1 and u_2 are equal up to a constant. If $\beta/\alpha < 0$ we can not conclude the uniqueness. $\square$

2.5 Mean value and maximum

2.5.1 Finite differences and the Mean value

We can consider the approximation of the Laplace operator using the formula, (for $h > 0$, $h \to 0$)

$$w''(x) = \frac{w(x+h) - 2w(x) + w(x-h)}{h^2} + O(h^2). \tag{21}$$

The discretization of the Laplacian in 2D, with $h_x, h_y > 0$, becomes

$$\begin{aligned} \Delta u(x,y) &= \frac{u(x+h_x,y) - 2u(x,y) + u(x-h_x,y)}{h_x^2} + \frac{u(x,y+h_y) - 2u(x,y) + u(x,y-h_y)}{h_y^2} \\ &\quad + O(h_x^2) + O(h_y^2) \end{aligned}$$

taking $h_x = h_y = h$, and neglecting the remainder in $O(h^2)$, we obtain

$$\tilde{\Delta} u(x,y) = \frac{u(x+h,y) + u(x-h,y) + u(x,y+h) + u(x,y-h) - 4u(x,y)}{h^2} \tag{22}$$

Thus, when $\Delta u = f$, we obtain the discretized version $\tilde{\Delta} u(x,y) = f(x,y)$ leading to a discrete Poisson equation:

$$u(x+h,y) + u(x-h,y) + u(x,y+h) + u(x,y-h) - 4u(x,y) = h^2 f(x,y)$$

This can lead to a numerical method, with $u_{ij} = u(x_i, y_j)$ (updating with a Jacobi or Gauss-Seidel iteration).

But here, our main interest is to show that if $f = 0$, the harmonic case, gives

$$u(x,y) = \frac{u(x+h,y) + u(x-h,y) + u(x,y+h) + u(x,y-h)}{4} \tag{23}$$

This means that the central point will became the average of the 4 neighbors in this numerical scheme.

This is a discrete version of a known continuous property.

2.5.2 Continuous mean value and maximum principle

Theorem 2.12. *(Mean value for harmonic functions) If u is harmonic in $\Omega \supset B(x_0, r)$ we have*

$$u(x_0) = \frac{1}{|B(x_0, r)|} \int_{B(x_0,r)} u(x)dx = \frac{1}{|\partial B(x_0, r)|} \int_{\partial B(x_0,r)} u(x)ds_x. \tag{24}$$

From this property we deduce a Maximum-Minimum property

Theorem 2.13. *(Maximum/minimum principle) If u is harmonic in Ω, we have*

$$\max_{x\in\bar{\Omega}} u(x) = \max_{x\in\partial\Omega} u(x), \quad \min_{x\in\bar{\Omega}} u(x) = \min_{x\in\partial\Omega} u(x). \tag{25}$$

Proof. Suppose that the maximum/minimum was some $x_0 \in \Omega$. Using the previous theorem, there is a ball $B(x_0, r) \subset \Omega$ (with r small enough) such that $u(x_0)$ is the average in that ball. If it is the average, $u(x_0)$ it is not the maximum nor the minimum, unless u is constant. If u is not constant we conclude that $x_0 \notin \Omega$ and the result follows, $x_0 \in \partial\Omega$. If it is constant the value is the same, and the result also holds. □

Remark 2.14. This property also implies the uniqueness for the Dirichlet problem, as the null boundary values would be maximum/minimum and the interior had to be null by consequence. It also implies a continuous dependence from the boundary data.

2.6 Fundamental solution

2.6.1 Dirac delta and convolution

The fundamental solution is a concept related to the notion of Dirac δ functional.

Definition 2.15. The Dirac δ is the linear functional$\delta : C(\mathbb{R}^N) \to \mathbb{R}$ given by

$$\delta(f) = f(0)$$

and centered at $y \in \mathbb{R}^N$ is given by $\delta_y(f) = f(y)$.

Remark 2.16. This functional is also written as $\delta(f) = \langle \delta,\ f \rangle = \int_{\mathbb{R}^N} \delta(x) f(x) dx = f(0)$. This introduces the δ as a generalized function, in the sense that it does not coincide to a classical function.

However we can consider that $\delta(x) = 0$ if $x \neq 0$ and $\delta(0) = \infty$. This unusual identification can be established by the pointwise limit of μ_ε functions (when $\varepsilon \to 0$)

$$\mu_\varepsilon(x) = \begin{cases} 1/\varepsilon, & x \in [-\varepsilon, \varepsilon] \\ 0, & \text{otherwise} \end{cases}$$

In fact, by the intermediary value theorem for integrals,

$$\langle \mu_\varepsilon,\ f \rangle = \int_{\mathbb{R}} \mu_\varepsilon(x) f(x) dx = \frac{1}{\varepsilon} \int_{-\varepsilon}^{\varepsilon} f(x) dx = f(\xi_\varepsilon),\ \text{with}\ \xi_\varepsilon \in [-\varepsilon, \varepsilon].$$

Now when $\varepsilon \to 0$, we have $f(\xi_\varepsilon) \to f(0)$, and the pointwise convergence $\mu_\varepsilon \to \delta$ is established.

Notice also that in this sense, $\delta_y(x) = \delta(x - y) = \delta(y - x)$, and

$$\delta_y(f) = \langle \delta_y,\ f \rangle = \int_{\mathbb{R}^N} \delta(y - x) f(x) dx = f(y).$$

Definition 2.17. We recall the notion of product of convolution

$$(f * g)(x) = \int_{\mathbb{R}^N} f(x - z) g(z) dz = \langle f(x - \bullet), g \rangle \tag{26}$$

that has the distributives and commutative properties of a product $f * g = g * f$, $(f_1 + f_2) * g = f_1 * g + f_2 * g$.

This notion allows us to write $f(x) = \delta_x(f) = \int_{\mathbb{R}^N} \delta(x - z) f(z) dx = (\delta * f)(x)$, and we conclude that

$$\delta * f = f,$$

which means that the Dirac δ is the identity element of the convolution product.

Another important property of the convolution is related to the derivatives.

In the following we will consider differential operators that are linear with constant coefficients, for instance of the form

$$Df = A_0 f + (\nabla f) \cdot A_1 + (\nabla^2 f) : A_2 + \cdots + (\nabla^m f) : A_m$$

with A_0 a constant, A_1 a vector, A_2 a matrix, ... , A_m a tensor of order m. In particular, the Laplacian is given by taking A_2 to be the identity matrix, which is dot-multiplied (:) by the Hessian matrix $\nabla^2 f$.

Proposition 2.18. *Let D be a constant coefficient differential operator, we have*

$$D(f * g) = (Df) * g = f * (Dg). \tag{27}$$

Proof. Consider $D = \nabla$, then

$$\nabla(f * g)(x) = \nabla \int_{\mathbb{R}^N} f(x-z)g(z)dz = \int_{\mathbb{R}^N} \nabla f(x-z)g(z)dz = ((\nabla f) * g)(x),$$

likewise $\nabla(f * g) = f * (\nabla g)$. Since this holds for the first derivatives, it will be similar for linear combination of higher order derivatives. □

2.6.2 Fundamental solution concept

Definition 2.19. Given a differential operator D, we say that Φ is a fundamental solution of A if it verifies

$$D\Phi = \delta. \tag{28}$$

Remark 2.20. Notice that if Φ is a fundamental solution, also $\phi = \Phi + v$ will be if $Dv = 0$, i.e. if we add v, solutions of the homogeneous differential equation, these will also be fundamental solutions.

This notion is of particular importance to obtain solutions of the equation $Du = f$ using the convolution product.

Theorem 2.21. *If Φ is a fundamental solution of D, the convolution*

$$u = \Phi * f \tag{29}$$

is a solution of $Du = f$.

Proof. This is an immediate consequence of the previous properties, because

$$Du = D(\Phi * f) = D(\Phi) * f = \delta * f = f.$$

□

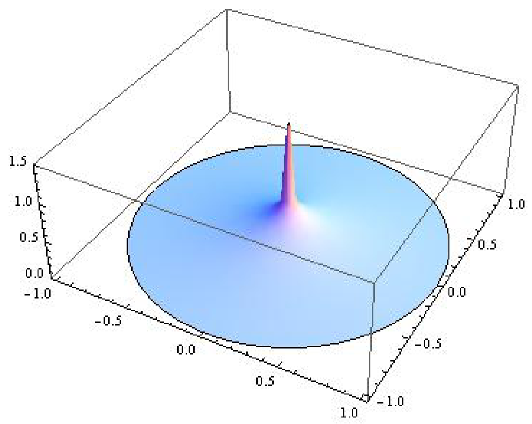

Figure 4: Laplace operator fundamental solution in 2D (singularity at the origin).

There are known fundamental solutions for some differential operators. We give here some that will be useful in this course

- Laplace operator $-\Delta\Phi = \delta$, (for convenience, we take $-\Delta$ instead of Δ)
  - in 2D
  $$\Phi(x) = -\frac{1}{2\pi}\log ||x|| \tag{30}$$
  - in 3D
  $$\Phi(x) = \frac{1}{4\pi||x||} \tag{31}$$
  -
- Heat operator, $(\partial_t - \alpha\Delta)\Phi = \delta$,
  $$\Phi(t,x) = \frac{1}{(4\pi\alpha t)^{N/2}}\exp(-\frac{||x||^2}{4\alpha t}), \quad (\text{and if } t<0, \Phi(t,x)=0)$$
-
- Helmholtz operator (harmonic waves), $-(\Delta+\kappa^2)\Phi = \delta$,

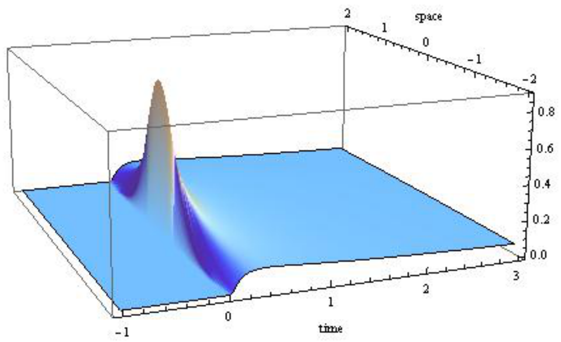

Figure 5: Heat operator fundamental solution with $N = 1, \alpha = 5$.

– in 2D (here $H_0^{(1)}$ denotes a Hänkel function)

$$\Phi(x) = \frac{i}{4} H_0^{(1)}(\kappa||x||) \tag{32}$$

– in 3D

$$\Phi(x) = \frac{e^{i\kappa||x||}}{4\pi||x||} \tag{33}$$

Remark 2.22. For instance, from the previous results, we have as a particular solution

$$u(x) = (\Phi * f)(x) = \int_{\mathbb{R}^N} \Phi(x - y) f(y) dy,$$

and in the Laplace 3D case, this resumes to

$$u(x) = \int_{\mathbb{R}^3} \frac{f(y)}{4\pi||x - y||} dy$$

which is known as the Newtonian potential, due to its relation to the gravity field. In fact, considering the characteristic function

$$\chi_\Omega(y) = \begin{cases} 1, & x \in \Omega \\ 0, & \text{otherwise} \end{cases}$$

we see that $f = \chi_\Omega m$ leads to the integral sum of each point $y \in \Omega$, with mass $m(y)$, in the gravitational field,

$$u(x) = \int_\Omega \frac{m(y)}{4\pi||x - y||} dy.$$

2.6.3 Fourier Transform

To deduce the fundamental solution we recall the notion of Fourier Transform.

Definition 2.23. The Fourier Transform of a function f is given by

$$\mathcal{F}(f)(\xi) = \int_{\mathbb{R}^N} e^{-i(\xi\cdot x)} f(x)dx = \left\langle f,\, e^{i(\xi\cdot\bullet)}\right\rangle \tag{34}$$

The inversion of the Fourier Transform is defined in a similar way

$$\mathcal{F}^{-1}(f)(x) = \tfrac{1}{(2\pi)^N} \int_{\mathbb{R}^N} e^{i(\xi\cdot x)} f(\xi)d\xi = \tfrac{1}{(2\pi)^N} \left\langle f,\, e^{-i(\xi\cdot\bullet)}\right\rangle \tag{35}$$

But the most important property is related to the differentiation

$$\mathcal{F}(\nabla f)(\xi) = i\xi\mathcal{F}(f)(\xi), \tag{36}$$

as this gives for the Laplacian

$$\mathcal{F}(\Delta f)(\xi) = \mathcal{F}(\nabla\cdot\nabla f)(\xi) = i\xi\cdot\mathcal{F}(\nabla f)(\xi) = -||\xi||^2\mathcal{F}(f)(\xi).$$

Now we also recall that the Fourier Transform has an important property related to the convolution.

Proposition 2.24. $\mathcal{F}(f*g) = \mathcal{F}(f)\mathcal{F}(g)$.

In particular, from here it is clear that the Fourier Transform of the Dirac delta must be 1, because

$$\mathcal{F}(f) = \mathcal{F}(f*\delta) = \mathcal{F}(f)\mathcal{F}(\delta) \Longrightarrow \mathcal{F}(\delta) = 1.$$

Now we can establish that the Fourier Transform of the fundamental solution of the Laplace operator should verify

$$1 = \mathcal{F}(\delta) = \mathcal{F}(-\Delta\Phi) = +||\xi||^2\mathcal{F}(\Phi)(\xi)$$

$$\Phi(x) = \mathcal{F}^{-1}(\frac{1}{||\xi||^2})(x) = \tfrac{1}{(2\pi)^N}\int_{\mathbb{R}^N} \frac{e^{i(\xi\cdot x)}}{||\xi||^2}dx$$

2.7 Newtonian Potentials

The existence of a potential means that a force field F can be expressed with a gradient

$$F = \nabla u,$$

because in this case we can apply the divergence to obtain $\Delta u = \nabla \cdot \nabla u = \nabla \cdot F$, a Poisson equation.

2.7.1 Newtonian Potential in gravity

We saw that the solution through the convolution with the fundamental solution the leads to Newtonian potential

$$u(x) = \int_\Omega \frac{m(y)}{4\pi||x-y||} dy \tag{37}$$

in the case of the Laplace operator in 3D, in the interpretation of the gravitational field.

In fact, it is well known that the interaction force between a particle of mass 1 located at x, and a body of mass m located at y, is given by the force inverse proportional to the square of the distance $||x-y||$ between the two:

$$F = G\frac{m}{||x-y||^2}$$

where G is the gravitational constant (that may hold a mass different to 1).

The gravitational force holds along the direction of $r = x - y$, normalized

$$\hat{r} = \frac{x-y}{||x-y||}$$

and therefore we can write

$$F = -G\frac{m}{||x-y||^2}\hat{r} = -Gm\frac{x-y}{||x-y||^3}.$$

Now the Laplace observation concerning the fundamental solution is that

$$\nabla\Phi(x) = \frac{1}{4\pi}\nabla\frac{1}{||x||} = -\frac{1}{4\pi}\frac{x}{||x||^3}$$

and therefore we can write

$$F = 4\pi Gm\nabla\Phi(x-y).$$

This is just for a single particle. If we consider a sum, it would became

$$F = 4\pi G \sum_{k=0}^{n} m_k \nabla\Phi(x - y_k) = -4\pi G \sum_{k=0}^{n} m_k \frac{x - y_k}{||x - y_k||^3}.$$

Moreover, taking an integration over a mass distribution $m(y)$ for each point $y \in \Omega$, this leads to

$$F = 4\pi G \int_\Omega m(y)\nabla\Phi(x - y)dy = 4\pi G\nabla u(x) = 4\pi G\nabla_x \int_\Omega \frac{m(y)}{4\pi||x - y||}dy.$$

We see that this enough to calculate the potential gravitational field u to obtain the gravitational force.

The Poisson equation

$$\Delta u = 4\pi G m \tag{38}$$

establishes the gravitational field u, given a mass distribution m.

2.7.2 Newtonian potential in the electric field

Another well known interpretation of the Newtonian potential is given within the electric field. In the mathematical point of view, the situation is pratically the same, since the electrostatic force, between a particle of electrical charge 1 and a particle of charge q is given by Coulomb's law

$$E = K\frac{q}{||x - y||^2}\hat{r} = Kq\frac{x - y}{||x - y||^3}$$

and the only difference with respect to gravity is that K is now Coulomb's constant for the units, and ulinke the mass, the electrical charge q can have positive or negative values, leading to repulsion and not only attraction forces.

Again we can define the forces in term of the gradients of the electric field

$$E = -\nabla v,$$

and by Gauss' Law we have

$$\nabla \cdot E = \frac{\rho}{\varepsilon_0}$$

where ρ is electric charge density (instead of mass density) and ε_0 is the vacuum permittivity constant (notice that the relation between Coulomb's constant and this one is simply given by $4\pi K\varepsilon_0 = 1$).

This leads immediately to the Poisson equation

$$-\Delta v = \frac{\rho}{\varepsilon_0}, \tag{39}$$

and again we have the Newtonian potential for the electric field

$$v(x) = K \int_\Omega \frac{q(y)}{||x-y||} dy.$$

Remark 2.25. Due to the divergence Gauss theorem, the Gauss law has also an integral boundary form

$$\int_\Omega \nabla \cdot E = \int_{\partial\Omega} n \cdot E = \frac{\rho}{\varepsilon_0}.$$

Remark 2.26. Notice that if we considered a discrete set of electric charges q_k at locations x_k then we may consider the charge density in terms of a sum of Dirac deltas

$$\rho = \sum_{k=1}^{n} q_k \delta_{x_k} \tag{40}$$

this would give

$$v(x) = K \int_{\mathbb{R}^N} \frac{1}{||x-y||} \sum_{k=1}^{n} q_k \delta_{x_k}(y) dy = K \sum_{k=1}^{n} q_k \int_{\mathbb{R}^N} \frac{1}{||x-y||} \delta_{x_k}(y) dy = K \sum_{k=1}^{n} \frac{q_k}{||x-x_k||}$$

and therefore, as expected,

$$E = -\nabla v = K \sum_{k=1}^{n} q_k \frac{x-x_k}{||x-x_k||^3}.$$

The charges given by the δ_{x_k} are called monopolar sources, and it is also possible to consider $\nabla\delta_{x_k}$ which correspond to dipolar sources, and this can also be treated in a similar way.

2.8 Boundary potentials

We saw the discrete potentials as a simple sum of the contributions of each particle, and we also considered the integration all over a domain Ω, now we will be interest in the integration through the boundary $\partial\Omega$ or through a surface Γ, which corresponds to the exchange of mass, of charge, of temperature, on the boundaries of the domain.

2.8.1 Single and Double layer potentials

Definition 2.27. Given a part of a boundary $\gamma \subseteq \partial\omega$, of a domain ω, we define a *single layer potential* with a boundary density ψ, using the fundamental solution Φ,

$$u(x) = (\mathcal{L}_\gamma \psi)(x) = \int_\gamma \Phi(x-y)\psi(y)ds_y. \tag{41}$$

Likewise, we define a *single layer potential* with a boundary density φ,

$$v(x) = (\mathcal{M}_\gamma \varphi)(x) = \int_\gamma \frac{\partial \Phi}{\partial n_y}(x-y)\varphi(y)ds_y \tag{42}$$

(where n_y represents the normal vector at point $y \in \partial\omega$).

Remark 2.28. We can consider this potentials modelling a charge distribution on a surface panel γ. The single layer potential corresponds to a monopolar distribution, in the sense that we can approximate the integral using a numerical quadrature

$$u_h(x) = \int_\gamma \Phi(x-y)\psi(y)ds_y = \sum_{y_k \in \gamma} w_k \Phi(x-y_k)\psi(y_k) + O(h^p)$$

where w_k are quadrature weights associated to quadrature knots y_k and $O(h^p)$ is the error of a p-order quadrature rule, with some discretization step $h > 0$. Notice that

$$Du_h = \sum_{y_k \in \gamma} w_k \psi(y_k)\delta_{y_k} \tag{43}$$

Likewise, the double layer potential will correspond to a dipolar distribution.

3 Heat equation

We now consider the *heat equation*, also called *diffusion equation*, where the unknown $u(t,x)$ verifies

$$\frac{\partial u}{\partial t} = \alpha \Delta u \tag{44}$$

where $\alpha > 0$ is the *diffusion permittivity*. Notice that:

- with very small permittivity, when $\alpha \to 0$, we will have $\frac{\partial u}{\partial t} \to 0$ and the solution tends to be constant in time, given by the initial $u(x,0)$.
- with very high permittivity, when$\alpha \to \infty$, we have $\Delta u = \frac{1}{\alpha}\frac{\partial u}{\partial t} \to 0$, and the solution tends to be harmonic.
- when u is time invariant, $\frac{\partial u}{\partial t} = 0$, and we have the previous Laplace equation, $\Delta u = 0$.

Remark 3.1. There is a more general version of this equation where the diffusion coefficient is not considered to be constant. In that case, α can be a matrix (of mass or heat diffusivity), and the equation becames

$$\frac{\partial u}{\partial t} = \nabla \cdot (\alpha \nabla u) = \alpha \Delta u + \nabla \alpha : \nabla u,$$

but we will not consider that case here.

3.1 Particular solutions

Considering a separation of variables $u(t,x) = w(t)v(x)$, the heat equation gives

$$w'(t)v(x) = \frac{\partial u}{\partial t}(t,x) = \alpha \Delta_x u(t,x) = \alpha w(t) \Delta_x v(x),$$

and assuming that $v, w \neq 0$, this gives

$$\frac{w'(t)}{w(t)} = \alpha \frac{\Delta_x v(x)}{v(x)} = \text{const.} = \kappa$$

one equation on w, and one equation on v :

$$\begin{cases} w' = \kappa w \\ \Delta_x v = \frac{\kappa}{\alpha} v \end{cases}$$

We have an exponential solution on w

$$w(t) = w_0 e^{\kappa t},$$

and a Helmholtz equation on v. In both cases the behavior of the solution depends on the chosen sign of κ :

If $\kappa > 0$, the solution would increase when $t \to +\infty$, and we get the modified-Helmholtz equation on v. This case has no physical meaning in the heat dissipation or diffusion, unless we invert the sense of time and $t \to -\infty$.

Thus $\kappa < 0$ is the correct sign, unless we invert the sign of time.

To simplify calculations, since $\alpha > 0$, we consider $\kappa = -\alpha\mu^2 < 0$.

Thus, in the 1D case, we get

$$\begin{cases} w' = (-\alpha\mu^2)w \\ v'' + \mu^2 v = 0 \end{cases}$$

$$w(t) = w_0 e^{-\alpha\mu^2 t}, \quad v(x) = v_0 e^{i\mu x} + v_1 e^{-i\mu x}.$$

and particular solutions (1D+1T), can be expressed in the trigonometric form

$$u(t, x) = e^{-\alpha\mu^2 t}(a\cos(\mu x) + b\sin(\mu x)).$$

A combination of these particular solutions, for instance

$$u(t, x) = \sum_{k=0}^{\infty} e^{-\alpha k^2 t} a_k \cos(kx) + \sum_{k=1}^{\infty} e^{-\alpha k^2 t} b_k \sin(kx) \tag{45}$$

can lead to a solution of the initial problem, if

$$u(0, x) = u_0(x) = \sum_{k=0}^{\infty} a_k \cos(kx) + \sum_{k=1}^{\infty} b_k \sin(kx),$$

which means a Fourier expansion of the initial condition.

This requires a definition of the full transient problem, which includes an initial condition, beside the boundary condition.

3.2 Transient domain - initial and boundary conditions

In the diffusion, or heat phenomena, we may also consider an internal heat source $f(t,x)$ leading to the non homogeneous equation

$$\frac{\partial u}{\partial t}(t,x) = \Delta_x u(t,x) + f(t,x). \tag{46}$$

The full problem will be considered in a time-cylinder domain which corresponds to the cartesian multiplication of the time interval (t_0, t_f) and the space domain Ω :

$$\Omega_T = (t_0, t_f) \times \Omega.$$

The initial time $t = t_0$ (usually $t_0 = 0$) holds the *initial condition*

$$u(t_0, x) = u_0(x), \quad \text{for } x \in \Omega,$$

for some prescribed function u_0 in Ω. Thus, this holds at the bottom of the time-cylinder $\{t_0\} \times \Omega$. There is no particular restriction to the end of measurements, and therefore we can establish the end at $t = t_f$, or we can also defined the full domain as $\Omega_T = (t_0, +\infty) \times \Omega$.

The boundary conditions are placed on the boundary of Ω but change in time, along $(t_0, t_f) \times \partial\Omega$. For instance, a Dirichlet boundary condition would became

$$u(t,x) = u_D(t,x), \quad \text{for } (t,x) \in (t_0, t_f) \times \partial\Omega. \tag{47}$$

This can also be substituted by a boundary condition of the Neumann type:

$$\frac{\partial u}{\partial n}(t,x) = u_N(t,x), \quad \text{for } (t,x) \in (t_0, t_f) \times \partial\Omega. \tag{48}$$

Or, we can also mix the two type of boundary conditions, depending on part of the boundary, $\partial\Omega = \Gamma_D \cup \Gamma_N$, where a Dirichlet boundary condition is assumed on Γ_D and a Neumann type on Γ_N.

The full problem then becames

$$(HP) \left\{ \begin{array}{ll} \frac{\partial u}{\partial t}(x,t) = \alpha \Delta_x u(x,t) + f(x,t), & (t,x) \in (t_0, t_f) \times \Omega \\ u(t_0, x) = u_0(x), & x \in \Omega \\ u(t,x) = u_D(t,x), & (t,x) \in (t_0, t_f) \times \Gamma_D \\ \frac{\partial u}{\partial n}(t,x) = u_N(t,x), & (t,x) \in (t_0, t_f) \times \Gamma_N \end{array} \right. \tag{49}$$

Theorem 3.2. *The heat problem (HP) defined above has an unique solution.*

Proof. Consider two different solutions u_1 and u_2 of (HT) and take $u = u_1 - u_2$. Then u verifies the homogeneous problem

$$\begin{cases} \frac{\partial u}{\partial t}(x,t) = \alpha \Delta_x u(x,t), & (t,x) \in (t_0,t_f) \times \Omega \\ u(t_0,x) = 0, & x \in \Omega \\ u(t,x) = 0, & (t,x) \in (t_0,t_f) \times \Gamma_D \\ \frac{\partial u}{\partial n}(t,x) = 0, & (t,x) \in (t_0,t_f) \times \Gamma_N \end{cases}$$

Now take $E(t)$ a variation of energy through time

$$E(t) = \frac{1}{2}||u(t,\cdot)||^2_{L^2(\Omega)} = \frac{1}{2}\int_\Omega u(t,x)^2 dx. \tag{50}$$

and we have

$$\begin{aligned} E'(t) &= \frac{1}{2}\int_\Omega \frac{d}{dt}(u(t,x)^2)dx = \frac{1}{2}\int_\Omega 2\frac{\partial u}{\partial t}(t,x)u(t,x)dx \\ &= \alpha \int_\Omega \Delta_x u(t,x)u(t,x)dx = -\alpha \int_\Omega \nabla_x u(t,x) \cdot \nabla_x u(t,x)dx + \alpha \int_{\partial\Omega} \frac{\partial u}{\partial n}(t,x)u(t,x)dx, \end{aligned}$$

and $\int_{\partial\Omega} \frac{\partial u}{\partial n}(t,x)u(t,x)dx = 0$ because $u = 0$ on the boundary part Γ_D and $\frac{\partial u}{\partial n} = 0$ on Γ_N. Therefore, since $\alpha > 0$,

$$E'(t) = -\alpha||\nabla_x u||^2_{L^2(\Omega)} \leq 0.$$

This means that the energy quantity $E(t) \geq 0$ decreases in time

$$0 \leq E(t) \leq E(t_0) = \frac{1}{2}||u(t_0,\cdot)||^2_{L^2(\Omega)} = \frac{1}{2}||u_0||^2_{L^2(\Omega)} = 0,$$

because the initial condition of the difference is null.

Now we conclude that $E(t) = 0$ for all time, and this means $||u(t,\cdot)||_{L^2(\Omega)} = 0$, meaning $u(t,x) = 0$ for all time and space. Uniqueness is proven. $\square$

Theorem 3.3. *The Maximum Principle still holds in the transient heat equation (with $f = 0$)*

$$\max_{([t_0,t_f]\times\partial\Omega)\cup(\{0\}\times\bar{\Omega})} u = \max_{[t_0,t_f]\times\bar{\Omega}} u \tag{51}$$

and an analogous identity holds for the minimum. This also implies uniqueness and continuous dependence from the initial and boundary data.

3.3 Advection-diffusion equation

This is a model problem that combines transport with the diffusion (heat) equation.

3.3.1 Transport equation

The transport equation in its more general form can be written as

$$\frac{\partial u}{\partial t} + \nabla \cdot (\mathbf{v}u) = 0 \tag{52}$$

where $\mathbf{v}$ denotes the velocity vector and u the quantity to be transfered, usually the mass or concentration of a substance. Since

$$\nabla \cdot (\mathbf{v}u) = \mathbf{v} \cdot \nabla u + (\nabla \cdot \mathbf{v})u$$

the term $(\nabla \cdot \mathbf{v})u$ can not be ignored unless $\mathbf{v}$ is constant, or has null divergence (incompressible flow).

Here we will assume that the velocity is constant and therefore we just write the transport equation as

$$\frac{\partial u}{\partial t} + \mathbf{v} \cdot \nabla u = 0. \tag{53}$$

Remark 3.4. We already mentioned that in this simplest case a general solution is

$$u(t, x) = u_0(x - \mathbf{v}t),$$

where u_0 stands for an initial condition at time $t = 0$. In fact,

$$\frac{\partial u}{\partial t}(t, x) = -\mathbf{v} \cdot \nabla u_0(x - \mathbf{v}t) = -\mathbf{v} \cdot \nabla u(t, x).$$

3.3.2 Advection-diffusion with constant velocity and constant diffusivity

In the *advection-diffusion* phenomena (also called *convection-diffusion*), the right hand side of the equation is ruled by the diffusion term:

$$\frac{\partial u}{\partial t}(t, x) + \mathbf{v} \cdot \nabla u(t, x) = \alpha \Delta u(t, x), \tag{54}$$

as we may understand that in the limit case, when $\alpha \to 0$, when no diffusion occurs, there is only a transport phenomena, and when there is no transport, then $V = 0$, and we get the previous diffusion (or heat) equation.

Remark 3.5. We can also understand the transport term using the material derivative concept. In fact, if x depends on t, the derivative in terms of t would became

$$\frac{d}{dt}u(t,x(t)) = \frac{\partial u}{\partial t}(t,x(t)) + \frac{dx}{dt}(t) \cdot \nabla_x u(t,x(t))$$

and taking the velocity $\mathbf{v} = \frac{dx}{dt}$ we get the previous form $\frac{d}{dt}u = \frac{\partial u}{\partial t} + \mathbf{v} \cdot \nabla_x u$.

3.3.3 Pollution problems

The advection-diffusion equation is often used to model pollution problems, where $u(t,x)$ denotes the concentration of a substance in time t at the location x. An initial concentration is considered

$$u_0(x) = \chi_\omega(x)w(x)$$

where χ_ω denotes the characteristic function on the location ω, a compact set where the initial concentration exists. For instance, in the case of a pollution problem, this corresponds to the origin of the pollutant source, that varies in ω according to some concentration w.

Thus we may consider the problem in free space as

$$\begin{cases} \frac{\partial u}{\partial t}(t,x) + \mathbf{v} \cdot \nabla u(t,x) = \alpha \Delta u(t,x), & (t,x) \in (0,+\infty) \times \mathbb{R}^3 \\ u(0,x) = u_0(x), & x \in \mathbb{R}^3 \end{cases} \tag{55}$$

and with no boundary conditions being specified.

3.4 Black-Scholes equation

The Black-Scholes equation, introduced in 1973, was an important tool in financial mathematics, as it was widely used to establish the prices of option contracts in the financial markets. The model used can be reduced to a heat equation problem, and we will see why.

3.4.1 Option contracts in finance

An investor could buy a stock (or a portfolio of stocks) at a certain price S and risk his investment through some chaotic flow of the stock market. To suppress some risk of the investment, option contracts were devised, in such a way that the investor, by paying a price for the option contract, would guarantee the right to buy (call option) or sell (put option) at an agreed *strike price.*

The option value $V(t, S)$ is therefore a function of time t and of the stock price S.

At a certain time T the option value $V(T, S)$ reflects the difference between the spot price of the stock S and the expected strike price E. The owner of the call option has the right to buy at the strike price E, but no one would exert the option of buying if $E > S$, because he could buy cheaper at the market price - in that case the option has no value.

Call option. Therefore at the time the option contract is exerted the value of the call option is

$$V(T, S) = \max\{S - E, 0\} \tag{56}$$

meaning that the option of buying worths nothing if the strike price is higher than the spot price, and it will payoff $S - E$ in the other case.

Put option. Similar process is the right to sell at a fixed strike price E, but then it will worth nothing to sell at the price E if you can sell it the market at a higher price S. Thus, the put option value at the contract time T_f will be

$$V(T, S) = \max\{E - S, 0\}. \tag{57}$$

Remark 3.6. *(European and American Options).* The difference between these two type of option contracts is the time when the option right can be used. In the european options this can only be done at a final time T_f (expiration time), while in the american options the right can be exerted (almost any time) before the contract ends.

The previous discussion is clear in what concerns the value of the option in the future, at the end of the contract, but it does not establish what is the value of the option contract before, at present time $t = 0$. The option value $V(0, S)$ should define the option price presented to the investor. This also depends on the volatility of the market, because the call option can turn out to worth nothing if the market drops the price of the stocks below the strike price. Black and Scholes in 1973 presented a model for option contracts that allowed to do these calculations, which was based in stochastic calculus, and it could be reduced to a partial differential equation, in particular to the heat equation.

3.4.2 Risk-free rate

If we have an asset S that adds an interest rate r, at each step we get an increase
$$S_{m+1} = (1+r)S_m,$$
which leads to the return $S_m = (1+r)^m S_0$, where S_0 is the initial value. Instead of discrete time steps, we may consider in the limit a continuous flow. In that case the original rate μmust be divided for the number of N steps, giving instead $r = \frac{\mu}{N}$, and

$$S_N = (1+\frac{\mu}{N})^N S_0 \implies S_N \to e^{\mu} S_0$$

This behavior of exponencial increase of interest rates over an original asset gives the evolution
$$S(t) = e^{\mu t} S(0),$$
solution of $\frac{dS}{dt} = \mu S$, or in terms of differential forms

$$dS = \mu S\, dt \tag{58}$$

which is the continuous version of $S_{m+1} - S_m = rS_m = \mu S_m(t_{m+1} - t_m)$, since $t_{m+1} - t_m = \frac{1}{N}$.

Now this means an evolution of stock price with expected rate μ and no other oscillation.

If we want to add a chaotic oscillation, we need to consider random variables.

3.4.3 Itô's Lemma

The typical setting for the evolution of a random variable X is to consider a Itô process
$$dX = \mu dt + \sigma dB \tag{59}$$
this means that instead of having a linear deterministic behavior $dX = \mu dt$ that would lead to $X(t) = \mu t\, X(0)$, we now add a random behavior, like in the Brownian motion, being B_t a Wiener process.

This Wiener process verifies $B(0) = 0$, B is continuous and $B(t+\varepsilon) \simeq B(t) + \mathcal{N}(0, \varepsilon)$, where $\mathcal{N}(\mu, \sigma)$ is a normal distribution with expected value μ and variance σ^2.

Therefore $E(B_t) = 0$ (the expectation is null) and $Var(B_t) = E(B_t^2) - E(B_t)^2 = E(B_t^2) = t$.

It is now important to evaluate the infinitesimal variation of a function of a random variable, that is also a random variable.

Theorem 3.7. *(Itô Lemma). Consider $f \in C^2$, and $dX = \mu dt + \sigma dB$, then the differential form of f is*

$$df(t, X) = \left(\frac{\partial f}{\partial t} + \mu \frac{\partial f}{\partial X} + \frac{\sigma^2}{2} \frac{\partial^2 f}{\partial X^2} \right) dt + \sigma \frac{\partial f}{\partial X} dB \tag{60}$$

Proof. We sketch the idea of the proof because it mainly relies on the Taylor expansion of f and on stochastic calculus. The standard two variable Taylor expansion gives

$$df(t, X) = \frac{\partial f}{\partial t} dt + \frac{\partial f}{\partial X} dX + \frac{1}{2} \frac{\partial^2 f}{\partial X^2} (dX)^2 + O(dtdX) + O(dX^2) + O(dt^2)$$

Since $dX^2 = (\mu dt + \sigma dB)^2 = O(dt^2) + O(dtdB) + \sigma^2 dB^2$ and $dB^2 = dt$ (because $E(B_t^2) = t$), neglecting the the terms $O(dt^2), O(dtdB)$ converging to zero faster than $O(dt)$, we get

$$\begin{aligned} df(t, X) &= \frac{\partial f}{\partial t} dt + \frac{\partial f}{\partial X} (\mu dt + \sigma dB) + \frac{1}{2} \frac{\partial^2 f}{\partial X^2} (\mu dt + \sigma dB)^2 \\ &= \frac{\partial f}{\partial t} dt + \frac{\partial f}{\partial X} (\mu dt + \sigma dB) + \frac{\sigma^2}{2} \frac{\partial^2 f}{\partial X^2} (dB)^2 \end{aligned}$$

and the result follows (as $dB^2 = dt$). □

3.4.4 Black-Scholes equation

Now we can consider the stochastic model, adding a random variable perturbation σdB,

$$dS = S(\mu \, dt + \sigma dB) \tag{61}$$

instead of the deterministic evolution $dS = S\mu \, dt$. Thus, the value of the option $V(t, S)$ will give by Itô's Lemma

$$dV = \left(\frac{\partial V}{\partial t} + \mu S \frac{\partial V}{\partial S} + \frac{\sigma^2}{2} S^2 \frac{\partial^2 V}{\partial S^2} \right) dt + S\sigma \frac{\partial V}{\partial S} dB$$

and given the stock portfolio $P = S\frac{\partial V}{\partial S} - V$ (S increase at the rate of V compared to it) , we get

$$\begin{aligned} dP &= dS\frac{\partial V}{\partial S} - dV = S(\mu\, dt + \sigma dB)\frac{\partial V}{\partial S} - \left(\frac{\partial V}{\partial t} + \mu S\frac{\partial V}{\partial S} + \frac{\sigma^2}{2}S^2\frac{\partial^2 V}{\partial S^2}\right) dt - S\sigma\frac{\partial V}{\partial S}dB \\ &= -\left(\frac{\partial V}{\partial t} + \frac{\sigma^2}{2}S^2\frac{\partial^2 V}{\partial S^2}\right) dt. \end{aligned}$$

On the other hand, at a risk-free rate r the portfolio behaves as $dP = rPdt = r\left(S\frac{\partial V}{\partial S} - V\right) dt$, and therefore we conclude

$$r\left(S\frac{\partial V}{\partial S} - V\right) = \frac{dP}{dt} = -\frac{\partial V}{\partial t} - \frac{\sigma^2}{2}S^2\frac{\partial^2 V}{\partial S^2}$$

and this is the Black-Scholes equation

$$\frac{\partial V}{\partial t} - \frac{\sigma^2}{2}S^2\frac{\partial^2 V}{\partial S^2} + r\left(S\frac{\partial V}{\partial S} - V\right) = 0 \tag{62}$$

3.4.5 Conditions on European Call Options

Black-Scholes equation has been established as a parabolic differential equation, now we will define the full problem, considering not an initial condition, but a condition at the final time of the contract, T_f. If E is the strike price, in the case of a **call option** (*opção de compra*), we already saw that

$$V(T_f, S) = \max\{S - E, 0\}, \tag{63}$$

We also need to establish boundary conditions on S.

One of them is quite obvious, if the stock value is null, the option to buy it also worths nothing. Therefore

$$V(t, 0) = 0. \tag{64}$$

On the other hand when S increases much the option value will basically worth the same, because the strike price will be too small. Suppose that the call option had the strike price $E = 1$ and that the stock has raised the value to $S = 1000$, if this does not change much, the call option value will be $S - E = 999$, because the stocks will be bought at 1€ and their market value is 1000€.

In fact, when $S \to \infty$,

$$V(T_f, S)/S = (S - E)/S \to 1$$

and we can consider $V(t, S) - S \to 0$, when $S \to \infty$.

Therefore the full problem for the value of a call option, let us call it $C(t, S)$ instead of $V(t, S)$, is the following

$$\begin{cases} \dfrac{\partial C}{\partial t} - \dfrac{\sigma^2}{2} S^2 \dfrac{\partial^2 C}{\partial S^2} + r\left(S\frac{\partial C}{\partial S} - C\right) = 0, & (t, S) \in (0, T_f) \times (0, \infty) \\ C(T_f, S) = \max\{S - E, 0\} & S \in [0, \infty[\\ C(t, 0) = 0 & t \in (0, T_f) \\ C(t, S) - S \to 0 & \text{when } S \to \infty \end{cases} \tag{65}$$

and the aim is to know the value of the call option at the initial time, meaning $C(0, S)$.

3.4.6 Reduction to the Heat Equation

With some variable substitution we can reduce the Black-Scholes equation to the heat equation.

We will consider first the following change of variables (notice the inversion sign on time)

$$\begin{cases} S = Ee^x \\ t = T_f - \frac{\tau}{\sigma^2/2} \\ C = Ev \end{cases} \quad \begin{cases} x = \log(S/E) \\ \tau = \frac{\sigma^2}{2}(T_f - t) \\ v = C/E \end{cases} \tag{66}$$

and we now have $v(\tau, x)$ instead of $C(t, S)$, which verifies

$$\frac{\partial v}{\partial \tau} = \frac{\partial^2 v}{\partial x^2} + (k - 1)\frac{\partial v}{\partial x} - kv$$

with $k = \frac{r}{\sigma^2/2}$, and in a second step, using

$$u(\tau, x) = \exp\left(\frac{1}{2}(k - 1)x + \frac{1}{4}(k + 1)^2\tau\right) v(\tau, x).$$

we can reduce it to the heat equation

$$\frac{\partial u}{\partial \tau} = \frac{\partial^2 u}{\partial x^2}.$$

Also, this change of variables introduces a difference in the domain and on the boundary and initial conditions.

Since $\tau = \frac{\sigma^2}{2}(T_f - t)$, we have $t = T_f \implies \tau = 0$ and $t = 0 \implies \tau = \frac{\sigma^2}{2}T_f$. This means that we will have an initial condition on u, and that the measurement time will be $\tau_f = \frac{\sigma^2}{2}T_f$ instead of zero.

Since $x = \log(S/E)$, we have $S \to 0 \implies x \to -\infty$, and of course $S \to +\infty \implies x \to +\infty$.

Therefore the new time-space domain is with$-\infty < x < +\infty$, and $\tau \in (0, \tau_f)$.

Finally, notice that

$$C(t,S) = u(\tau,x)E/\exp\left(\frac{1}{2}(k-1)x + \frac{1}{4}(k+1)^2\tau\right)$$

and since at final time $\tau = 0$,

$$C(T_f,S) = u(0,x)E/\exp\left(\frac{1}{2}(k-1)x\right)$$

and the condition $C(T_f,S) = \max\{S-E,0\}$ becames

$$u(0,x)E/\exp\left(\frac{1}{2}(k-1)x\right) = \max\{Ee^x - E, 0\}$$

that is $u(0,x) = \max\left\{(e^x-1)\exp\left(\frac{1}{2}(k-1)x\right), 0\right\}$ or also

$$u(0,x) = \max\left\{\exp\left(\frac{1}{2}(k+1)x\right) - \exp\left(\frac{1}{2}(k-1)x\right), 0\right\}. \tag{67}$$

Considering the boundary-asymptotic conditions, since $C = 0 \Leftrightarrow u = 0$, the condition $C(t,0) = 0$ becames

$$\lim_{x\to-\infty} u(\tau,x) = 0 \tag{68}$$

and the other condition $C(t,S) - S \to 0$, which is

$$u(\tau,x)E/\exp\left(\frac{1}{2}(k-1)x + \frac{1}{4}(k+1)^2\tau\right) - Ee^x \to 0$$

becames $u(\tau,x) - e^x\exp\left(\frac{1}{2}(k-1)x + \frac{1}{4}(k+1)^2\tau\right) \to 0$, and therefore

$$\lim_{x\to+\infty} u(\tau,x) - \exp\left(\tfrac{1}{2}(k+1)x + \tfrac{1}{4}(k+1)^2t\right) = 0. \tag{69}$$

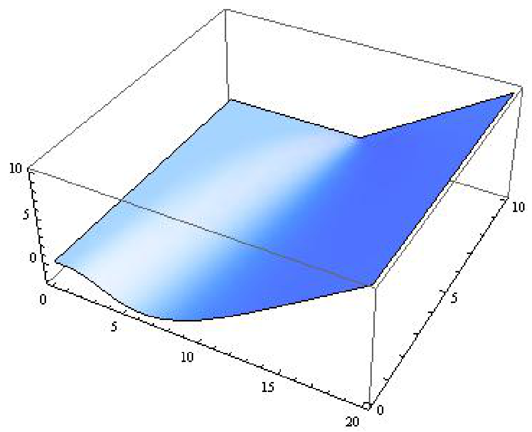

Figure 6: Black-Scholes solution with $E = 10, r = 0.01, \sigma = 0.2, T_f = 10$

3.4.7 Solution to the Black-Scholes equation

It is possible to deduce an explicit form for the Black-Scholes solution for an European call option

$$C(t, S) = S\mathcal{N}(R^+(t, S)) - \frac{E\mathcal{N}(R^-(t, S))}{\exp(r(T_f - t))} \tag{70}$$

where $\mathcal{N}(x) = \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{x} \exp(-\frac{y^2}{2}) dy$ is the cumulative normal probability distribution and where

$$R^{\pm}(t, S) = \frac{\log(S/E) + (r \pm \sigma^2/2)(T_f - t)}{\sigma\sqrt{T_f - t}}. \tag{71}$$

We now plot the solution of the Black-Scholes equation

4 Wave propagation

We now consider the propagation of waves. This leads to second order hyperbolic equations in the transient case. Now we have a second order derivative in time, and the simplest case is the 1D model for the vibrating string

$$\frac{\partial^2 u}{\partial t^2}(t,x) = c^2 \frac{\partial^2 u}{\partial x^2}(t,x) \tag{72}$$

where c denotes the velocity of propagation and u the amplitude.

Since a second derivative occurs in time, we impose two initial conditions

$$\begin{cases} u(t_0,x) = u_0(x), & x \in \Omega, \\ \frac{\partial u}{\partial t}(t_0,x) = u_1(x), & x \in \Omega, \end{cases} \tag{73}$$

instead of a single one initial condition, as in the parabolic heat equation.

Concerning the boundary conditions, we consider the same type of Dirichlet, Neumann, Robin or mixed, as considered previously.

4.1 Vibrating Strings

In the 1-dimensional case, given any functions $v_R, v_P \in C^2(\mathbb{R})$ we get particular solutions for the wave equation

$$u(x,t) = v_R(x+ct) + v_P(x-ct), \tag{74}$$

since $\partial_t^2 u(x,t) = c^2(v_R''(x+ct) + v_P''(x-ct)) = c^2 \partial_x u(x,t)$.

It is easy to check that the D'Alembert formula

$$u(x,t) = \frac{u_0(x+ct) + u_0(x-ct)}{2} + \frac{1}{2c}\int_{x-ct}^{x+ct} u_1(\tau)d\tau, \tag{75}$$

also verifies the two initial conditions (73).

4.1.1 Separation of variables

Using separation of variables $u(t,x) = w(t)v(x)$ in $\frac{\partial^2 u}{\partial t^2}(t,x) = c^2 \frac{\partial^2 u}{\partial x^2}(t,x)$ we get

$$c^2 \frac{v''(x)}{v(x)} = \frac{w''(t)}{w(t)} = K.$$

Considering $K = -c^2\mu^2$ we get two equations

$$\begin{aligned} v''(x) + \mu^2 v(x) = 0 \\ w''(t) + (\mu c)^2 w(t) = 0 \end{aligned}$$

leading to

$$\begin{aligned} v(x) = A_1 \cos(\mu x) + B_1 \sin(\mu x) \\ w(t) = A_2 \cos(c\mu t) + B_2 \sin(c\mu t) \end{aligned}$$

Therefore

$$u(t,x) = \cos(\mu x)\cos(c\mu t), \quad \text{or} \quad u(x,t) = \sin(\mu x)\sin(c\mu t)$$

are particular solutions of the vibrating string equation.

A combination of these particular solutions, for instance

$$u(t,x) = \sum_{k=0}^{\infty} a_k \cos(kx)\cos(ckt) + \sum_{k=1}^{\infty} b_k \sin(kx)\cos(ckt) \tag{76}$$

can lead to verify one initial condition

$$u(0,x) = u_0(x) = \sum_{k=0}^{\infty} a_k \cos(kx) + \sum_{k=1}^{\infty} b_k \sin(kx), \tag{77}$$

using the Fourier expansion.

4.2 Acoustic Waves

For acoustic waves, propagating in 3D, the equation is similar, now with the Laplace operator:

$$\frac{\partial^2 u}{\partial t^2}(t,x) = c^2 \Delta u(t,x) \tag{78}$$

and u is the amplitude associated to the pressure.

The wave operator is some times called D'Alembertian and denoted $\Box$:

$$\Box u(t,x) = \left(\frac{\partial^2}{\partial t^2} - c^2 \Delta \right) u(t,x) \tag{79}$$

Thus, the full acoustic wave propagation problem inside a domain Ω, with Dirichlet boundary conditions, is given by

$$(WP) \begin{cases} \Box u(t,x) = f(t,x), & (t,x) \in (t_0,t_f) \times \Omega \\ u(t_0,x) = u_0(x), \quad \partial_t u(t_0,x) = u_1(t), & x \in \Omega \\ u(t,x) = u_D(t,x), & (t,x) \in [t_0,t_f] \times \partial\Omega \end{cases} \tag{80}$$

Theorem 4.1. *There is uniqueness of solution for the problem (WP).*

Proof. We follow the steps of the heat equation uniqueness proof. Taking $u = u_1 - u_2$, the difference of solutions we now consider the energy function

$$E(t) = \frac{1}{2}\int_\Omega \left(\left| \frac{\partial u}{\partial t}(t,x) \right|^2 + c^2 \left| \nabla_x u(t,x) \right|^2 \right) dx. \tag{81}$$

Now, since $\partial_t^2 u(t,x) = c^2 \Delta_x u(t,x)$, we have

$$\begin{aligned} E'(t) &= \int_\Omega \partial_t^2 u(t,x)\partial_t u(t,x)dx + c^2 \int_\Omega \nabla_x u(t,x)\cdot\nabla_x \partial_t u(t,x)dx \\ &= c^2\int_\Omega \Delta_x u(t,x)\partial_t u(t,x)dx - c^2\int_\Omega \Delta_x u(t,x)\partial_t u(t,x)dx \\ &\quad -c^2\int_{\partial\Omega} \frac{\partial u}{\partial n_x}(t,x)\partial_t u(t,x)dx = 0 \end{aligned}$$

because $u(x,t) = 0\ \forall x \in \partial\Omega$ (Dirichlet b.c., for Neumann is similar) also implies $\partial_t u(x,t) = \partial_t 0 = 0$ in $\partial\Omega$.

Therefore $E(t)$ is constant, but the initial condition gives $\partial_t u(t_0,x) \equiv 0$, and $u(t_0,x) = 0$ for all $x \in \Omega$, which means that $E(t_0) = 0$ and E constant means $E(t) \equiv 0$. Therefore, from (81) we have $\frac{\partial u}{\partial t}(t,x) \equiv 0$, meaning that u is constant through time, and the null initial condition gives $u \equiv 0$. □

4.3 Helmholtz equation

We will now consider the time-harmonic case, in which

$$u(t,x) = e^{i\omega t} v(x), \tag{82}$$

that reflects a separation of the time variable with frequency $\omega > 0$.

This corresponds to a solution of the acoustic wave equation if the Helmholtz equation is verified for v:

$$\Delta v + (\frac{\omega}{c})^2 v = 0, \tag{83}$$

because $\frac{\partial^2 u}{\partial t^2} = -\omega^2 e^{i\omega t} v$, and $c^2 \Delta u = c^2 e^{i\omega t}\Delta v$.

Therefore, for time-harmonic waves the transient case is reduced to the Helmholtz equation.

The quantity $\kappa = \omega/c$ is called the wavenumber and it will be equal to the frequency as we consider an unitary wave speed $c = 1$.

4.3.1 Resonance frequencies

The Helmholtz equation does not provide uniqueness results always. In 1D this would correspond to

$$\frac{\partial^2 v}{\partial x^2} + \omega^2 v = 0 \Leftrightarrow v'' + \omega^2 v = 0$$

with general solution $v(x) = a\cos(\omega x) + b\sin(\omega x)$. Therefore, even if we consider null Dirichlet boundary conditions, for instance $v(0) = 0 = v(1)$, we can still find a solution $v(x) = \sin(\pi x)$ which is not null and verifies

$$v'' + \pi^2 v = 0.$$

Thus, there are certain frequencies for which uniqueness does not hold, depending on the domain that we consider.

In this case, taking $\Omega = (0, 1)$ we see that not only $\omega = \pi$ will lead to non uniqueness, but also any $\omega = n\pi$ with integers $n \in \mathbb{N}$.

If the domain was $\Omega = (0, \pi)$ we would get the same thing using any $\omega = n \in \mathbb{N}$. It is easy to see that this could be done in any interval, with an appropriate shift. It is not only a problem of the Dirichlet boundary condition, as $v(x) = \cos(\pi x)$ would give $v'(0) = v'(1) = 0$, leading to non null solutions for the null Neumann problem.

In 2D, notice that

$$v(x_1, x_2) = \sin(nx_1)\sin(mx_2)$$

verifies the Helmholtz equation with $\omega^2 = n^2 + m^2$, and that $v = 0$ on the boundary of $\Omega = (0, \pi)^2$, because $\sin(n\pi) = \sin(m\pi) = 0$ when $n, m \in \mathbb{N}$, and these are non null solutions.

The frequencies ω for which there are no uniqueness solutions are called *resonance frequencies.*

In the case of the square $\Omega = (0, \pi)^2$ these are

$$\omega \in \{\sqrt{2}, \sqrt{5}, \sqrt{8}, \sqrt{10}, \sqrt{13}, \ldots, \sqrt{n^2 + m^2}, ...\} \tag{84}$$

and the set of these resonance frequencies is called the spectrum

Each of these resonance frequencies corresponds to an eigenvalue of the Laplace operator with Dirichlet boundary conditions, because

$$\Delta v = \lambda v$$

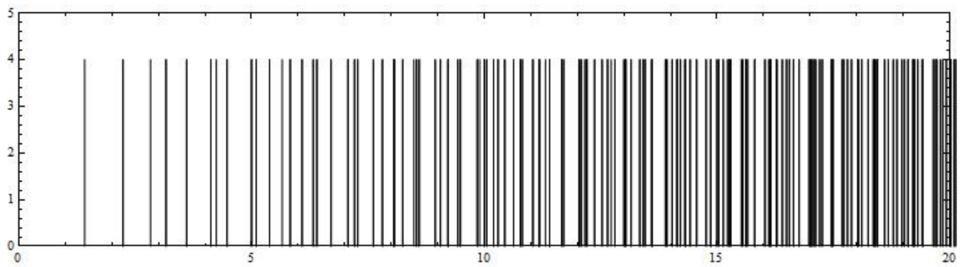

Figure 7: The spectrum of the first resonance frequencies for $\Omega = (0, \pi)^2$.

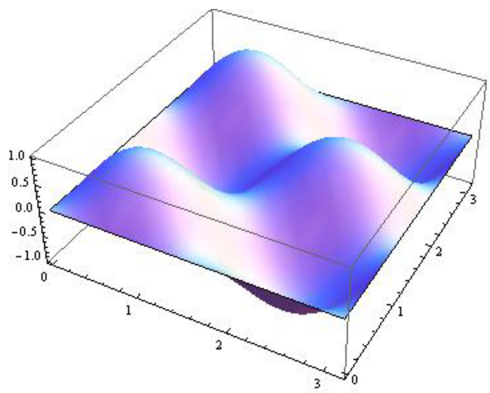

Figure 8: A Dirichlet eigenmode for $\omega = \sqrt{13}$.

with $\lambda = -\omega^2 = -(n^2 + m^2)$.

Associated to each eigenvalue λ (or *eigenfrequency*ω) there are eigenfunctions v (also called *eigenmodes*).

For instance for $\lambda = -13 = -(2^2 + 3^2)$, we can consider

$$v(x_1, x_2) = \sin(2x_1)\sin(3x_2) \quad \text{or} \quad v(x_1, x_2) = \sin(3x_1)\sin(2x_2)$$

If it is easy to calculate the eigenfrequencies in the case of the square, or a rectangle, it is not so easy to calculate it for other shapes. The full eigenfrequencies are only given for rectangles, balls and equilateral or rectangle triangles.

Remark 4.2. An interesting problem is to associate the set of frequencies to a certain shape. This was a famous problem raised by Kac in 1966:

Can one hear the shape of a drum? - The problem was only partially solved in 1992 (Gordon, Webb, and Wolpert) by presenting a negative result

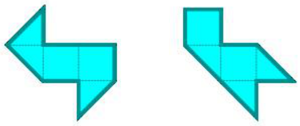

Figure 9: Isospectral drums - same eigenfrequencies, and a different shape.

- two polygonal shapes that have the same set of eigenfrequencies but that have different shapes.

4.3.2 Interior Helmholtz problems

From the previous discussion, we conclude that the Helmholtz Dirichlet (or Neumann) problem for a bounded (interior) domain Ω

$$\begin{cases} \Delta v + \omega^2 v = 0, & \text{in } \Omega, \\ v = g, & \text{on } \partial\Omega, \end{cases} \tag{85}$$

may not have an unique solution for a certain number of eigenfrequencies that depend on the domain.

However, for all the other frequencies the solution exists and it is unique.

4.4 Exterior Helmholtz problems

A different setting consists in taking the complementary set of a compact set D. Now our domain is unbounded

$$\Omega = \mathbb{R}^3 \backslash \bar{D}.$$

These are called exterior Helmholtz problems. There is a new "boundary" which is *infinity*...

Beside the boundary $\partial\Omega = \partial D$ we must consider an asymptotic behavior at infinity.

This behavior is given by the *Sommerfeld radiation condition* (in 3D)

$$\frac{\partial u}{\partial r} - i\omega u = o(r^{-1}) \quad \text{when } r = ||x|| \to \infty, \tag{86}$$

and it is verified by the Helmholtz fundamental solution

$$\Phi(x) = \frac{e^{i\omega ||x||}}{4\pi ||x||}. \tag{87}$$

4.4.1 Incident and scattered waves

The scattering problem consists in evaluating the effect of an incident wave u^{inc} on an object D, which produces a scattering wave u^{sc}. The total wave becames the sum of the two

$$u^{tot} = u^{inc} + u^{sc}.$$

The usual boundary conditions are of the Dirichlet type

$$u^{tot} = 0 \Leftrightarrow u^{sc} = -u^{inc}, \tag{88}$$

or of the Neumann type

$$\frac{\partial u^{tot}}{\partial n} = 0 \Leftrightarrow \frac{\partial u^{sc}}{\partial n} = -\frac{\partial u^{inc}}{\partial n} \tag{89}$$

(there are also Robin-impedance or mixed type conditions).

Typical incident waves are

- Plane waves in a direction d (with $||d|| = 1$)

$$u^{inc}(x) = e^{i\omega x\cdot d} \tag{90}$$

- Spherical waves centered at a source point y

$$u^{inc}(x) = \Phi(x-y) = \frac{e^{i\omega||x-y||}}{4\pi||x-y||}. \tag{91}$$

Remark 4.3. The plane waves verify the Helmoltz equation in the whole space, because

$$\nabla \cdot \nabla(e^{i\omega x\cdot d}) = i\omega d \cdot \nabla(e^{i\omega x\cdot d}) = -\omega^2||d||^2 e^{i\omega x\cdot d}$$

and $||d|| = 1$. The spherical waves verify it everywhere except at the center y.

Remark 4.4. We can also see that, asymptotically, the spherical wave behaves like a plane wave

$$\Phi(x-y) = \frac{e^{i\omega||x-y||}}{4\pi||x-y||} = \frac{e^{i\omega||x||}}{4\pi||x||}\left(e^{-i\omega\frac{x}{||x||}\cdot y} + O(||x||^{-1})\right) \tag{92}$$

4.4.2 Scattering problem

The scattered wave must verify the Helmholtz equation in the exterior domain Ω, the boundary conditions (here we considered Dirichlet), and the Sommerfeld radiation condition

$$\begin{cases} \Delta u^{sc} + \omega^2 u^{sc} = 0, & \text{in } \Omega, \\ u^{sc} = g = -u^{inc}, & \text{on } \partial\Omega, \\ \frac{\partial u^{sc}}{\partial r} - i\omega u^{sc} = o(r^{-1}) & \text{when } r = ||x|| \to \infty \end{cases} \tag{93}$$

The Sommerfeld radiation condition ensures that this exterior problem has an unique solution.

Moreover the resulting scattered wave decreases in a similar manner as the fundamental solution

$$u^{sc}(x) = \frac{e^{i\omega||x||}}{||x||}\left(u_\infty(\hat{x}) + O(||x||^{-1})\right) \tag{94}$$

where $\hat{x} = \frac{x}{||x||}$ has norm 1. The quantity u_∞ is called the far field pattern of u^{sc}. In fact if $u^{sc}(x) = \Phi(x-y)$ then we have

$$u_\infty(\hat{x}) = \frac{1}{4\pi} e^{-i\omega\hat{x}\cdot y}. \tag{95}$$

Also, by taking a linear combination of spherical waves

$$u^{sc}(x) = \sum_m \alpha_m \Phi(x - y_m) \tag{96}$$

the corresponding far field pattern would became

$$u_\infty(\hat{x}) = \frac{1}{4\pi}\sum_m \alpha_m e^{-i\omega\hat{x}\cdot y_m}. \tag{97}$$

Remark 4.5. A representation with boundary layers (like we did for the Laplace equation), holds in the same manner for the Helmholtz equation. The single layer potential would became

$$u^{sc}(x) = \int_{\partial\Omega} \Phi(x-y)\psi(y)ds_y \tag{98}$$

and this would lead to the following far field pattern

$$u_\infty(\hat{x}) = \frac{1}{4\pi}\int_{\partial\Omega} e^{-i\omega\hat{x}\cdot y}\psi(y)ds_y. \tag{99}$$

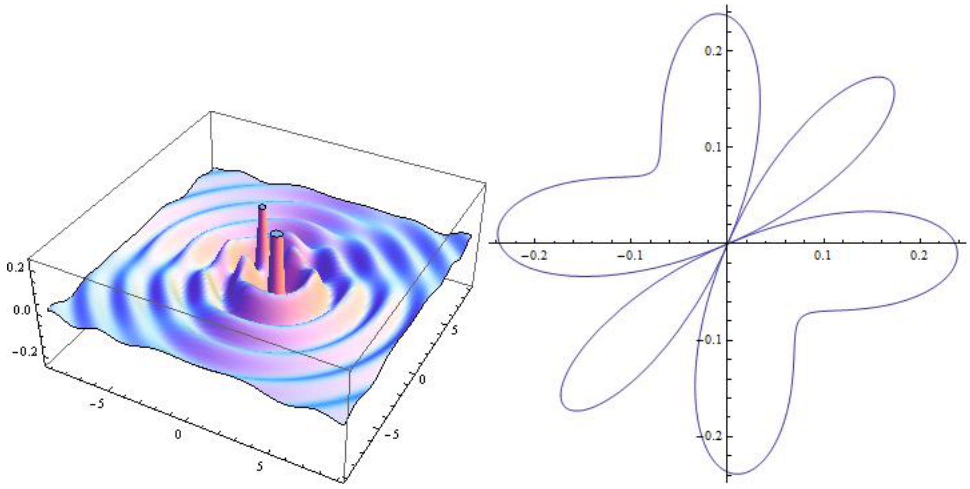

Figure 10: The scattered field by two sources and its far field pattern, as in the example.

Example 4.6. Suppose that we have a scattered field given by

$$u^{sc}(x) = \Phi(x - y_1) + 2\Phi(x - y_2)$$

with $y_1 = (-1, 1, 0)$ and $y_2 = -y_1$. Then its far field pattern will be given by

$$u_\infty(\hat{x}) = \frac{1}{4\pi}\left(e^{-i\omega\hat{x}\cdot y_1} + 2e^{-i\omega\hat{x}\cdot y_2}\right)$$

In Fig. 10 we plot the real part of u^{sc} (with singularities at y_1, y_2) and the real part of u_∞ (as a polar graphic for $\hat{x}_3 = 0$).

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