Introduction to the boundary element method. A case study: the Helmholtz equation

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Introduction

These are classnotes for the

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Although the course will be taught in Spanish, these notes have been prepared in English to reach a wider audience and to encourage Spanish speaking students to read scientific texts in English.

These notes are prepared so that the reader gets a feeling of what Boundary Element Methods are and to have a taste of their analysis, which is, let us put it simply, a bit hard. I firmly believe in understanding things first with an example and then organising your ideas to have a wider view of the problem. If you come from a very Mathematically oriented background, you will need faith to follow some of the steps, which are just sketched. Make the effort and get yourself a general idea of what this is about. If then you want to learn more, go for the many books on the subject. At the end I give some references where you can go on.

Instead of doing the theory with Laplace's equation, I've preferred to work with the Helmholtz equation as an excuse to introduce some topics (Fredholm theory, compact operators) and because Helmholtz fields are steady state waves that mix mathematics and physics in an attractive way. The style is easy–going and I propose several exercises. Most of them are quite simple and they are provided so that you are given some time to handle with these mathematical objects.

1 The Helmholtz equation

Consider a complex number k such that $\operatorname{Im} k \geq 0$. The equation

$$\Delta u + k^2 u = 0$$

is called the Helmholtz equation. Usually k is called the wave number. Even if $k^2 \in \mathbb{R}$ we will always look for **complex valued solutions** to this equation. Notice that the restriction to $\operatorname{Im} k \geq 0$ is immaterial, since what we are using is k^2 and not k, so what we are doing is restricting (arbitrarily) to one of the square roots.

Remark. When $k = \imath\, r$, we obtain the following equation (I've changed signs to make it look clearer):

$$-\Delta u + r^2 u = 0.$$

This is a typical elliptic equation, similar as those one obtains in reaction–diffusion systems. This equation is usually called the Yukawa equation. Wave–oriented people find it bad taste to call this equation the Helmholtz equation. More on this later. □

The most important appearance of the Helmholtz equation is in the study of time–harmonic waves. Consider the wave equation

$$c^2 \Delta v = \rho\, v_{tt},$$

where c and ρ are positive numbers (again, that c is not negative is irrelevant, but ρ has to be positive). A time–harmonic (or steady) solution to the wave equation is a solution of the form:

$$v(\mathbf{x},t) = \mathrm{Re}\left[u(\mathbf{x})\, e^{-\imath\, t\, \omega}\right] = u_{\mathrm{re}}(\mathbf{x})\, \cos(\omega\, t) + u_{\mathrm{im}}(\mathbf{x})\, \sin(\omega\, t).$$

Remark. A physicist would write this in terms of a positive amplitude and a phase

$$v(\mathbf{x},t) = A(\mathbf{x})\, \cos(\omega\, (t - \phi(\mathbf{x}))\,), \qquad A \geq 0.$$

Written in this way, one sees clearly that the solution is oscillating at the same frequency in all points (ω is the frequency), but there is a different amplitude (maximum oscillation) and a different phase (the time where oscillation reaches its maximum) in each point. Seeing things as linear combinations of a sine and a cosine leads to a simpler mathematical statement: no restriction on positivity for the amplitude; no angular redundancy for the phase; and, above all, linearity! Notice also that u is not a proper amplitude, since it is not a positive real function; u is called a **complex amplitude**. □

If a time–harmonic wave solves the wave equation, necessarily

$$c^2 \Delta u = -\rho\, \omega^2 u$$

that is,

$$\Delta u + k^2 u = 0, \qquad k := \sqrt{\rho}\, \frac{\omega}{c},$$

and u has to satisfy the Helmholtz equation. Notice that the wave number k is real, proportional to frequency and inversely proportional to c (velocity of transmission in the medium). It is also proportional to the square root of ρ (the density).

Exercise. *Instead of the wave equation, consider the following equation:*

$$c^2 \Delta v = \rho\, v_{tt} + \gamma\, v_t,$$

where $\gamma, \rho > 0$. If this equation has a time–harmonic solution, what steady–state equation has to satisfy its amplitude? Write explicitly the wave number.

Remark. The equation in the exercise above is a wave equation with damping. The one–dimensional case (one dimension in space) is called the telegrapher's equation. When the wave number in the Helmholtz equation has a non–trivial imaginary part, the medium is said to be absorbing. The case $k \in \mathbb{R}$ is usually called the acoustic case. Notice also that high frequencies correspond to high wave numbers: one usually speaks of high frequencies. However, when the medium transmits waves very fast (c is large), high frequencies correspond to moderate wave numbers. □

Exercise. *Look for time–harmonic solutions to the heat equation:* ($\kappa, \rho > 0$)

$$\kappa\, \Delta v = \rho\, v_t$$

How is the wave number in this case?

Exercise. *Consider the Helmholtz equation*

$$\Delta u + k^2 u = 0$$

in a bounded domain Ω. Prove that any classical boundary value problem (Dirichlet, Neumann) can be given a variational formulation by means of the sesquilinear form

$$a(u,v) := \int_\Omega \nabla u \cdot \nabla \overline{v} - k^2 u\, \overline{v}.$$

If $k^2 = \alpha + \imath\, \beta$ with $\beta > 0$, prove that there exists θ and $C > 0$ such that

$$\mathrm{Re}\left[e^{\imath\theta} a(u,u)\right] \geq C \|u\|^2_{1,\Omega}, \qquad \forall u \in H^1(\Omega).$$

(here $\|\cdot\|_{1,\Omega}$ is the classical $H^1(\Omega)-$norm).

2 Scattering

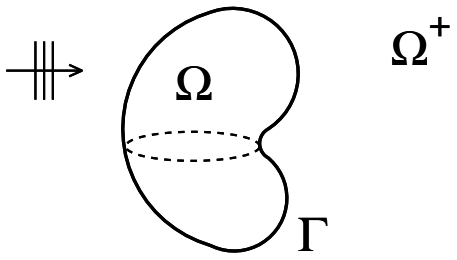
Let now Ω be a bounded domain in $\mathbb{R}^3$ with Lipschitz boundary Γ. Consider the exterior of Ω, denoted Ω^+. We fix a wave number k and consider the Helmholtz equation

$$\Delta u + k^2 u = 0, \qquad \text{in } \Omega^+.$$

Let us assume that we have a solution of the same equation in the whole of the space, that is, a function $u_{\mathrm{inc}} : \mathbb{R}^3 \to \mathbb{C}$ satisfying

$$\Delta u_{\mathrm{inc}} + k^2 u_{\mathrm{inc}} = 0, \qquad \text{in } \mathbb{R}^3.$$

The wave–field u_{inc} is called an **incident field**, or more generally, the corresponding wave is called an incident wave (recall that the complex amplitude defines a wave after multiplication with the time–oscillating term).



For instance,

$$u_{\mathrm{inc}}(\mathbf{x}) := e^{\imath\, k\, \mathbf{d}\cdot\mathbf{x}}, \qquad |\mathbf{d}| = 1$$

is an incident wave–field, corresponding to a plane wave. Then we decompose the total complex amplitude (the unknown of our problem) as

$$u = u_{\text{inc}} + u_{\text{scat}}.$$

By linearity

$$\Delta u_{\text{scat}} + k^2 u_{\text{scat}} = 0, \qquad \text{in } \Omega^+,$$

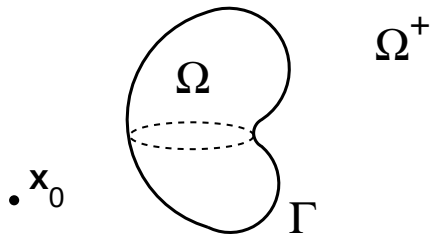
that is, the **scattered field** is a solution to the Helmholtz equation with the same wave number. The scattering measures the influence of the presence of the obstacle Ω in the wave–field u_{inc}.

Exercise. *Prove that plane waves are solutions to the Helmholtz equation. What is the corresponding incident wave in the time domain?*

Exercise. *If $\mathbf{x}_0$ is a fixed point in $\mathbb{R}^3$, prove that the function*

$$u_{\text{inc}}(\mathbf{x}) := \frac{1}{4\pi} \frac{e^{\imath\, k\, |\mathbf{x}-\mathbf{x}_0|}}{|\mathbf{x}-\mathbf{x}_0|}$$

satisfies the Helmholtz equation in $\mathbb{R}^3 \backslash \{\mathbf{x}_0\}$. These incident waves are called point sources. In general we will not demand that incident waves satisfy the Helmholtz equation in the whole space (as plane waves do), but only on a volume including the obstacle (as point sources with $\mathbf{x}_0 \in \Omega^+$ do).



We then have to give a boundary condition. The obstacle is called **sound–soft** when

$$u|_\Gamma = 0$$

or, seeing u_{scat} as unknown

$$u_{\text{scat}}|_\Gamma = -u_{\text{inc}}|_\Gamma.$$

Sound–hard bodies are those for which

$$\partial_\nu u|_\Gamma = 0,$$

or equivalently

$$\partial_\nu u_{\text{scat}}|_\Gamma = -\partial_\nu u_{\text{inc}}|_\Gamma.$$

Here ∂_ν is the normal derivative, where the normal vector points always outwards.

The partial differential equation plus a boundary condition for u_{scat} are not enough since we are dealing with a problem in an unbounded domain. We will have to give some kind of condition at infinity. This is what comes now.

Let us consider again the point source (spherical wave) defined in the last exercise, taking the origin as source, i.e., the function

$$u = \frac{1}{4\pi}\frac{e^{\imath\, k\, r}}{r}, \qquad r = |\mathbf{x}|.$$

Then

$$\partial_r u - \imath\, k\, u = -\frac{1}{4\pi}\frac{e^{\imath\, k\, r}}{r^2},$$

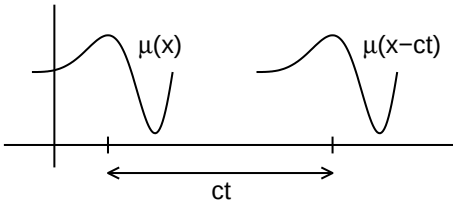
which means that the leading term of the radial derivative of this function is $\imath\, k\, u$. In the time domain this corresponds to

$$\text{Re}\left[\frac{e^{\imath\, k\, r}}{4\,\pi\, r}\, e^{-\imath\,\omega\, t}\right] = \frac{1}{4\,\pi\, r}\cos(k\, r - \omega\, t) = \frac{1}{4\,\pi\, r}\cos\Big(k\,(r - \frac{\omega}{k}t)\Big).$$

Notice that ω/k is proportional to c (the factor is related to the density ρ). Notice also that the process

$$\mu(x) \qquad \longmapsto \qquad \mu(x - c\, t)$$

moves the (graph of the) function μ, c units to the right every unit of time, that is, μ is moving rightwards at speed c.



Coming back to

$$\frac{1}{4\pi\, r}\cos\Big(k\,(r - \frac{\omega}{k}t)\Big),$$

this is a function moving radially outwards at speed $\omega/k \sim c$. Besides, the function is itself oscillating in space: it is a cosine with decreasing amplitude (amplitude decreases proportional to distance to the origin), the wave number being the number of oscillations per space unit. Again: c is related to how fast the waves travel (speed) and k is related to how oscillating it is. If one stays in a point, what one sees is an oscillation with frequency ω, but if one moves with the oscillation, the perceived frequency is different. Complicated, isn't it?

If we consider instead the function

$$\frac{e^{-\imath\, k\, r}}{4\,\pi\, r},$$

or in the time domain,

$$\mathrm{Re}\left[\frac{e^{-\imath k r}}{4\pi r}\, e^{-\imath \omega t}\right] = \frac{1}{4\pi r}\cos(k r + \omega t),$$

we obtain an **incoming wave**, travelling from infinity to the origin. The **outgoing wave** satisfies the condition

$$\lim_{r\to\infty} r\,(\partial_r u - \imath k u) = 0.$$

This limit is uniform in all directions. This is usually written

$$\partial_r u - \imath k u = o(r^{-1}), \qquad r \to \infty$$

(with the implicit understanding that a radial limit is uniform along all radii). The incoming wave does not satisfy this condition. This condition at infinity is usually called the **Sommerfeld radiation condition**.

The full scattering problem is written in terms of the scattering amplitude (we call it simply $u \equiv u_{\mathrm{scat}}$): we impose the Helmholtz equation in the exterior of the obstacle

$$\Delta u + k^2 u = 0, \qquad \text{in } \Omega^+,$$

the Sommerfeld radiation condition

$$\partial_r u - \imath k u = o(r^{-1}), \qquad r \to \infty.,$$

a Dirichlet boundary condition

$$u|_\Gamma = g_0$$

if the obstacle is sound–soft ($g_0 = -u_{\mathrm{inc}}|_\Gamma$) or a Neumann boundary condition

$$\partial_\nu u|_\Gamma = g_1$$

if the obstacle is sound–hard ($g_1 = -\partial u_{\mathrm{inc}}|_\Gamma$).

Recall that the true unknown of the problem is the total complex amplitude $u + u_{\mathrm{inc}}$, but we will always consider the amplitude of the scattered wave as unknown.

Remark. In scattering problems, typically right–hand sides are smooth functions restricted to the boundary (why solutions to the Helmholtz equation are smooth is a question we will deal with later on). However, both theory and numerics are always worked out with general right–hand sides. As incident waves one considers mainly plane waves and point sources placed on points outside the obstacle. □

There are also some other interesting problems related to scattering with more complicated boundary or transmission conditions. One of them, of great relevance when we move from acoustic to electromagnetic waves, is the use of impedance conditions, of the form

$$\partial_\nu u + \lambda u = g.$$

Helmholtz transmission problems stem from situations when the wave is transmitted inside the obstacle, which has different material properties (density and speed of transmission of waves).

3 Single–layer acoustic potentials

Let us consider the following function:

$$\phi(\mathbf{x}, \mathbf{x}_0) := \frac{e^{\imath\, k\, |\mathbf{x}-\mathbf{x}_0|}}{4\pi\, |\mathbf{x}-\mathbf{x}_0|}.$$

This function (of 2×3 variables) is called the outgoing fundamental solution to the Helmholtz equation, because it satisfies

$$\Delta\phi(\,\cdot\,, \mathbf{x}_0) + k^2\phi(\,\cdot\,, \mathbf{x}_0) = \delta_{\mathbf{x}_0}$$

(we will propose a proof of this in a forthcoming exercise) and the Sommerfeld radiation condition at infinity. If we place a finite number of point sources on Γ ($\mathbf{x}_j \in \Gamma$, $\forall j$), with different *charges/masses* ψ_j, its superposition

$$\sum_j \phi(\mathbf{x}, \mathbf{x}_j)\psi_j = \sum_j \frac{e^{\imath\, k\, |\mathbf{x}-\mathbf{x}_j|}}{4\pi\, |\mathbf{x}-\mathbf{x}_j|}\, \psi_j,$$

also satisfies the Helmholtz equation in Ω^+ together with the Sommerfeld radiation condition. The basic idea is to convert this sum into an integral by using a density $\psi : \Gamma \to \mathbb{C}$ and proposing

$$\int_\Gamma \phi(\mathbf{x}, \mathbf{x}_0)\psi(\mathbf{x}_0)\mathrm{d}\gamma(\mathbf{x}_0) = \int_\Gamma \frac{e^{\imath\, k\, |\mathbf{x}-\mathbf{x}_0|}}{4\pi\, |\mathbf{x}-\mathbf{x}_0|}\psi(\mathbf{x}_0)\mathrm{d}\gamma(\mathbf{x}_0)$$

as a candidate to solve our scattering problem:

$$\begin{aligned} \Delta u + k^2 u = 0, &\qquad \text{in } \Omega^+, \\ \partial_r u - \imath\, k\, u = o(r^{-1}), &\qquad r \to \infty \\ u|_\Gamma = g_0. & \end{aligned}$$

Notice (prove it!) that it satisfies automatically the differential equation and the radiation condition. What is left to impose is the boundary condition. But first, some nomenclature: the function (or class of functions)

$$(\mathcal{S}_\Gamma\psi)(\mathbf{x}) := \int_\Gamma \phi(\mathbf{x}, \mathbf{x}_0)\psi(\mathbf{x}_0)\mathrm{d}\gamma(\mathbf{x}_0) = \int_\Gamma \frac{e^{\imath\, k\, |\mathbf{x}-\mathbf{x}_0|}}{4\pi\, |\mathbf{x}-\mathbf{x}_0|}\psi(\mathbf{x}_0)\mathrm{d}\gamma(\mathbf{x}_0)$$

is called a **single–layer potential** and ψ is called the density.

Exercise. *Let $\varphi \in \mathcal{D}(\mathbb{R}^3)$ and $\phi_0(\mathbf{x}) := e^{\imath\, k\, |\mathbf{x}|}/(4\pi\, |\mathbf{x}|)$. Prove that*

$$\int_{\mathbb{R}^3} \phi_0(\Delta\varphi + k^2\varphi) = \lim_{\varepsilon \to 0} \int_{\partial B(0;\varepsilon)} (\partial_r\phi_0)\, \varphi - \phi_0(\partial_r\varphi).$$

Write down the explicit expression for

$$\partial_r\phi_0|_{\partial B(0;\varepsilon)} \qquad \textit{and} \qquad \phi_0|_{\partial B(0;\varepsilon)}.$$

Use them to prove that

$$\lim_{\varepsilon\to 0}\int_{\partial B(0;\varepsilon)}(\partial_r\phi_0)\,\varphi=\varphi(0)$$

and that

$$\lim_{\varepsilon\to 0}\int_{\partial B(0;\varepsilon)}\phi_0(\partial_r\varphi)=0.$$

Conclude that

$$\Delta\phi_0+k^2\phi_0=\delta_0,\qquad \textit{in } \mathcal{D}'(\mathbb{R}^3).$$

Deduce that

$$\Delta\phi(\,\cdot\,,\mathbf{x}_0)+k^2\phi(\,\cdot\,,\mathbf{x}_0)=\delta_{\mathbf{x}_0},\qquad \textit{in } \mathcal{D}'(\mathbb{R}^3).$$

Remark. Since we are solving the exterior problem, we could think of using a potential generated with a density defined on the whole of the obstacle, not only on its boundary, that is, something of the form

$$\int_\Omega \phi(\mathbf{x},\mathbf{x}_0)\psi(\mathbf{x}_0)\mathrm{d}\mathbf{x}_0.$$

Electrostatics (formally the case $k=0$) say clearly that we shouldn't do this: in the equilibrium charges are placed on the boundary. Mathematically this is a bit more complicated and you have to go to deep results of potential theory to prove that trying to solve our problem with a potential defined on the obstacle leads to a (distributional) solution supported on the boundary. Anyway, from our point of view, we are only trying with a class of functions. The fact that the class will be large enough to include a solution will be sufficient for us. □

Remark. Another possibility would be considering a surface (or a volume) Γ_0 strictly contained in the obstacle and trying a potential from there:

$$\mathcal{S}_{\Gamma_0}\psi.$$

Notice that on Γ (the true boundary of the scatterer) this function is very smooth. Imposing the boundary condition is extremely simple

$$\int_{\Gamma_0}\phi(\mathbf{x},\mathbf{x}_0)\psi(\mathbf{x}_0)\mathrm{d}\gamma(\mathbf{x}_0)=g_0(\mathbf{x}),\qquad \mathbf{x}\in\Gamma.$$

The approach looks correct but leads to a very ill–posed problem. But a very interesting problem though! If we change the point of view, assuming that Γ_0 is the boundary of the scatterer and that we have information on a surface surrounding the obstacle Γ, then we are dealing with a problem of *acoustic holography*, one of the simple–to–state but difficult–to–solve ill–posed problems of acoustics. We will not look further into this issue. □

We go then back to the definition of the potential

$$u:=\mathcal{S}_\Gamma\psi:=\int_\Gamma\phi(\,\cdot\,,\mathbf{y})\psi(\mathbf{y})\mathrm{d}\gamma(\mathbf{y}),$$

and notice again that

$$u \in \mathcal{C}^\infty(\mathbb{R}^3 \backslash \Gamma)$$
$$\Delta u + k^2 u = 0, \qquad \text{in } \Omega \cup \Omega^+ = \mathbb{R}^3 \backslash \Gamma$$

and that u is an outgoing wave–field (u satisfies the Sommerfeld condition at infinity). To simplify things, assume now that Γ and ψ are as smooth as you need them to be for what is coming. A simple argument using Lebesgue's theorem (the dominated convergence theorem) proves that the following limit exists

$$\lim_{\mathbf{x} \to \mathbf{x}_0^\pm} (\mathcal{S}_\Gamma \psi)(\mathbf{x}) = \int_\Gamma \phi(\mathbf{x}_0, \mathbf{y}) \psi(\mathbf{y}) \mathrm{d}\gamma(\mathbf{y}),$$

i.e., the same expression (now with an isolated singularity in the integrand; we are not integrating something smooth anymore) gives the interior (denoted with the sign $-$) and exterior ($+$) limits of the potential on the boundary. If we take the difference of the normal derivatives from inside and outside, we find this other fact ($\nu(\mathbf{x}_0)$ is the normal vector at $\mathbf{x}_0$ pointing outwards)

$$(\partial_\nu^- \mathcal{S}_\Gamma \psi)(\mathbf{x}_0) - (\partial_\nu^+ \mathcal{S}_\Gamma \psi)(\mathbf{x}_0) = \lim_{\mathbf{x} \to \mathbf{x}_0^+} \nabla \mathcal{S}_\Gamma \psi(\mathbf{x}) \cdot \nu(\mathbf{x}_0) - \lim_{\mathbf{x} \to \mathbf{x}_0^-} \nabla \mathcal{S}_\Gamma \psi(\mathbf{x}) \cdot \nu(\mathbf{x}_0) = \psi(\mathbf{x}_0),$$

which means that ψ is the jump of the normal derivative of the potential. Notice that the gradient is continuous (formally at least) in tangential directions, which means that the discontinuity of the gradient of the potential when approaching the boundary is a normal field proportional to density.

Remark. If we were dealing with electrostatics we would say that electric charges create continuous potentials but discontinuous electric fields. □

Then we define the single–layer operator

$$(V_\Gamma \psi)(\mathbf{x}) := \int_\Gamma \phi(\mathbf{x}, \mathbf{y}) \psi(\mathbf{y}) \mathrm{d}\gamma(\mathbf{y}), \qquad \mathbf{x} \in \Gamma.$$

You can be wondering now: but was this not $\mathcal{S}_\Gamma \psi$? In a way it was, but there is an important difference. Given a density $\psi : \Gamma \to \mathbb{C}$, $\mathcal{S}_\Gamma \psi$ is a function defined on the whole of $\mathbb{R}^3$ (a priori, we are interested only in $\Omega \cup \Omega^+$ or even only on Ω^+), whereas $V_\Gamma \psi$ is a function defined on Γ. In fact, $V_\Gamma \psi$ is the value on Γ of $\mathcal{S}_\Gamma \psi$. We recall names again: $\mathcal{S}_\Gamma \psi$ is a single–layer **potential** and $V_\Gamma \psi$ is a single–layer **operator**. The important thing is not the name or the letter we use (you'll find all kind of possibilities in the literature), but the concept: one is the field defined in the space, the other is a function defined in the same surface as the density. The operator

$$\psi \qquad \longmapsto \qquad V_\Gamma \psi := \int_\Gamma \phi(\,\cdot\,, \mathbf{y}) \psi(\mathbf{y}) \mathrm{d}\gamma(\mathbf{y})$$

is a linear integral operator. It is the first occurrence of what we call a **boundary integral operator**. We finally close the circle. The problem: find a density ψ such that

$$V_\Gamma \psi = g_0 \qquad \text{in } \Gamma$$

and then define

$$u := \mathcal{S}_\Gamma \psi$$

is a boundary integral method. One first solves an integral equation and then inputs its solution in a potential expression. An integral equation involving a boundary integral operator is called a **boundary integral equation** (BIE for short). Notice that after solving this BIE, we have obtained a solution of the exterior Dirichlet problem for the Helmholtz equation and that this solution is defined by means of a potential. The fact that we used an artificial device as a single–layer potential, where a non–physical quantity (the density) is involved, justifies why this kind of approach is called an **indirect method**.

Exercise. *Prove that if $\psi \in L^1(\Gamma)$, both $\mathcal{S}_\Gamma \psi$ and $V_\Gamma \psi$ are well defined. Prove also the limiting expressions on Γ for $\mathcal{S}_\Gamma \psi$ and its gradient.*

4 The Sobolev setting

Remark. If you are an engineer, you would be willing to have some numbers (a discretization) as fast as possible. Skip this section and move on to finding a numerical scheme. But then come back here, even if you have to ignore the difficult parts with all the Sobolev spaces, because there are some non–trivial solvability questions to be taken into account. Non–trivial and important. □

Recall first your Sobolev spaces. $H^1(\Omega)$ is the classical Sobolev space of order one (its elements and their first distributional derivatives are in $L^2(\Omega)$). The norm of $H^1(\Omega)$ is denoted $\| \cdot \|_{1,\Omega}$ and the one of $L^2(\Omega) = H^0(\Omega)$ as $\| \cdot \|_{0,\Omega}$. $H^{1/2}(\Gamma)$ is the trace space. The trace operator

$$\gamma : H^1(\Omega) \to H^{1/2}(\Gamma)$$

is continuous and onto. Since the inclusion

$$H^{1/2}(\Gamma) \subset L^2(\Gamma)$$

is dense and continuous, we can add the dual space of $H^{1/2}(\Gamma)$ to the other side of this inclusion and obtain something like

$$H^{1/2}(\Gamma) \subset L^2(\Gamma) \subset H^{-1/2}(\Gamma).$$

In this way, $H^{-1/2}(\Gamma)$ is the dual space to $H^{1/2}(\Gamma)$ (the set of continuous linear maps from $H^{1/2}(\Gamma) \to \mathbb{C}$), seen in a way such that any $g \in L^2(\Gamma)$ defines an element of $H^{-1/2}(\Gamma)$ by means of the expression

$$H^{1/2}(\Gamma) \ni \varphi \qquad \longmapsto \qquad \int_\Gamma g(\mathbf{y})\, \varphi(\mathbf{y}) \mathrm{d}\gamma(\mathbf{y}),$$

and this element (a bounded linear functional $H^{1/2}(\Gamma) \to \mathbb{C}$) is also called g. The duality product will be denoted

$$\langle g, \varphi \rangle_\Gamma.$$

A priori $g \in H^{-1/2}(\Gamma)$ and $\varphi \in H^{1/2}(\Gamma)$, but if $g \in L^2(\Gamma)$ (which is a proper dense subset of $H^{-1/2}(\Gamma)$ with the identification above), this is just

$$\langle g, \varphi \rangle_\Gamma = \int_\Gamma g(\mathbf{y})\, \varphi(\mathbf{y}) \mathrm{d}\gamma(\mathbf{y}).$$

We are not going to dive very deep into this, since this course is introductory. Nevertheless, if you are really willing to understand the mathematics of boundary elements, there is no way round.

Remark. A triple $V \subset H \subset V'$ defined as above (the key is that the injection of V into H is continuous and dense) is called a Gelfand triple or Courant triple (or triad). □

The weak normal derivative is defined as follows: if $u \in H^1(\Omega)$ and $\Delta u \in L^2(\Omega)$, then the expression

$$\int_\Omega \Delta u \; v + \int_\Omega \nabla u \cdot \nabla v$$

is a continuous function of the trace of $v \in H^1(\Omega)$ (not of v itself). Thus, we define

$$\langle \partial_\nu u, \varphi \rangle_\Gamma := \int_\Omega \Delta u \; v + \int_\Omega \nabla u \cdot \nabla v$$

where v is any element of $H^1(\Omega)$ such that $\gamma v = \varphi$. Maybe it looks simpler if we write it as follows

$$\langle \partial_\nu u, \gamma v \rangle_\Gamma := \int_\Omega \Delta u \; v + \int_\Omega \nabla u \cdot \nabla v, \qquad \forall v \in H^1(\Omega).$$

Then $\partial_\nu u \in H^{-1/2}(\Gamma)$ and

$$\|\partial_\nu u\|_{-1/2,\Gamma} \leq C \Big[\|\nabla u\|_{0,\Omega} + \|\Delta u\|_{0,\Omega} \Big].$$

It is not very obvious at first sight, but to define $\partial_\nu u$ on Γ we only need that ∇u and Δu are in L^2 in a region near the boundary Γ, since distant parts of the domain do not play any role in the definition.

We are going to need a new set. We say that

$$u \in H^1_{\mathrm{loc}}(\overline{\Omega^+})$$

if the restriction of u to any bounded open subset of Ω^+ (possibly touching the boundary Γ) is in H^1. This *local* space keeps functions with locally H^1 behaviour, ignoring the rate of decay at infinity necessary to have square–integrability. Since the trace operator is local, we can define the exterior trace

$$\gamma : H^1_{\mathrm{loc}}(\overline{\Omega^+}) \to H^{1/2}(\Gamma).$$

Also we can define the exterior normal derivative for functions in $H^1_{\mathrm{loc}}(\overline{\Omega^+})$ whose laplacian is in $L^2_{\mathrm{loc}}(\overline{\Omega^+})$.

Remark. The exterior trace is the same as the interior trace operator, but for functions defined on the other side of the boundary. It is, let me emphasize this, the same operator. The same thing applies for the exterior normal derivative. The key to a good understanding of these operators is that, even if their definition looks global (it is done in an operational way), finally the operators are local, taking into account what happens around the boundary and not far from it. □

Remark. The notation $H^1_{\rm loc}(\overline{\Omega^+})$ is the correct one. I'd be tempted to write the simpler form $H^1_{\rm loc}(\Omega^+)$, but what this really means is local H^1 behaviour strictly inside Ω^+, that is, not only ignoring the infinity but also the limits on Γ. A very smooth function with a very strong singularity on Γ belongs to $H^1_{\rm loc}(\Omega^+)$ but not to $H^1_{\rm loc}(\overline{\Omega^+})$. □

Theorem *For arbitrary $\psi \in H^{-1/2}(\Gamma)$,*

$$\mathcal{S}_\Gamma \psi \in H^1(\Omega) \times H^1_{\rm loc}(\overline{\Omega^+}),$$

is an outgoing solution of $\Delta u + k^2 u = 0$. The interior and exterior traces coincide

$$\gamma(\mathcal{S}_\Gamma \psi) = V_\Gamma \psi$$

and the gradient has a jump in the normal direction:

$$\partial_\nu^- \mathcal{S}_\Gamma \psi - \partial_\nu^+ \mathcal{S}_\Gamma \psi = \psi.$$

Finally,

$$V_\Gamma : H^{-1/2}(\Gamma) \to H^{1/2}(\Gamma)$$

is linear and bounded.

Remark. Notice that for any $\mathbf{x} \in \mathbb{R}^3 \backslash \Gamma$, the potential can be defined by duality

$$(\mathcal{S}_\Gamma \psi)(\mathbf{x}) = \langle \psi, \phi(\mathbf{x}, \cdot\,) \rangle_\Gamma.$$

The smooth part of the proposition above (that this function satisfies the Helmholtz equation plus the Sommerfeld radiation condition at infinity) can be proven with very classical arguments. The part related to traces and normal derivatives requires a higher level of analysis. □

Uniqueness for boundary value problems for the Helmholtz equation is not straightforward. This is what can be obtained.

- The exterior problem has uniqueness of radiating solution:

$$\begin{aligned} \Delta u + k^2 u = 0, &\qquad \text{in } \Omega^+, \\ \partial_r u - \imath\, k\, u = o(r^{-1}), &\qquad r \to \infty \\ u|_\Gamma = 0 & \end{aligned}$$

  implies that $u \equiv 0$

- There is a sequence of eigenvalues for which the interior problem has no unique solution, i.e.,

$$\begin{aligned} \Delta u + k^2 u &= 0, \qquad \text{in } \Omega, \\ u|_\Gamma &= 0 \end{aligned}$$

  implies that $u \equiv 0$ if and only if $-k^2$ is not a Dirichlet eigenvalue of the Laplacian in Ω.

- The Dirichlet eigenvalues of the Laplace operator form a sequence of numbers

$$0 < k_1^2 < k_2^2 < \ldots < k_n^2 < \ldots \to \infty$$

  for which the problems

$$\begin{aligned} -\Delta u &= k_n^2 u, \qquad \text{in } \Omega, \\ u|_\Gamma &= 0 \end{aligned}$$

  have non–unique solution. To each eigenvalue corresponds a finite dimensional eigenspace.

Remark. One can say a lot more about the Dirichlet eigenvalues and eigenfunctions of the Laplacian. For instance, the first eigenvalue is simple. Also, taking an $L^2(\Omega)-$orthonormal basis of each eigenspace we obtain a Hilbert basis of $L^2(\Omega)$. Upon normalization this basis is also a Hilbert basis of $H_0^1(\Omega)$. This is precisely the origin of the method of separation of variables that can be found in any classical text of differential equations. □

Assume now that

$$V_\Gamma \psi = 0.$$

Defining $u := \mathcal{S}_\Gamma \psi$, we have

$$\begin{aligned} \Delta u + k^2 u &= 0, \qquad \text{in } \Omega^+ \cup \Omega, \\ \partial_r u - \imath\, k\, u &= o(r^{-1}), \qquad r \to \infty \\ u|_\Gamma = V_\Gamma \psi &= 0 \end{aligned}$$

and therefore $u^+ \equiv 0$. If $-k^2$ is not a Dirichlet eigenvalue of the Laplacian (in the interior of the obstacle), then $u^- \equiv 0$. Hence

$$\psi = \partial_\nu^- u - \partial_\nu^+ u = 0,$$

and we just proved that V_Γ is injective.

If on the other hand, $-k^2$ is a Dirichlet eigenvalue of the Laplace operator, and we take $0 \neq \xi$ such that

$$\begin{aligned} -\Delta \xi &= k^2 \xi, \qquad \text{in } \Omega, \\ \xi|_\Gamma &= 0, \end{aligned}$$

then $\psi = \partial_\nu \xi \neq 0$. The reason why a non–trivial Dirichlet eigenfunction of the Laplace operator cannot be at the same time a Neumann eigenfunction, i.e., why

$$\begin{aligned} -\Delta \xi = k^2 \xi, \quad & \text{in } \Omega, \\ \xi|_\Gamma = 0, \qquad & \Longrightarrow \qquad \xi \equiv 0 \\ \partial_\nu \xi|_\Gamma = 0, & \end{aligned}$$

will be derived from a result we will see in a forthcoming section. With precisely that result it is possible to see that $V_\Gamma \psi = 0$.

The preceding (formal) argument proves that

$$V_\Gamma \textit{ is injective} \qquad \Longleftrightarrow \qquad -k^2 \textit{ is not a Dirichlet eigenvalue of } \Delta \textit{ in } \Omega.$$

In particular, when k^2 has non–trivial imaginary part (the medium is absorbing), V_Γ is injective.

Remark. Invertibility of V_Γ can be trivially used to show existence of solution to the exterior Helmholtz problem with Dirichlet condition. Then the remaining point is showing invertibility (surjectivity!) of V_Γ, which follows a more complicated path. We'll sketch the proof in due time. Anyway, you will definitely not learn here all the details of the proofs and I'll be very careful to hide some complicated facts. □

As mentioned, if $V_\Gamma : H^{-1/2}(\Gamma) \to H^{1/2}(\Gamma)$ is invertible we can solve the exterior Helmholtz equation (the sound–soft scattering problem)

$$\begin{aligned} \Delta u + k^2 u = 0, \qquad & \text{in } \Omega^+, \\ \partial_r u - \imath\, k\, u = o(r^{-1}), \qquad & r \to \infty \\ u|_\Gamma = g & \end{aligned}$$

for arbitrary $g \in H^{1/2}(\Gamma)$ as follows: first we solve the integral equation on Γ

$$V_\Gamma \psi = g$$

and the we input ψ in the potential expression

$$u = \mathcal{S}_\Gamma \psi$$

to obtain the solution of the scattering problem. By looking at the integral equation (formally; in truth ψ is not a function)

$$(V_\Gamma \psi)(\mathbf{x}) := \int_\Gamma \phi(\mathbf{x}, \mathbf{y}) \psi(\mathbf{y}) \mathrm{d}\gamma(\mathbf{y}) = g(\mathbf{x}), \qquad \mathbf{x} \in \Gamma$$

we observe the very non–local character of the equation, that is, the value of ψ in some region influences the value of $V_\Gamma \psi$ in the whole of Γ.

5 Discretization

We begin by showing the simplest Galerkin scheme for the integral equation

$$(V_\Gamma \psi)(\mathbf{x}) = \int_\Gamma \phi(\mathbf{x},\mathbf{y})\psi(\mathbf{y})\mathrm{d}\gamma(\mathbf{y}) = g(\mathbf{x}), \qquad \mathbf{x}\in\Gamma.$$

Let us decompose the boundary Γ into a finite set of curved patches

$$\Gamma = \cup\{\overline{\Gamma}_i \,|\, i = 1,\ldots,N\}$$

with trivial overlappings: $\overline{\Gamma}_i \cap \overline{\Gamma}_j$ is one–dimensional for $i \neq j$. We point out that we are looking for ψ in the space $H^{-1/2}(\Gamma)$ and that

$$L^2(\Gamma) \subset H^{-1/2}(\Gamma).$$

This implies that we will not need any degree of continuity in the discrete space here. Consequently, we can work with basically any partition of the boundary in curved polygons without the classical rules of *either–full–sides–or–vertices match* of finite element spaces. A traditional triangulation of the surface is however the typical choice.

Remark. A highly non–trivial question when we are dealing with triangulations of surfaces is what do we consider as a triangulation and how can we manage the fact that we usually lack a parameterization valid for the whole surface. The following is a theoretical setting which corresponds to what we usually find in practice. Related to the real boundary Γ there is a closed polyhedron $\widehat{\Gamma}$ and a bijection

$$\boldsymbol{\eta} : \widehat{\Gamma} \to \Gamma$$

which is: (a) continuous; (b) globally Lipschitz with globally Lipschitz inverse ; (c) smooth (for instance $\mathcal{C}^2$) on each face of the polyhedron $\widehat{\Gamma}$. The second hypothesis means that we can estimate distances on the surface (geodesic distances) by distances on the polyhedron or by joining points through the three–dimensional space. The estimate can be bad but does not degenerate. The polyhedron is composed of M polygonal faces $\{P_1,\ldots,P_M\}$ and their images $\{\boldsymbol{\eta}(P_n)|n = 1,\ldots,M\}$ define a level zero partition of Γ. We do not plan to discretize here. Then we can define a triangulation of the polyhedral surface $\widehat{\Gamma}$ in the usual triangles or quadrilaterals with the common rules (not really necessary here, but...). These planar elements on the straight faces are then mapped onto the surface and define the partition of the surface. □

Instead of a generic density $\psi : \Gamma \to \mathbb{R}$ we take $\psi_h : \Gamma \to \mathbb{R}$ such that

$$\psi_h(\mathbf{x}) \equiv \psi_j, \qquad \mathbf{x}\in\Gamma_j,$$

that is, ψ_h is constant on each element. Then

$$\begin{aligned}
(V_\Gamma\psi_n)(\mathbf{x}) &= \int_\Gamma \phi(\mathbf{x},\mathbf{y})\psi_h(\mathbf{y})\mathrm{d}\gamma(\mathbf{y}) \\
&= \sum_{j=1}^N \int_{\Gamma_j} \phi(\mathbf{x},\mathbf{y})\psi_h(\mathbf{y})\mathrm{d}\gamma(\mathbf{y}) \\
&= \sum_{j=1}^N \Big[\int_{\Gamma_j} \phi(\mathbf{x},\mathbf{y})\mathrm{d}\gamma(\mathbf{y})\Big]\,\psi_j.
\end{aligned}$$

Obviously $V_\Gamma \psi_h$ will not match g everywhere. We only demand that the average value of both functions on each element Γ_i coincide, that is, we demand that

$$\int_{\Gamma_i} (V_\Gamma \psi_h)(\mathbf{x}) \mathrm{d}\gamma(\mathbf{x}) = \int_{\Gamma_i} g(\mathbf{x}) \mathrm{d}\gamma(\mathbf{x}), \qquad i = 1, \ldots, N$$

or equivalently

$$\sum_{j=1}^{N} \Big[\int_{\Gamma_i} \Big[\int_{\Gamma_j} \phi(\mathbf{x}, \mathbf{y}) \mathrm{d}\gamma(\mathbf{y}) \Big] \mathrm{d}\gamma(\mathbf{x}) \Big] \psi_j = \int_{\Gamma_i} g(\mathbf{x}) \mathrm{d}\gamma(\mathbf{x}), \qquad i = 1, \ldots, N,$$

which is an $N \times N$ linear system, whose unknowns are the values of the piecewise constant density on the elements.

To avoid an excess of parentheses we will always adopt the following convention

$$\int_A \int_B f(\mathbf{x}, \mathbf{y}) \mathrm{d}\gamma(\mathbf{x}) \mathrm{d}\gamma(\mathbf{y}) := \int_A \left(\int_B f(\mathbf{x}, \mathbf{y}) \mathrm{d}\gamma(\mathbf{y}) \right) \mathrm{d}\gamma(\mathbf{x}),$$

that is, the variables and sets of integration are given in the same order.

Exercise. *Let*

$$a_{ij} := \int_{\Gamma_i} \int_{\Gamma_j} \frac{e^{\imath k |\mathbf{x}-\mathbf{y}|}}{4\pi |\mathbf{x}-\mathbf{y}|} \mathrm{d}\gamma(\mathbf{x}) \, \mathrm{d}\gamma(\mathbf{y})$$

be the matrix of the linear system above. Prove that it is symmetric but non–hermitian in general. For which values of k is this matrix hermitian? Notice that a priori $a_{ij} \neq 0$ for all i, j.

The method we just described can be easily understood as a **Galerkin method**. First, remark that

$$V_\Gamma \psi = g$$

is equivalent to

$$\langle V_\Gamma \psi, \varphi \rangle_\Gamma = \langle g, \varphi \rangle_\Gamma, \qquad \forall \varphi \in H^{-1/2}(\Gamma).$$

The angled brackets $\langle \cdot, \cdot \rangle_\Gamma$ represent the duality of $H^{-1/2}(\Gamma)$ on $H^{1/2}(\Gamma)$. In this case, the second component is the element of $H^{-1/2}(\Gamma)$ (the dual space) and the first is the element of $H^{1/2}(\Gamma)$ (the primal space).

We can then define a bilinear form $a : H^{-1/2}(\Gamma) \times H^{-1/2}(\Gamma) \to \mathbb{C}$

$$a(\psi, \varphi) := \langle V_\Gamma \psi, \varphi \rangle_\Gamma$$

and a linear form $\ell : H^{-1/2}(\Gamma) \to \mathbb{C}$

$$\ell(\varphi) := \langle g, \varphi \rangle_\Gamma$$

and write the whole problem as a typical variational problem in the Hilbert space $H^{-1/2}(\Gamma)$

$$\psi \in H^{-1/2}(\Gamma), \qquad a(\psi, \varphi) = \ell(\varphi), \quad \forall \varphi \in H^{-1/2}(\Gamma).$$

The bilinear and the linear forms are continuous. Notice also that the bilinear form can be formally written as

$$\int_\Gamma \int_\Gamma \phi(\mathbf{x},\mathbf{y})\,\psi(\mathbf{y})\,\varphi(\mathbf{x})\mathrm{d}\gamma(\mathbf{x})\,\mathrm{d}\gamma(\mathbf{y}),$$

that is, it involves a double integral on Γ.

Remark. This is not properly a variational formulation in the sense you will have found in elliptic PDE theory and finite element implementations, since we have not moved derivatives from the original equation to the tests. It is simply a straightforward testing of an integral equation. This is a common feature to most boundary integral equations. In some equations, however, after this straightforward testing, we apply some identities to rewrite the bilinear form without changing the regularity requirements of the unknown though. □

If we define now

$$X_h := \{\psi_h : \Gamma \to \mathbb{R} \,|\, \psi_h|_{\Gamma_j} \in \mathbb{P}_0, \quad \forall j\}$$

where $\mathbb{P}_0$ is the space of constant functions (polynomials of degree zero), then we can define a Galerkin scheme by

$$\psi_h \in X_h, \qquad a(\psi_h,\varphi_h) = \ell(\varphi_h), \quad \forall \varphi_h \in X_h.$$

Exercise. *Prove that this Galerkin scheme is equivalent to the method we derived before. Why can we properly write*

$$a(\psi_h,\varphi_h) = \int_\Gamma \int_\Gamma \phi(\mathbf{x},\mathbf{y})\,\psi_h(\mathbf{y})\,\varphi_h(\mathbf{x})\,\mathrm{d}\gamma(\mathbf{x})\,\mathrm{d}\gamma(\mathbf{y})$$

without needing duality products?

Assume again that we approximate ψ by $\psi_h \in X_h$. Instead of requiring that $V_\Gamma\psi_h$ and g have equal averages on the elements, we do the following: we choose a point $\mathbf{x}_i \in \Gamma_i$ on each element; we demand that

$$(V_\Gamma\psi_h)(\mathbf{x}_i) = g(\mathbf{x}_i), \qquad i = 1,\ldots,N.$$

The method thus derived is called a **collocation method**. The points $\{\mathbf{x}_i\}$ are called **collocation nodes**.

Exercise. *Write this method as an equivalent system of linear equations. Is the corresponding matrix symmetric?*

Remark. Generally speaking engineers prefer the collocation method to the Galerkin method. The essential reason is that we have simpler integrals to compute or approximate and that the deduction is somewhat simpler in the sense that we are neither averaging on the cells nor considering an intermediate variational formulation. □

There are however some aspects (pros and cons) to be taken into account:

- Not every choice of collocation nodes is going to work. For instance, taking a vertex per triangle is not a judicious choice.
- There is not a satisfactory theory for this method working even for smooth surfaces. This should not worry too much a practitioner of the method: most people are convinced that the theory will arrive in due time. However, the Galerkin setting gives more confidence to mathematically (or theoretically) oriented users of the boundary element method.
- If g has discontinuities, where one places nodes is also relevant.
- In some instances, practitioners of the method use many more collocation nodes than elements and solve the (incompatible) equations by mean squares. This has the advantage that we have to solve a Hermitian positive definite system. If we are going to use conjugate gradient iterates we don't even have to create the normal matrix A^*A. There is a big drawback to this nevertheless. The conditioning of the systems we have obtained is not very good (it is not dramatically bad) and the normal equations have it squared, which makes everything worse–off by making iterative methods far too slow. The other point in favour of taking many more collocation points than elements (two or three per element) is that maybe a subset of them is stable and compensates the bad choice of other sets. My point here is then: don't do this!

Sometimes, one sees in texts the collocation method written in a variational form as

$$\psi_h \in X_h, \qquad \langle V_\Gamma \psi_h, \delta_i \rangle_\Gamma = \langle g, \delta_i \rangle_\Gamma, \quad i = 1, \ldots, N$$

or even as a Petrov–Galerkin method

$$\psi_h \in X_h, \qquad \langle V_\Gamma \psi_h, \rho_h \rangle_\Gamma = \langle g, \rho_h \rangle_\Gamma, \quad \forall \rho_h \in Y_h = \operatorname{span}\{\delta_i \,|\, i = 1, \ldots, N\}$$

where Y_h is the space of linear combinations of the Dirac delta distributions δ_i on the collocation nodes $\mathbf{x}_i$. One has to take this with more than a bit of salt. It is formally okay and makes the method look a particular case of the Petrov–Galerkin method, but the angled brackets are not really correct and one is in fact using a far more complicated theoretical setting.

In Section 8 we will work a bit more on the matrices for the Galerkin and collocation method as well as proposing a method based on point sources.

6 Theoretical aspects: the continuous case

The theory of boundary integral formulations and boundary element methods is based both on the well–known elliptic theory and in the Fredholm theory, which is in a way the branch of functional analysis that studies the effect of compact perturbations to operator equations. Let us first expose the main results concerning this theory at the continuous level. For the next section we leave the effect of compact perturbations at the discrete level.

Let H_1 and H_2 be Hilbert spaces. A linear operator $K : H_1 \to H_2$ is **compact** if any of the three following equivalent conditions hold:

(a) K transforms weakly convergent sequences into strongly convergent sequences.

(b) If (ψ_n) is a bounded sequence in H_1, then the image sequence $(K\psi_n)$ has a convergent subsequence.

(c) There exist two orthonormal sequences, (ψ_n) in H_1 and (φ_n) in H_2, and a sequence of positive numbers $\sigma_n \to 0$ such that

$$K = \sum_n \sigma_n(\,\cdot\,, \psi_n)\,\varphi_n,$$

where the bracket denotes the inner product in H_1 and convergence of the series holds in operator norm.

In the last characterization, the sum can be limited to a finite number of terms, in which case the operator is called **degenerate** or **of finite rank**.

Remark. That these three characterizations are equivalent is not obvious at all and requires some effort of applying well–known but strong results of Hilbert space theory. It is not very difficult to prove that (b) is equivalent to: *The image of any bounded set is relatively compact, that is, has a compact closure.* This formulation allows for extensions of the definition to Banach or even normed spaces, and also to non–linear operators. Characterizations (a) and (c) are Hilbertian in essence. The series decomposition in (c) is called the Singular Value Decomposition of K and shows very clearly the ill–posed character of equations of the form $K\psi = \varphi$. □

From the point of view of what we are doing, the most important result of this theory is the following.

Theorem *Let H be a Hilbert space and $K : H \to H$ be compact. Then:*

$$I + K \text{ is injective} \qquad \Longleftrightarrow \qquad I + K \text{ is surjective.}$$

In this case, the inverse of $I + K$ is bounded.

Remark. The last part of the theorem is of general application for any bounded invertible operator between Hilbert spaces: its inverse is always bounded. This result holds in Banach spaces, where it is often called the **Banach isomorphism theorem**, and it is a consequence of a more general result called the **Banach open mapping theorem**. You can find this type of result in any book of basic functional analysis. □

Exercise. *Let H_1, H_2 and H_3 be Hilbert spaces. Prove the following results:*

*(a) If $A : H_1 \to H_2$ is bounded and $K : H_2 \to H_3$ is compact, then $K\,A : H_1 \to H_3$ is compact. (***Hint.*** Use characterization (b) of compactness). If $A : H_1 \to H_2$ is bounded and $K : H_3 \to H_1$ is compact, then $A\,K : H_3 \to H_2$ is compact.*

(b) If $A : H_1 \to H_2$ is bounded and inversible and $K : H_1 \to H_2$ is compact, then

$$A + K \text{ is injective} \qquad \Longleftrightarrow \qquad A + K \text{ is surjective.}$$

Remark. The theorem we enounced above is the first part of a very important result in functional analysis with huge relevant applications to elliptic theory, even if it does not look like that at first sight. The theorem is called **the Fredholm alternative** and, in its simplest form, states the following. If $K : H \to H$ is compact then:

either $I + K$ is invertible with continuous inverse,

or $\ker(I + K)$ is finite dimensional and $\mathrm{im}(I + K)^\top$ has the same finite dimension.

In the second case, there exist $\psi_1, \ldots, \psi_N$ linearly independent (a basis of the orthogonal complement of $\mathrm{im}(I + K)^\perp$ such that the equation

$$\psi + K\psi = \varphi$$

is solvable if and only if φ is orthogonal to ψ_i for all i. □

The final definition of this theory is given also in a set of equivalent characterizations. Let again H_1 and H_2 be Hilbert spaces. A bounded linear operator $V : H_1 \to H_2$ is a **Fredholm operator** (short for a Fredholm operator of index zero) if any of the following equivalent conditions hold:

(a) $\dim(\ker V) = \dim(\mathrm{im}V)^\perp < \infty$.

(b) There exists $W : H_2 \to H_1$ bounded and invertible such that $W\,V - I$ is compact.

(c) There exists $W : H_1 \to H_2$ bounded and invertible such that $V - W$ is compact.

In the jargon used by people who use this theory one simply says that an operator is Fredholm, instead of saying that an operator is a Fredholm operator.

If V is Fredholm (of index zero), then

$$V \text{ is injective} \qquad \Longleftrightarrow \qquad V \text{ is surjective.}$$

Remark. In fact, there exist Fredholm operators of other indices (since we will just be dealing with index zero, we are going to ignore this). Fredholm operators are those for which $\dim(\ker V)$ and $\dim(\mathrm{im}V)^\perp$ are finite. The difference between these numbers is called the index. Instead of using the quantity $\dim(\mathrm{im}V)^\perp$, it is common to use the co–dimension of $\mathrm{im}V$, which is the dimension of any supplementary subspace to $\mathrm{im}V$. □

Finally, let us mention how all this applies to our theory. Consider the operator $V_0 : H^{-1/2}(\Gamma) \to H^{1/2}(\Gamma)$ defined by

$$(V_0\psi)(\mathbf{x}) := \int_\Gamma \frac{1}{4\,\pi\,|\mathbf{x} - \mathbf{y}|}\psi(\mathbf{y})\mathrm{d}\gamma(\mathbf{y}).$$

This operator corresponds formally to that case $k = 0$, which gives the Laplace equation. I say formally, because the case $k = 0$ is a singular case in all this theory and does not follow easily as a limit of the remaining cases. The two important facts about this operator are:

- V_0 is elliptic, that is, there exists $\alpha > 0$ such that

$$\langle V_0\,\psi, \psi\rangle_\Gamma \geq \alpha \|\psi\|_{-1/2,\Gamma}, \qquad \forall \psi \in H^{-1/2}(\Gamma).$$

- $V_\Gamma - V_0$ is compact.

Hence, V_Γ is Fredholm of index zero and we have that

$$V_\Gamma \text{ is injective} \qquad \Longleftrightarrow \qquad V_\Gamma \text{ is surjective.}$$

Moreover, we can write $V_\Gamma = V_0 + (V_\Gamma - V_0)$ and therefore we have a decomposition

$$V_\Gamma = V_0 + K,$$

where V_0 is elliptic and K is compact. This will be relevant in the numerical approximation.

We now can collect the pieces so far:

- We had begun with the exterior scattering problem

$$\begin{aligned} \Delta u + k^2 u = 0, &\qquad \text{in } \Omega^+, \\ \partial_r u - \imath\, k\, u = o(r^{-1}), &\qquad r \to \infty \\ u|_\Gamma = g. & \end{aligned}$$

  A priori $g = -u_{\text{inc}}$ on Γ, but we had widened our interest to arbitrary data in the trace space: $g \in H^{1/2}(\Gamma)$. The problem with $g = 0$ only admitted the trivial solution, so we have **uniqueness**.

- Our proposal to solution was a single–layer acoustic potential

$$u := \mathcal{S}_\Gamma \psi = \int_\Gamma \frac{e^{\imath\, k\, |\,\cdot\, - \mathbf{y}|}}{4\,\pi\,|\,\cdot\, - \mathbf{y}|} \psi(\mathbf{y}) \mathrm{d}\gamma(\mathbf{y}).$$

  This expression gives also a definition of solution inside the obstacle. (By the way, if you really can sound as if you know your business with boundary integral formulations, you don't give a proposal of solution; you give an **ansatz**, which is German for proposal).

- We have proved that $u = \mathcal{S}_\Gamma \psi$ solves the scattering problem if and only if $V_\Gamma \psi = g$, that is

$$\int_\Gamma \frac{e^{\imath\, k\, |\mathbf{x} - \mathbf{y}|}}{4\,\pi\,|\mathbf{x} - \mathbf{y}|} \psi(\mathbf{y}) \mathrm{d}\gamma(\mathbf{y}) = g(\mathbf{x}), \qquad \mathbf{x} \in \Gamma.$$

  (The equation has to be understood with the integral operator in a weak sense, $\psi \in H^{-1/2}(\Gamma)$ and holding almost everywhere in Γ).

- The operator V_Γ is injective if and only if $-k^2$ is not a Dirichlet eigenvalue of the Laplace operator in the interior domain. Injectivity was a consequence of uniqueness of the exterior (always) and interior (with the exception of eigenvalues!) boundary value problems.

- Hence, except in the singular cases, V_Γ is invertible. Therefore we can give a solution (the unique solution) of the exterior scattering problem.

The preceding argument furnishes a proof of **existence of solution** of the exterior scattering problem except for some values that correspond to interior Dirichlet eigenvalues. The usual proof for existence uses this kind of argumentation, only with a more complicated potential (ansatz) that does not fail to be invertible for some wave numbers.

Before going any further, let us examine what happens with more than one obstacle. Two will be enough. Assume that the obstacle is not a single domain, but the union of two disjoint domains Ω_1 and Ω_2 with boundaries Γ_1 and Γ_2. All the integrals over Γ can be decomposed

$$\int_\Gamma = \int_{\Gamma_1} + \int_{\Gamma_2}.$$

Let $g_i := g|_{\Gamma_i} \in H^{1/2}(\Gamma_i)$. Consider the following operators

$$V_{ij}\psi := \int_{\Gamma_i} \phi(\,\cdot\,,\mathbf{y})\psi(\mathbf{y})\mathrm{d}\gamma(\mathbf{y}) \,:\, \Gamma_j \to \mathbb{C}, \qquad i,j = 1,2.$$

The notation is taken so that V_{ij} goes from Γ_i to Γ_j. The density of the potential is generated in Γ_i and observed in Γ_j. This is is very similar to what we had in numerical approximation, but here Γ_1 and Γ_2 are closed disjoint surfaces.

Exercise. *In the notations above, answer these questions:*

(a) When are V_{ii} inversible?

(b) Using that the inclusion of $H^1(\Gamma_i)$ into $H^{1/2}(\Gamma_i)$ is compact, prove that V_{12} and V_{21} are compact.

(c) If $\psi_i \in H^{-1/2}(\Gamma_i)$, prove that

$$u = \mathcal{S}_{\Gamma_1}\psi_1 + \mathcal{S}_{\Gamma_2}\psi_2$$

solves the sound–soft scattering problem exterior to $\Omega_1 \cup \Omega_2$ is and only if

$$\begin{bmatrix} V_{11} & V_{12} \\ V_{21} & V_{22} \end{bmatrix} \begin{bmatrix} \psi_1 \\ \psi_2 \end{bmatrix} = \begin{bmatrix} g_1 \\ g_2 \end{bmatrix}.$$

(d) Prove that

$$\begin{bmatrix} V_{11} & V_{12} \\ V_{21} & V_{22} \end{bmatrix}$$

is Fredholm as an operator $H^{-1/2}(\Gamma_1) \times H^{-1/2}(\Gamma_2) \to H^{1/2}(\Gamma_1) \times H^{1/2}(\Gamma_2)$.

(e) Prove that if V_{11} and V_{22} are invertible, then the whole matrix of operators is invertible.

This looks new but follows directly from the theory by admitting Γ not to be a single surface but a set of boundaries of non–intersecting domains (one surface enclosed by another gives a very different problem though!). The point is that Dirichlet eigenvalues in $\Omega_1 \cup \Omega_2$ are those of Ω_1 and those of Ω_2, since the problems are completely decoupled.

One can arrange (theoretically) the system of boundary integral equations

$$\begin{bmatrix} V_{11} & V_{12} \\ V_{21} & V_{22} \end{bmatrix} \begin{bmatrix} \psi_1 \\ \psi_2 \end{bmatrix} = \begin{bmatrix} g_1 \\ g_2 \end{bmatrix}$$

by 'multiplying' each row by V_{ii}^{-1}, obtaining thus,

$$\begin{aligned} \psi_1 + V_{11}^{-1} V_{12} \psi_2 &= V_{11}^{-1} g_1, \\ V_{22}^{-1} V_{21} \psi_1 + \psi_2 &= V_{22}^{-1} g_2. \end{aligned}$$

Iterations to this formal system (that is, Jacobi iterations to the first system) involve solving scattering problems exterior to each domain, not to the group of both obstacles. This is the origin of a technique often used by physicists and called multiple scattering. Each object reacts to the scattering produced by others. You can always think in the following terms: densities emit a time–harmonic wave from each Γ_i; the operators V_{ij} with $i \neq j$ correspond to emissions from Γ_i heard in Γ_j; the operators V_{ii}^{-1} are the reactions of each obstacle to emissions (something is received in Γ_i and the boundary emits something just to compensate). Iterations happen till an asymptotic equilibrium is reached. Even if you are not going to use this kind of iterations, acquiring this language will help you to make yourself better understood.

7 Theoretical aspects: the discrete case

The Galerkin method we exposed two sections ago fits into a very general framework of Galerkin methods for operator equations. Consider an invertible operator $A : H \to H'$, where H is a Hilbert space and H' is its dual. We want to study the numerical approximation for the operator equation

$$A\psi = g.$$

Let H_h be a sequence of finite dimensional subspaces of H, directed in the parameter h, that tends to zero.

Remark. The parameter h can be a geometrical parameter (as it happens often in finite element analysis) or not. With it we simply want to describe that there are several subspaces and that, in general, they become richer as $h \to 0$. From now on we will use a common convention when writing numerical mathematics: $C > 0$, with possible subscripts, will be a constant independent of h and of any other quantity it is multiplied by. The constant can be different in different occurrences, unless we state the opposite. □

The Galerkin approximation is the solution (if it exists and if it is unique) to the discrete problem:

$$\psi_h \in H_h, \qquad \langle A\psi_h, \varphi_h \rangle = \langle g, \varphi_h \rangle, \quad \forall \varphi_h \in H_h.$$

Before going on, let us point out some simple facts:

(a) If $\xi_1, \ldots, \xi_N$ is a basis of H_h, the discrete problem is equivalent to the linear system

$$\sum_{j=1}^{N} \langle A\xi_j, \xi_i \rangle \, \psi_j = \langle g, \xi_i \rangle, \qquad i = 1, \ldots, N$$

where $(\psi_1, \ldots, \psi_N)$ is the vector of coefficients of $\psi_h \in H_h$ in that basis:

$$\psi_h = \sum_{j=1}^{N} \psi_j \, \xi_j.$$

(b) Therefore existence–and–uniqueness (both together) do not depend on the right–hand side. They only depend on the invertibility of the matrix

$$\langle A\xi_j, \xi_i \rangle, \qquad i, j = 1, \ldots, N.$$

(c) If the operator A is self–adjoint

$$\langle A\psi, \varphi \rangle = \langle A\varphi, \psi \rangle^*, \qquad \forall \psi, \varphi \in H,$$

then the corresponding matrix at the discrete level is hermitian. If the operator is symmetric

$$\langle A\psi, \varphi \rangle = \langle A\varphi, \psi \rangle, \qquad \forall \psi, \varphi \in H,$$

the matrix is symmetric.

(d) The method is based on reduction to finite dimension of the operator equation $A\psi = g$ written in variational form

$$\psi \in H, \qquad \langle A\psi, \varphi \rangle = \langle g, \varphi \rangle, \quad \forall \varphi \in H.$$

As we had already mentioned in the particular case of the single–layer equation, there is no additional effort in obtaining this formulation. It simply states that since $A\psi$ and g are the same element of the dual space H', they coincide when acting for arbitrary $\varphi \in H$.

Exercise. *Assume that for a particular h, the exact solution belongs to H_h. Prove that $\psi_h = \psi$ for that value of h.*

Assume that the system is invertible at least **for h small enough**. The method is said to be **stable** if there exists C_1 such that

$$\|\psi_h\| \leq C_1 \|g\|.$$

(Notice that the norm for ψ_h is that of H, but the norm for g is that of H'). Since A is bounded, then stability can be written as a bound of the discrete solutions in terms of the continuous solution

$$\|\psi_h\| \leq C_2 \|\psi\|,$$

by simply taking $C_2 = C_1 \|A\|$. Stability implies the existence of $C_3 > 0$ such that

$$\|\psi - \psi_h\| \leq C_3 \inf_{\varphi_h \in H_h} \|\psi - \varphi_h\|.$$

Let us prove this. Take a particular $\widetilde{\varphi}_h \in H_h$ and let $f := A(\psi - \widetilde{\varphi}_h)$. Then, the exact solution to the equation

$$A\rho = f$$

is $\rho = \psi - \widetilde{\varphi}_h$ and the Galerkin solution

$$\rho_h \in H_h, \qquad \langle A\rho_h, \varphi_h \rangle = \langle f, \varphi_h \rangle, \quad \forall \varphi_h \in H_h$$

is $\psi_h - \widetilde{\varphi}_h$. Then

$$\|\psi - \psi_h\| \leq \|\psi - \widetilde{\varphi}_h\| + \|\psi_h - \widetilde{\varphi}_h\| \leq (1 + C_2)\|\psi - \widetilde{\varphi}_h\|,$$

and therefore

$$\|\psi - \psi_h\| \leq (1 + C_2)\|\psi - \varphi_h\|, \qquad \forall \varphi_h \in H_h.$$

Since H_h is finite dimensional, it can be proved that in the bound

$$\|\psi - \psi_h\| \leq C_3 \inf_{\varphi_h \in H_h} \|\psi - \varphi_h\|$$

the infimum is a minimum. Anyway, the conventional wisdom is writing an infimum, and we are not going to challenge common uses. In the world of Galerkin approximation to elliptic boundary value problems, this bound is known as **Céa's lemma**. As we will see later on, for elliptic equations stability is for free (all Galerkin methods satisfy it). In the non–elliptic world, the bound is known as a **Céa estimate**. The interesting fact is that this bound implies stability, which follows the following very simple argument

$$\|\psi_h\| \leq \|\psi\| + \|\psi - \psi_h\| \leq \|\psi\| + C_3 \inf_{\varphi_h \in H_h} \|\psi - \varphi_h\| \overset{\varphi_h = 0}{\leq} (1 + C_3)\|\psi\|.$$

A subtler argument shows that in the inequalities

$$\|\psi_h\| \leq C_2 \|\psi\|$$

and

$$\|\psi - \psi_h\| \leq C_3 \inf_{\varphi_h \in H_h} \|\psi - \varphi_h\|$$

one can always have $C_2 = C_3$. The Céa estimate moves the problem of studying the Galerkin error to one purely of approximation theory, namely to prove that

$$\inf_{\varphi_h \in H_h} \|\psi - \varphi_h\| \qquad \overset{h \to 0}{\longrightarrow} \quad 0.$$

If this holds for arbitrary $\psi \in H$, then we know that

$$\|\psi - \psi_h\| \quad \overset{h \to 0}{\longrightarrow} \quad 0$$

for all possible right–hand sides in the equation. This property is called **convergence** of the method.

Since

$$\inf_{\varphi_h \in H_h} \|\psi - \varphi_h\| \leq \|\psi - \psi_h\|,$$

convergence implies the **approximation property**

$$\|\psi - \psi_h\| \quad \stackrel{h\to 0}{\longrightarrow} \quad 0, \qquad\qquad \forall \psi \in H.$$

By using a well–known but non–trivial theorem of functional analysis (the principle of uniform boundedness or the Banach–Steinhaus theorem), it is possible to prove that convergence implies stability. Therefore, we have

Convergence = Stability + Approximation property.

Remark. It is also possible to prove that stability is equivalent to the following condition on the discrete bilinear form: there exists $C > 0$

$$\sup_{0 \neq \varphi_h \in H_h} \frac{|\langle A\psi_h, \varphi_h \rangle|}{\|\varphi_h\|} \geq C \, \|\psi_h\|, \qquad \forall \psi_h \in H_h.$$

This condition is usually called a **discrete inf–sup condition** or **Babuška–Brezzi** condition. In relation to the first stability inequality

$$\|\psi_h\| \leq C_1 \|g\|$$

it is simple to prove that $C_1 = 1/C$. An advantage of using the discrete inf–sup condition is that it implies invertibility of the system of linear equations and therefore the definition of the discrete solution. □

Remark. The underlying idea of this kind of analysis of Galerkin methods by showing stability and the approximation property is by no means necessary to prove that this kind of numerical methods work properly. Notice that if we want to show convergence for arbitrary right–hand sides (arbitrary solutions), the paradigm

Convergence = Stability + Approximation property

is the correct one. Stability plus knowing that

$$\|\psi - \psi_h\| \quad \stackrel{h\to 0}{\longrightarrow} \quad 0,$$

for our unknown solution is enough to prove convergence for our sequence of solutions. It could happen that the sequence of discrete spaces is correct from the point of view of stability and to approximate some solutions, but not all.

There's more, however. Convergence for some solutions can be attained without the requirement of stability. This is the key to many numerical methods based on adaptivity, where the sequence of subspaces is chosen progressively depending on the behaviour of the discrete solutions obtained. The sequence of spaces depends then on the particular right–hand side, is

constructed to satisfy the approximation property for the concrete solution but can fail to satisfy the inf–sup condition (stability). The nice paradigm is thus broken into pieces. Things are however not moving fast enough to justify forgetting all the good old theories to have something newer and better, so stability is here to stay, at least for a while. □

Remark. There are many other possible generalizations of operator equations that fit in a framework suitable for Galerkin approximations. For instance one can work with $A : H \to H$ and test the equation either with H itself (via the inner product). The Riesz–Fréchet representation theorem says that it doesn't matter which of them you use. However, the way the operator equation is written down allows to use a Galerkin method or not. The Galerkin methods form a family in the wider class of Petrov–Galerkin or projection methods. Sometimes a clever rewriting of the discrete and continuous equations allow to understand a discretization scheme as a projection method, even if it is not self–evident. □

If the operator A is elliptic

$$\mathrm{Re}\langle A\psi, \psi\rangle \geq \alpha\|\psi\|^2, \qquad \forall \psi \in H,$$

stability of Galerkin schemes follows readily: it is no longer a hypothesis. First, since ellipticity is inherited by the discrete spaces

$$\mathrm{Re}\langle A\psi_h, \psi_h\rangle \geq \alpha\|\psi_h\|^2, \qquad \forall \psi_h \in H_h,$$

(the constant is the same), then the solution to the Galerkin equations

$$\psi_h \in H_h, \qquad \langle A\psi_h, \varphi_h\rangle = \langle g, \varphi_h\rangle, \quad \forall \varphi_h \in H_h$$

is unique (this is very simple to prove). Also

$$\alpha\|\psi_h\|^2 \leq \mathrm{Re}\langle A\psi_h, \psi_h\rangle \leq |\langle A\psi_h, \psi_h\rangle| = |\langle g, \psi_h\rangle| \leq \|g\|\,\|\psi_h\|,$$

so we obtain

$$\|\psi_h\| \leq (1/\alpha)\|g\|$$

and consequently

$$\|\psi_h\| \leq (\|A\|/\alpha)\|\psi\|$$

and the Céa estimate

$$\|\psi - \psi_h\| \leq (\|A\|/\alpha) \inf_{\varphi_h \in H_h} \|\psi - \varphi_h\|.$$

Convergence then follows from the approximation property.

The following key result relates convergence (not stability!) of Galerkin approximations with the Fredholm theory.

Theorem *Assume that the Galerkin method based on the sequence of spaces $\{H_h\}$ is convergent for the operator A. If K is compact and $A + K$ is invertible (it is enough that $A + K$ is injective), then the method is convergent for $A + K$. Moreover, the stability constant is proportional to that of the method applied to A multiplied by $\|(A + K)^{-1}\|$.*

The theorem can be looked at with positive eyes and asserts that your method is going to work well if it works well adding or taking compact terms. For instance, a Galerkin method for an operator $A+K$, where A is elliptic, is going to be stable if the approximation property holds. Nevertheless, the stability constant can be quite bad if $\|(A+K)^{-1}\|$ is large and the asymptotic regime (the hs small enough where all the inequalities hold) can be beginning somewhat late. This is a drawback of a certain relevance in some (but by no means all) applications to scattering problems. More on this in the following section.

8 Discretization revisited

In this section we are going to apply the theory above to our case and to examine with more detail some aspects related to implementation of the Galerkin and collocation methods.

Let us return to the equation

$$\psi \in H^{-1/2}(\Gamma), \qquad V_\Gamma \psi = g$$

and its Galerkin discretization

$$\psi_h \in X_h, \qquad \langle V_\Gamma \psi_h, \varphi_h \rangle = \langle g, \psi_h \rangle, \quad \forall \varphi_h \in X_h$$

by means of the space

$$X_h := \{\psi_h : \Gamma \to \mathbb{C} \,|\, \psi_h|_{\Gamma_j} \in \mathbb{P}_0, \quad \forall j\}.$$

We know that

$$V_\Gamma = \text{elliptic} + \text{compact}$$

and that V_Γ is invertible if $-k^2$ is not an interior Dirichlet eigenvalue. In this case, for h small enough, the corresponding matrix is invertible, we have a stability bound

$$\|\psi_h\|_{-1/2,\Gamma} \leq C \, \|\psi\|_{-1/2,\Gamma}$$

and the Céa estimate

$$\|\psi - \psi_h\|_{-1/2,\Gamma} \leq C \inf_{\varphi_h \in X_h} \|\psi - \varphi_h\|_{-1/2,\Gamma}.$$

Remark. The constant C deserves some additional attention. It is a stability constant that depends on the ellipticity constant for V_0 and on the norm of the inverse of V_Γ. The first of these constants depends only on the boundary Γ, but the second depends on the wave number. The constant will blow–up if we approach one of the Dirichlet eigenvalues. Also, when the asymptotic regime (the h small enough so that all inequalities hold) begins depends on the wave number, both on its size and on the proximity to a bad eigenvalue.

The problem with the proximity to a Dirichlet eigenvalue can be solved using a better integral equation. I emphasize that we are still on a first step in an introductory course. It takes time to see all the difficulties and more time to solve them.

There is another question on the ability of the space X_h to approximate the exact solution. For high wave numbers, the solution can be highly oscillating, and the triangulation has to be

very fine to cope will all the oscillations of the exact solution. Keep in mind that high frequencies require specific techniques! □

If

$$h := \max\{h_j \,|\, j = 1, \ldots, N\}, \qquad h_j := \operatorname{diam}(\Gamma_j)$$

converges to zero and we assume a maximum flattening hypothesis on the triangulation, then

$$\inf_{\varphi_h \in X_h} \|\psi - \varphi_h\|_{-1/2,\Gamma} \quad \stackrel{h\to 0}{\longrightarrow} 0,$$

no matter how singular ψ is. To see that, first approximate ψ by an element in $L^2(\Gamma)$ (which is dense in $H^{-1/2}(\Gamma)$) and then make the $L^2(\Gamma)-$orthogonal projection of this function. Both terms can be made as small as desired.

If $\psi \in H^1(\Gamma)$, with some additional analytic effort, we can prove that

$$\inf_{\varphi_h \in X_h} \|\psi - \varphi_h\|_{-1/2,\Gamma} \leq Ch^{3/2}\|\psi\|_{1,\Gamma}.$$

Notice that we have the norm of ψ in the right–hand side and not the typical seminorm you find in finite element analysis. This is not really important and sometimes the bounds for approximation on surfaces can be worked out a little bit to make them resemble more like finite element estimates. But one has to acknowledge that curvature of the surface is always a bore and lower order derivatives are due to appear most of the time in precise bounds. This approximation estimate (which has nothing to do with the boundary integral equation; it is simply 'interpolation' theory) together with the Céa estimate, give order to the method

$$\|\psi - \psi_h\|_{-1/2,\Gamma} \leq Ch^{3/2}\|\psi\|_{1,\Gamma}$$

under the hypothesis of sufficient regularity of the solution.

The order estimate for approximation is not really easy to prove. We are going to simply sketch how one can prove this kind of results in this very simple situation. The first try is classical: we bound in $H^0(\Gamma) = L^2(\Gamma)$ for $\psi \in H^1(\Gamma)$

$$\inf_{\varphi_h \in X_h} \|\psi - \varphi_h\|_{0,\Gamma} \leq Ch\|\psi\|_{1,\Gamma}.$$

This is easy to do by means of the $L^2(\Gamma)-$orthogonal projection and classical analysis. Then one tries this other one

$$\inf_{\varphi_h \in X_h} \|\psi - \varphi_h\|_{-1,\Gamma} \leq Ch^2\|\psi\|_{1,\Gamma}.$$

This one looks somewhat more difficult to prove since the $H^{-1}(\Gamma)-$norm is usually defined by duality, so we have to find a way of obtaining $\varphi_h \in X_h$ such that

$$\sup_{0\neq\rho\in H^1(\Gamma)} \frac{|\langle \psi - \varphi_h, \rho\rangle|}{\|\rho\|_{1,\Gamma}} \leq Ch^2\|\psi\|_{1,\Gamma}.$$

Nevertheless, the point here is simply to take again φ_h as the best $L^2(\Gamma)$ approximation and $\rho_h \in X_h$ as the one of an arbitrary $\rho \in H^1(\Gamma)$, and bound as follows:

$$\begin{aligned} |\langle \psi - \varphi_h, \rho\rangle_\Gamma| &= |\langle \psi - \varphi_h, \rho - \rho_h\rangle_\Gamma| \\ &\leq \|\psi - \varphi_h\|_{0,\Gamma}\, \|\rho - \rho_h\|_{0,\Gamma} \\ &\leq Ch^2\|\psi\|_{1,\Gamma}\, \|\rho\|_{1,\Gamma}. \end{aligned}$$

A key point here is that we could find a way of approximating ψ simultaneously in $H^0(\Gamma)$ and $H^{-1}(\Gamma)$, that is, the same approximation serves for both bounds. Then we apply this inequality

$$\|\psi - \varphi_h\|_{-1/2,\Gamma} \leq \|\psi - \varphi_h\|_{0,\Gamma}^{1/2} \|\psi - \varphi_h\|_{-1,\Gamma}^{1/2} \leq C h^{3/2} \|\psi\|_{1,\Gamma},$$

to obtain the desired bound.

Remark. The general bound

$$\|g\|_{-1/2,\Gamma} \leq \|g\|_{0,\Gamma}^{1/2} \|g\|_{-1,\Gamma}^{1/2}, \qquad \forall g \in H^0(\Gamma)$$

belongs to a very wide class of inequalities by Sobolev norms on the boundary. These are a consequence of the structure of the family of spaces $H^r(\Gamma)$ (for $-1 \leq r \leq 1$ or in wider intervals if the surface is smooth enough). This kind of inequalities are often referred to as **interpolation inequalities**, which has no relation at all with interpolation in the numerical sense, but on the very deep fact that all inner spaces are interpolated from the extremes. □

To avoid the repeated occurrence of the constant C, which may be different in each case, we will adopt the following convention. We write that

$$a \lesssim b$$

when there exists $C > 0$ (as usual independent on h and on particular data of the problem) such that

$$a \leq C\, b.$$

Exercise. *Prove that if the solution to $V_\Gamma \psi = g$ belongs to $H^0(\Gamma)$ we can bound*

$$\|\psi - \psi_h\|_{-1/2,\Gamma} \lesssim h^{1/2} \|\psi\|_{0,\Gamma}.$$

It is also possible to obtain error bounds of the numerical solution in **stronger norms**. For instance, it is possible to prove a bound

$$\|\psi - \psi_h\|_{0,\Gamma} \lesssim h \|\psi\|_{1,\Gamma}.$$

Nevertheless, this bound needs from more stringent conditions on the triangulation. If all the elements are triangles and the size of the largest triangle is asymptotically controlled by that of the smallest one

$$\max\{h_j\} \lesssim \min\{h_j\}$$

then the space X_h satisfies an inverse inequality

$$\|\varphi_h\|_{0,\Gamma} \lesssim h^{-1/2} \|\varphi_h\|_{-1/2,\Gamma}, \qquad \forall \varphi_h \in X_h,$$

which gives a bound on the equivalence constant for the $H^0(\Gamma)-$ and $H^{-1/2}(\Gamma)-$norms restricted to the discrete finite–dimensional space X_h (where all norms are equivalent!).

The fact that the size of the smallest triangle controls that of the largest one is called **quasi–uniformity**.

Then, take ψ to be the exact solution, ψ_h the numerical solution and φ_h the $H^0(\Gamma)-$orthogonal projection of ψ on X_h, and follow the chain of inequalities

$$\begin{aligned}
\|\psi-\psi_h\|_{0,\Gamma} &\leq \|\psi-\varphi_h\|_{0,\Gamma}+\|\varphi_h-\psi_h\|_{0,\Gamma}\\
&\lesssim \|\psi-\varphi_h\|_{0,\Gamma}+h^{-1/2}\|\varphi_h-\psi_h\|_{-1/2,\Gamma}\\
&\lesssim \|\psi-\varphi_h\|_{0,\Gamma}+h^{-1/2}\Big(\|\psi-\psi_h\|_{-1/2,\Gamma}+\|\psi-\varphi_h\|_{-1/2,\Gamma}\Big)\\
&\lesssim h\|\psi\|_{1,\Gamma}
\end{aligned}$$

that prove the desired convergence property. Notice that we have used the inverse inequality (which follows from quasi–uniformity, but could hold in more general cases) and again the simultaneous optimal approximation properties of the $H^0(\Gamma)-$orthogonal projection in two different norms.

Similar but more sophisticated arguments can be used to prove convergence in stronger Sobolev norms, although the lack of regularity of the discrete space X_h imposes that we cannot arrive to measure errors in $H^{1/2}(\Gamma)$, since this space does not contain piecewise smooth discontinuous functions.

Another line of analysis goes to prove convergence in even **weaker norms**. To the finite element oriented person, this can seem quite awkward, given the fact that $H^{-1/2}(\Gamma)$, the natural space in our analysis, is already a very weak space, endowed with a dual norm. We'll see in a while why weak norms are interesting. First, the bound. With some regularity requirements on the boundary, it is possible to prove that

$$\|\psi-\psi_h\|_{-2,\Gamma}\lesssim h^{3/2}\|\psi-\psi_h\|_{-1/2,\Gamma},$$

so in the optimal case of $\psi\in H^1(\Gamma)$,

$$\|\psi-\psi_h\|_{-2,\Gamma}\lesssim h^{3}\|\psi\|_{1,\Gamma},$$

which means that we have been able to double the order of convergence by looking at a much weaker norm. This result is a consequence of the so–called **Aubin–Nitsche** technique, which follows a very similar path as the one we use when we want to prove $L^2(\Omega)-$convergence of finite elements for elliptic problems of the second order.

But, why can this inequality be interesting for us? Assume that the boundary is smooth enough to avoid unnecessary complications. Fix a point $\mathbf{x}\in\Omega^+$. Then the function

$$\phi(\mathbf{x},\,\cdot\,):\Gamma\to\mathbb{C}$$

is very smooth (the singularity doesn't happen, since $\mathbf{x}$ is outside and the function moves on the boundary), so $\phi(\mathbf{x},\,\cdot\,)\in\mathcal{C}^2(\Gamma)\subset H^2(\Gamma)$. Hence

$$|(\mathcal{S}_\Gamma\psi)(\mathbf{x})-(\mathcal{S}_\Gamma\psi_h)(\mathbf{x})|=|\langle\phi(\mathbf{x},\,\cdot\,),\psi-\psi_h\rangle_\Gamma|\leq\|\phi(\mathbf{x},\,\cdot\,)\|_{2,\Gamma}\|\psi-\psi_h\|_{-2,\Gamma}$$

since the duality product $\langle\,\cdot\,,\,\cdot\,\rangle_\Gamma$ represents also the duality of $H^2(\Gamma)$ and $H^{-2}(\Gamma)$. Therefore if

$$u:=\mathcal{S}_\Gamma\psi,\qquad u_h:=\mathcal{S}_\Gamma\psi_h$$

(these are the quantities of interest for the problem; ψ is an artificial unknown), then

$$|u(\mathbf{x}) - u_h(\mathbf{x})| \lesssim h^3 \|\psi\|_{1,\Gamma} \, \|\phi(\mathbf{x}, \cdot)\|_{2,\Gamma}$$

The right–most constant can be uniformly bounded on compact sets not intersecting the boundary, which gives a very high order of convergence for the computed potentials, as long as we don't approach the boundary, since then the constant $\|\phi(\mathbf{x}, \cdot)\|_{2,\Gamma}$ blows–up.

For bounds near the boundary, we only can use the natural norm in $H^{-1/2}(\Gamma)$ for the density to obtain local H^1- bounds in the exterior of order at most $h^{3/2}$.

Remark. In boundary element computations you always have to keep in mind what you want to compute (in fact, you should be doing this all the time you compute something) and no what you are computing. For us the density is not a quantity of particular interest. In a forthcoming section we will see that in some boundary integral formulations the unknown has an interest of its own. Right now, our interest is limited to the scattering amplitude u and its approximation. If you are not interested in what happens very near the boundary, the optimal convergence order h^3 looks extremely promising for the method. This kind of weak norm estimates is very particular of Galerkin methods. For collocation, right now there is not a very satisfactory error analysis in any norm, and the duality argument to move to weaker norms does not apply so easily (actually the method does not exhibit numerically such good properties when we look at potentials). This makes the additional effort of the Galerkin method look more desirable, although the gain needs regularity in the boundary, so it isn't universal for all kind of scatterers. □

If we now turn our attention to the matrix terms of the Galerkin method

$$\int_{\Gamma_i} \int_{\Gamma_j} \phi(\mathbf{x}, \mathbf{y}) \mathrm{d}\gamma(\mathbf{x}) \, \mathrm{d}\gamma(\mathbf{y})$$

there are some details that deserve to be commented:

- The diagonal terms have a singularity all along the line $\mathbf{x} = \mathbf{y}$. If one applies numerical integration, one has to be very careful to avoid using the same rule in Γ_i for the inner and outer integrals, since we cannot evaluate $\phi(\mathbf{x}, \mathbf{x})$. Also, the integrand is not smooth and one cannot expect a very good behaviour of simple quadrature rules. Usually some transformations of variables are performed to improve the aspect of the integrand. It is also possible to do some kind of singularity extraction and perform part of the work analytically.

- When two elements share a side, the singularity is reduced to both arguments $\mathbf{x}$ and $\mathbf{y}$ belonging to that side. When elements share a vertex, the singularity is limited to a single point of the four–dimensional domain $\Gamma_i \times \Gamma_j$. Again, numerical quadrature cannot ignore these singularities.

- In other cases, the integrand is very smooth, but can be close to a singularity if the elements Γ_i and Γ_j are near each other.

- In any case, there is a necessary balance between having a qualified numerical integration procedure and not wasting a lot of computational effort in computing almost exactly some integrals, when we are approximating an integral equation with a low order method.

Exercise. *Let us now try another method. We also consider the partition in elements $\Gamma_1, \ldots, \Gamma_N$ and a choice of points $\mathbf{x}_j \in \Gamma_j$ (for instance barycenters if the elements are triangles). One can devise a method by approximating the integral by a quadrature rule where the densities act as weights:*

$$\int_\Gamma \phi(\,\cdot\,, \mathbf{x})\psi(\mathbf{x})\mathrm{d}\gamma(\mathbf{x}) \approx \sum_{j=1}^{N} \phi(\,\cdot\,, \mathbf{x}_j)\,\psi_j.$$

The quantities ψ_j approximate the value of ψ, taking into account the size of the element, which would give the correct weight if ψ was known (which is not the case). Then, we compare the data function g with this discrete potential generated by N sources by matching Galerkin–wise their averages over the elements Γ_i:

$$\sum_{j=1}^{N} \left(\int_{\Gamma_i} \phi(\mathbf{y}, \mathbf{x}_j)\mathrm{d}\gamma(\mathbf{y}) \right) \psi_j = \int_{\Gamma_i} g(\mathbf{y})\mathrm{d}\gamma(\mathbf{y}), \qquad i = 1, \ldots, N.$$

This is called a **delta** *or point–source method.*

(a) Compare the matrix and the right–hand side of this method with those of the collocation method.

(b) In comparison with collocation, can you decide whether this method needs more, less or the same regularity on the right–hand side to be applied with property?

(c) Compare the potentials obtained by the Galerkin, collocation and delta method. Which is simpler?

As we explained in Section 5, assume that our surface Γ is given by a series of patches from a polyhedron $\widehat{\Gamma}$ and that we have collected the transformations from each face of the polyhedron to the corresponding curved patch in a single map

$$\boldsymbol{\eta} : \widehat{\Gamma} \to \Gamma.$$

With some degree of notational freedom we can consider integrals over $\widehat{\Gamma}$ as integrals with respect to the two–dimensional Lebesgue measure, so we will write

$$\int_{\widehat{\Gamma}} f(\boldsymbol{\xi})\mathrm{d}\boldsymbol{\xi}$$

in the understanding that we are parameterizing each face of $\widehat{\Gamma}$ by simply moving (rotating and translating) it to the plane $\mathbb{R}^2$. The area element in Γ can be defined from $\boldsymbol{\eta}$ and thus

$$\int_\Gamma f(\mathbf{x})\mathrm{d}\gamma(\mathbf{x}) = \int_{\widehat{\Gamma}} f(\boldsymbol{\eta}(\boldsymbol{\xi}))\,\sigma(\boldsymbol{\xi})\,\mathrm{d}\boldsymbol{\xi}, \qquad \sigma := |\boldsymbol{\eta}_{\xi_1} \wedge \boldsymbol{\eta}_{\xi_2}|$$

where the same convention as to what we understand by $\boldsymbol{\xi}$.

Then, the elements in Γ, which we have called $\{\Gamma_1, \ldots, \Gamma_N\}$ are the images through $\boldsymbol{\eta}$ of elements in $\widehat{\Gamma}$, $\{\widehat{\Gamma}_1, \ldots, \widehat{\Gamma}_N\}$.

Exercise. *Prove that the space we used in the Galerkin method can be written equivalently as*

$$X_h := \{\psi_h : \Gamma \to \mathbb{C} \,|\, (\psi_h \circ \boldsymbol{\eta})|_{\widehat{\Gamma}_j} \in \mathbb{P}_0, \quad \forall j\}.$$

Consider instead a new Galerkin method with the following discrete space

$$Y_h := \{\psi_h : \Gamma \to \mathbb{C} \,|\, \sigma\,(\psi_h \circ \boldsymbol{\eta})|_{\widehat{\Gamma}_j} \in \mathbb{P}_0, \quad \forall j\}.$$

Write down what is the formula for the elements of the coefficient matrix and right–hand side vector of this new method. Devise a collocation method in the same spirit.

Higher order methods can be constructed by mapping higher order polynomials on the flat elements $\widehat{\Gamma}_j$ to the curved boundary Γ. Since the method does not require continuity of the discrete space, one can go further employing discontinuous elements. However, the computational effort to increase order is much higher (the number of degrees of freedom increases very fast) and it is customary to employ continuous piecewise polynomials to reduce the number of degrees of freedom, while retaining the higher order approximation properties of the method.

9 A word on the two–dimensional case

Most of what we have done so far works also in two dimensions. Now, boundaries are curves, which are much simpler to handle that surfaces. The fundamental solution is

$$\phi(\mathbf{x}, \mathbf{y}) := \frac{\imath}{4}\, H_0^{(1)}(k\,|\mathbf{x} - \mathbf{y}|).$$

The function $H_0^{(1)}$ is defined in terms of Bessel functions as

$$H_0^{(1)}(r) = J_0(r) + \imath\, Y_0(r)$$

(J_0 is the Bessel function of order zero; Y_0 is the Bessel function of the second kind and order zero, also called Neumann function of order zero) and called **Hankel function of the first kind and order zero**. As $r \to 0$, $H^{(1)}(r)$ has a logarithmic singularity, which is also integrable.

The Sommerfeld condition is now

$$\lim_{r\to\infty} r^{1/2}\,(\partial_r u - \imath\, k\, u) = 0.$$

One defines similarly single–layer potentials, the operator V_Γ and proves the equivalent properties. For the decomposition

$$V_\Gamma = V_0 + \text{compact}$$

we have to use

$$V_0\psi := -\frac{1}{2\pi}\int_\Gamma \log|\varepsilon(\,\cdot\,-\mathbf{y})|\psi(\mathbf{y})\mathrm{d}\gamma(\mathbf{y})$$

($\mathrm{d}\gamma(\,\cdot\,)$ is a length element, not area!) with $\varepsilon < 1/\mathrm{diam}(\Omega)$. The reason for this new parameter related to size is not entirely obvious but has a lot to do with the essential difference of electrostatics in two and three dimensions.

If the boundary is smooth and we have a smooth parameterization of the whole curve (not a collection of pieces of parameterizations), we can very easily use high order elements without increasing the number of degrees of freedom, such as splines and trigonometric polynomials.

10 A direct formulation

At this point we are going to restart and work with new formulations, to obtain new integral equations, which we will have to numerically solve and then (when possible) analyse the discrete method. So, hold your breadth ... Part of what we are going to do includes new concepts, but a lot of it is going to be a more or less step by step repetition of already studied techniques.

The departure point for our new formulation is the **third Green formula** adapted to the Helmholtz equation. Assume that u is the solution of an exterior scattering problem (for which we don't give the boundary condition yet):

$$\begin{aligned} \Delta u + k^2 u &= 0, \qquad \text{in } \Omega^+, \\ \partial_r u - \imath\, k\, u &= o(r^{-1}), \qquad r \to \infty. \end{aligned}$$

Then,

$$u(\mathbf{x}) = -\int_\Gamma \phi(\mathbf{x},\mathbf{y})\partial_\nu u(\mathbf{y})\mathrm{d}\gamma(\mathbf{y}) + \int_\Gamma \partial_{\nu(\mathbf{y})}\phi(\mathbf{x},\mathbf{y})\, u(\mathbf{y})\,\mathrm{d}\gamma(\mathbf{y}), \qquad \mathbf{x}\in\Omega^+.$$

The formula holds with ordinary integrals if u is smooth enough near the boundary and with a duality product for the first term if u is simply locally H^1. The formula says a lot of things. Among them:

- It says that the solution is $\mathcal{C}^\infty(\Omega^+)$, and that lack of regularity is limited to the proximities to the boundary of the scatterer. We already had this from the indirect formulation, excepting at Dirichlet eigenfrequencies.
- It also says that if we know both **Cauchy data** (Dirichlet and Neumann data), the solution is determined via an explicit formula. Taking this point of view, we say that this is a **representation formula**.

If we take the limit to $\mathbf{x}\in\Gamma$ we find something new: if $\mathbf{x}$ is a smooth point of Γ, then

$$\frac{1}{2}u(\mathbf{x}) = -\int_\Gamma \phi(\mathbf{x},\mathbf{y})\partial_\nu u(\mathbf{y})\mathrm{d}\gamma(\mathbf{y}) + \int_\Gamma \partial_{\nu(\mathbf{y})}\phi(\mathbf{x},\mathbf{y})\, u(\mathbf{y})\,\mathrm{d}\gamma(\mathbf{y}).$$

This means that if we evaluate verbatim the right–hand side formula we obtain $u(\mathbf{x})$ when $\mathbf{x} \in \Omega^+$, but only $\frac{1}{2}u(\mathbf{x})$ when $\mathbf{x} \in \Gamma$. Moreover,

$$0 = -\int_\Gamma \phi(\mathbf{x},\mathbf{y})\partial_\nu u(\mathbf{x})\mathrm{d}\gamma(\mathbf{y}) + \int_\Gamma \partial_{\nu(\mathbf{y})}\phi(\mathbf{x},\mathbf{y})\, u(\mathbf{y})\,\mathrm{d}\gamma(\mathbf{y}), \qquad \mathbf{x} \in \Omega.$$

Remark. The formula holds also true, but with opposite signs, for interior problems. If

$$\Delta u + k^2 u = 0, \qquad \text{in } \Omega,$$

then

$$u(\mathbf{x}) = \int_\Gamma \phi(\mathbf{x},\mathbf{y})\partial_\nu u(\mathbf{y})\mathrm{d}\gamma(\mathbf{y}) - \int_\Gamma \partial_{\nu(\mathbf{y})}\phi(\mathbf{x},\mathbf{y})\, u(\mathbf{y})\,\mathrm{d}\gamma(\mathbf{y}), \qquad \mathbf{x} \in \Omega.$$

Notice that the changes of signs makes sense since we are keeping the sense of the normal vectors (always pointing inside Ω^+), which means that they are now pointing outwards whereas before they where pointing inwards, given the fact that the domain was Ω^+. Notice also that this formula doesn't contradict the last one for the exterior problem: the Cauchy data in that formula where for the exterior problem and here they are for the interior problem. □

Exercise. *Using the representation formula for the interior problem, prove that a function cannot be simultaneously a Dirichlet and a Neumann eigenfunction for the Laplace operator in Ω. (Notice that we needed this to prove that invertibility of the single–layer operator V_Γ was equivalent to $-k^2$ not being a Dirichlet eigenvalue.)*

Let us simplify the aspect of all these formulas using a new potential

$$(\mathcal{D}_\Gamma\varphi)(\mathbf{x}) := \int_\Gamma \partial_{\nu(\mathbf{y})}\phi(\mathbf{x},\mathbf{y})\,\varphi(\mathbf{y})\,\mathrm{d}\gamma(\mathbf{y}), \qquad \mathbf{y} \in \Omega^+ \cup \Omega = \mathbb{R}^3\backslash\Gamma$$

and a new operator

$$(K_\Gamma\varphi)(\mathbf{x}) := \int_\Gamma \partial_{\nu(\mathbf{y})}\phi(\mathbf{x},\mathbf{y})\,\varphi(\mathbf{y})\,\mathrm{d}\gamma(\mathbf{y}), \qquad \mathbf{y} \in \Gamma.$$

As before, potential and operator are given by the same formula, only the potential is a function defined in $\mathbb{R}^3\backslash\Gamma$ and the operator gives a function defined on Γ.

Remark. The potential $\mathcal{D}_\Gamma\varphi$ is called a **double–layer potential** for reasons we will explore in the following section. □

If again

$$\begin{aligned} \Delta u + k^2 u &= 0, && \text{in } \Omega^+, \\ \partial_r u - \imath\, k\, u &= o(r^{-1}), && r \to \infty, \end{aligned}$$

and we denote

$$g := u|_\Gamma, \qquad \lambda := \partial_\nu^+ u|_\Gamma,$$

then the representation formula says that

$$u = \mathcal{D}_\Gamma g - \mathcal{S}_\Gamma \lambda, \qquad \text{in } \Omega^+.$$

I want to emphasize that the Sommerfeld condition has to be satisfied for this to be true, since the right–hand satisfies it even if g and λ are not the Cauchy data of a solution of the Helmholtz equation. The limiting value of this formula is

$$\tfrac{1}{2} g = K_\Gamma g - V_\Gamma \lambda.$$

For the Dirichlet problem (sound–soft scattering), we can try to solve the equation

$$V_\Gamma \lambda = -\tfrac{1}{2} g + K_\Gamma g$$

and then obtain u by means of the representation formula. I don't waste your time, so let's give fast facts. Bullet points!

- The equation has the same structure as that of the indirect method. The right–hand side is more complicated though.
- If $-k^2$ is not a Dirichlet eigenvalue in Ω, we have a unique solution of the problem. We can solve it with the same Galerkin method as before.
- Now the unknown is a physical quantity, not a density we have devised to solve the problem. Notice that if you know $u|_\Gamma$ and $\partial_\nu u|_\Gamma$, you also have a first order Taylor knowledge of u near the boundary.
- The exterior Dirichlet problem admits a unique solution. This fact can be proved independently of the value of k. Therefore, the integral equation always has a solution, but it can fail to be unique when V_Γ is not invertible. The null–space (also called kernel) of V_Γ is the set of normal derivatives of the eigenfunctions

  $$\begin{aligned} \Delta \xi + k^2 \xi = 0, &\qquad \text{in } \Omega, \\ \xi = 0, &\qquad \text{on } \Gamma \end{aligned}$$

  Since (see below to check the formulas for interior problems)

  $$0 = \mathcal{S}_\Gamma \partial_\nu \xi - \mathcal{D}_\Gamma \xi = \mathcal{S}_\Gamma \partial_\nu \xi,$$

  any solution of the integral equation works from the point of view of the representation formula. The problem is that only one of these solutions is the normal derivative of the solution, so if you are after the correct value of the normal derivative, you have to be extra careful here!

Exercise. *Using the same Galerkin method as exposed in Section 5, what is the form of the right–hand side? And for the collocation method?*

Exercise. *Write down the boundary integral equation you would have to solve for the sound–hard scattering problem (Neumann problem):*

$$\begin{aligned} \Delta u + k^2 u = 0, &\qquad \text{in } \Omega^+, \\ \partial_r u - \imath\, k\, u = o(r^{-1}), &\qquad r \to \infty, \\ \partial_\nu u|_\Gamma = \lambda. & \end{aligned}$$

For the interior problem, we have the same type of formulas: if

$$\Delta u + k^2 u = 0, \qquad \text{in } \Omega$$

and $g^- := u|_\Gamma$, $\lambda^- := \partial_\nu^- u|_\Gamma$, then we have the representation formula

$$u = \mathcal{S}_\Gamma \lambda^- - \mathcal{D}_\Gamma g^-, \qquad \text{in } \Omega,$$

the identity satisfied by Cauchy data

$$\tfrac{1}{2} g^- = V_\Gamma \lambda^- - K_\Gamma g^-$$

and

$$0 = \mathcal{S}_\Gamma \lambda^- - \mathcal{D}_\Gamma g^-, \qquad \text{in } \Omega^+.$$

Exercise. *Write down the integral equations you would have to solve for the interior Dirichlet and Neumann problems.*

Exercise. *Let*

$$\begin{aligned} \Delta u + k^2 u = 0, &\qquad \text{in } \Omega^+ \cup \Omega, \\ \partial_r u - \imath\, k\, u = o(r^{-1}), &\qquad r \to \infty. \end{aligned}$$

Prove that

$$u = \mathcal{S}_\Gamma(\partial_\nu^- u - \partial_\nu^+ u) - \mathcal{D}_\Gamma(u^- - u^+), \qquad \text{in } \Omega^+ \cup \Omega.$$

(Hint: use the representation formulas for the interior and exterior problems and also the identities satisfied by the right–hand side in the complementary domain). What is the value of the function defined by the right–hand side when restricted to the boundary Γ?

11 Sound–hard scattering

We end this course by showing more formulas and more techniques to numerically solve exterior scattering problems via boundary elements. Our new problem is the exterior Neumann problem,

$$\begin{aligned} \Delta u + k^2 u = 0, &\qquad \text{in } \Omega^+, \\ \partial_r u - \imath\, k\, u = o(r^{-1}), &\qquad r \to \infty, \\ \partial_\nu u|_\Gamma = \lambda & \end{aligned}$$

for given $\lambda \in H^{-1/2}(\Gamma)$. A proof of existence and uniqueness of this problem can be given by following similar steps to the Dirichlet problem: we prove uniqueness of the homogeneous problem ($\lambda = 0$); we propose a potential solution and obtain a related boundary integral equation and, finally, we use this equation and Fredholm theory to prove existence of solution.

We will give it several tries: an indirect method with a double–layer potential; an indirect method with a single layer potential and a direct method.

11.1 Double–layer potentials

The first possibility we explore is trying

$$u := \mathcal{D}_\Gamma \varphi, \qquad \varphi \in H^{1/2}(\Gamma).$$

The following exercise proves that in the boundary

$$\begin{aligned} \gamma^+(\mathcal{D}_\Gamma\varphi) &= \tfrac{1}{2}\varphi + K_\Gamma\varphi \\ \gamma^-(\mathcal{D}_\Gamma\varphi) &= -\tfrac{1}{2}\varphi + K_\Gamma\varphi \\ \partial_\nu^+(\mathcal{D}_\Gamma\varphi) &= \partial_\nu^-(\mathcal{D}_\Gamma\varphi). \end{aligned}$$

The last expression gives rise to a boundary integral operator

$$W_\Gamma\varphi := -\partial_\nu(\mathcal{D}_\Gamma\varphi)$$

or, written more explicitly

$$W_\Gamma\varphi := -\partial_\nu \int_\Gamma \partial_{\nu(\mathbf{y})}\phi(\,\cdot\,,\mathbf{y})\,\varphi(\mathbf{y})\,\mathrm{d}\gamma(\mathbf{y}).$$

The negative sign in front of the definition looks quite arbitrary. It is imposed to ensure a certain degree of positiveness, as we will see in a while.

Exercise. *Take an arbitrary $g \in H^{1/2}(\Gamma)$, solve the exterior Dirichlet problem and call $\lambda := \partial_\nu u$. The representation formulas of Section 10 read then:*

$$\begin{aligned} u &= -\mathcal{S}_\Gamma\lambda + \mathcal{D}_\Gamma g, && \text{in } \Omega^+ \\ \tfrac{1}{2}g &= -V_\Gamma\lambda + K_\Gamma g, && \text{on } \Gamma \\ 0 &= -\mathcal{S}_\Gamma\lambda + \mathcal{D}_\Gamma g, && \text{in } \Omega. \end{aligned}$$

(a) By writing $\mathcal{D}_\Gamma g = u + \mathcal{S}_\Gamma\lambda$ in Ω^+, prove that

$$\gamma^+(\mathcal{D}_\Gamma g) = \tfrac{1}{2}g + K_\Gamma g.$$

(b) Prove that

$$\gamma^-(\mathcal{D}_\Gamma g) = V_\Gamma\lambda = -\tfrac{1}{2}g + K_\Gamma g.$$

What is the discontinuity of the double–layer potential across Γ?

(c) Using the identities

$$\begin{aligned}\lambda &= -\partial_\nu^+(\mathcal{S}_\Gamma\lambda) + \partial_\nu^+(\mathcal{D}_\Gamma g),\\ 0 &= -\partial_\nu^-(\mathcal{S}_\Gamma\lambda) + \partial_\nu^-(\mathcal{D}_\Gamma g),\\ \lambda &= \partial_\nu^-(\mathcal{S}_\Gamma\lambda) - \partial_\nu^+(\mathcal{S}_\Gamma\lambda),\end{aligned}$$

(the last one was mentioned and used when studying the single–layer potential) prove that

$$\partial_\nu^+\mathcal{D}_\Gamma g = \partial_\nu^-\mathcal{D}_\Gamma g$$

and therefore the normal derivative of the double–layer potential is continuous.

Remark. We already mentioned that single–layer acoustic potentials extend to the Helmholtz equation (time–harmonic acoustic fields) the idea of electrostatic charges in equilibrium. Similarly, double–layer potentials extend the idea of dipoles. Now the potential is discontinuous (the dipole distribution on the surface creates the discontinuity) but the electric field is continuous in the normal direction across the boundary. □

It is very tempting to introduce the derivative under integral sign and write something like this

$$(W_\Gamma\varphi)(\mathbf{x}) = -\int_\Gamma \partial_{\nu(\mathbf{x})}\partial_{\nu(\mathbf{y})}\phi(\mathbf{x},\mathbf{y})\,\varphi(\mathbf{y})\,\mathrm{d}\gamma(\mathbf{y}).$$

But you have to be careful with this. By doing the two normal derivatives, the kernel function

$$\partial_{\nu(\mathbf{x})}\partial_{\nu(\mathbf{y})}\phi(\mathbf{x},\mathbf{y})$$

fails to be integrable. In order that the integral makes full sense, we have to subtract the singularity and integrate the regular part of the integrand. What we really do there is the Hadamard finite part of the integral. Independently of how this is computed, you write

$$W_\Gamma\varphi = -\text{f.p.}\int_\Gamma \partial_{\nu(\,\cdot\,)}\partial_{\nu(\mathbf{y})}\phi(\,\cdot\,,\mathbf{y})\,\varphi(\mathbf{y})\,\mathrm{d}\gamma(\mathbf{y}).$$

The important points about W_Γ are:

- W_Γ is bounded from $H^{1/2}(\Gamma)$ to $H^{-1/2}(\Gamma)$.
- W_Γ is invertible if and only if $-k^2$ is not a Neumann eigenvalue of the Laplace operator in Ω.
- There exists an operator W_0 such that

  $$\langle\varphi, W_0\varphi\rangle_\Gamma \geq \beta\,\|\varphi\|^2_{1/2,\Gamma}, \qquad \forall\varphi\in H^{1/2}(\Gamma)$$

  and $W_\Gamma - W_0$ is compact. Here is where the minus sign in the definition becomes relevant.

- Because of the last property, in the case where W_Γ is invertible, a Galerkin method with a sequence of subspaces of $Y_h \subset H^{1/2}(\Gamma)$ that satisfy

$$\inf_{\rho_h \in Y_h} \|\varphi - \rho_h\|_{1/2,\Gamma} \quad \stackrel{h\to 0}{\longrightarrow} \; 0, \qquad \forall \varphi \in H^{1/2}(\Gamma)$$

  defines a convergent method. This means that the method defined by

$$\varphi_h \in Y_h, \qquad \langle \rho_h, W_\Gamma \varphi_h \rangle_\Gamma = \langle \rho_h, \lambda \rangle_\Gamma, \quad \forall \rho_h \in Y_h$$

  satisfies

$$\|\varphi - \varphi_h\|_{1/2,\Gamma} \quad \stackrel{h\to 0}{\longrightarrow} \; 0.$$

- A piecewise smooth function defined on a partition of Γ into elements has to be continuous to be an element of $H^{1/2}(\Gamma)$. Therefore, boundary elements for this problem have the same continuity requirements as the typical finite elements for elliptic problems of the second order.

For instance if we use a space of continuous piecewise linear elements (the classical Courant finite elements) we obtain, with regularity assumptions on the solution, the bound

$$\|\varphi - \varphi_h\|_{1/2,\Gamma} \lesssim h^{3/2} \|\varphi\|_{2,\Gamma}.$$

Again, a duality argument (an more assumptions on the regularity of the domain), can be used to improve this bound in a weaker norm to obtain

$$\|\varphi - \varphi_h\|_{-1,\Gamma} \lesssim h^{3} \|\varphi\|_{2,\Gamma}.$$

This is the optimal bound we observe if we look at pointwise values of the approximated potential sufficiently far from the boundary.

11.2 Single layers

Another option for an indirect formulation is trying again with single–layer potentials:

$$u = \mathcal{S}_\Gamma \psi, \qquad \psi \in H^{-1/2}(\Gamma).$$

To do that, we have first to know what is the normal derivative of a single layer potential, which is going to be different from the inside to the outside, since its difference is precisely the density ψ. With some effort (not a lot) it can be proved that

$$\partial_\nu^+ u = -\frac{1}{2}\psi + \int_\Gamma \partial_{\nu(\,\cdot\,)} \phi(\,\cdot\,, \mathbf{y})\, \psi(\mathbf{y})\, \mathrm{d}\gamma(\mathbf{y}), \qquad \text{on } \Gamma.$$

Defining

$$(K_\Gamma^t \psi)(\mathbf{x}) := \int_\Gamma \partial_{\nu(\mathbf{x})} \phi(\mathbf{x}, \mathbf{y})\, \psi(\mathbf{y})\, \mathrm{d}\gamma(\mathbf{y}),$$

the expression simplifies to

$$\partial_\nu^+ \mathcal{S}_\Gamma \psi = -\tfrac{1}{2}\psi + K_\Gamma^t \psi.$$

Therefore, to solve the Neumann problem, we only have to try to find a solution to the new boundary integral equation

$$-\tfrac{1}{2}\psi + K_\Gamma^t \psi = \lambda$$

and then input ψ in the single–layer potential $u = \mathcal{S}_\Gamma \psi$ to obtain the scattered wave field.

Exercise. *Prove that*

$$\partial_\nu^- \mathcal{S}_\Gamma \psi = \tfrac{1}{2}\psi + K_\Gamma^t \psi.$$

The operators K_Γ and K_Γ^t are transposed to each other, meaning that

$$\langle K_\Gamma^t \psi, \varphi \rangle_\Gamma = \langle K_\Gamma \varphi, \psi \rangle_\Gamma, \qquad \forall \psi \in H^{-1/2}(\Gamma),\ \varphi \in H^{1/2}(\Gamma).$$

Remark. K_Γ and K_Γ^t are not adjoint to each other, but transposed. The only difference between these two concepts is conjugation in the complex plane. □

Remark. In an exercise in the previous section, you will have arrived to a very similar integral equation

$$-\tfrac{1}{2}\, g + K_\Gamma g = V_\Gamma \lambda$$

for the Neumann problem. In this equation the unknown is the Dirichlet datum (this is a direct method; no potentials are involved), we have K_Γ instead of K_Γ^t and an integral operator in the right–hand side. Independently on whether these integral equations are uniquely solvable or not (we will not deal with this now), the direct formulation has always a solution, even if it is not unique. □

With some regularity assumptions, that preclude polyhedra of the setting, it is possible to prove that

$$K_\Gamma : H^{1/2}(\Gamma) \to H^{1/2}(\Gamma) \ \textit{is compact}$$

and therefore

$$K_\Gamma^t : H^{-1/2}(\Gamma) \to H^{-1/2}(\Gamma) \ \textit{is compact.}$$

This means that equations with operator of the form

$$-\tfrac{1}{2}\, I + K_\Gamma^t$$

satisfy always the Fredholm alternative. There is however a somewhat difficult point here when we want to do numerical approximation. The question is ellipticity: trying an inequality like

$$\langle I\, \psi, \psi \rangle_\Gamma \geq \alpha \|\psi\|^2_{-1/2,\Gamma}$$

is not possible, since in the bracket one component has to be in $H^{1/2}(\Gamma)$ and the other in $H^{-1/2}(\Gamma)$. A solution would be using the inner product of $H^{-1/2}(\Gamma)$, where ellipticity is trivial

$$(I\,\psi,\psi)_{-1/2,\Gamma} = \|\psi\|^2_{-1/2,\Gamma}.$$

However, the numerical approximation by a Galerkin scheme requires then using the variational formulation

$$\psi \in H^{-1/2}(\Gamma), \qquad (-\tfrac{1}{2}\psi + K^t_\Gamma\psi,\varphi)_{-1/2,\Gamma} = (\lambda,\varphi)_{-1/2,\Gamma}, \qquad \forall\varphi \in H^{-1/2}(\Gamma)$$

as a starting point and the inner product in $H^{-1/2}(\Gamma)$ is not easy to handle.

The simplest thing to do is trying a Galerkin scheme in the spirit of what we did in previous sections. We define X_h to be the space of piecewise constant functions and look for

$$\psi_h \in X_h, \qquad -\frac{1}{2}\int_\Gamma \psi_h\,\varphi_h + \int_\Gamma (K^t_\Gamma\psi_h)\,\varphi_h = \int_\Gamma \lambda\,\varphi_h, \qquad \forall\varphi_h \in X_h.$$

For this we need the additional assumption that the Neumann datum λ belongs to $L^2(\Gamma)$, which is not true for the Neumann problem in full generality, but certainly is for the sound–hard scattering problem. This is tantamount to moving the integral equation

$$-\tfrac{1}{2}\psi + K^t_\Gamma\psi = \lambda$$

to be happening in $H^0(\Gamma)$ instead of in $H^{-1/2}(\Gamma)$. Here the identity is elliptic with respect to the $H^0(\Gamma)-$inner product and therefore, assuming unique solvability, we obtain asymptotic stability plus the convergence bound

$$\|\psi-\psi_h\|_{0,\Gamma} \lesssim \inf_{\varphi_h\in X_h}\|\psi-\varphi_h\|_{0,\Gamma},$$

which, when $\psi \in H^1(\Gamma)$, yields the convergence rate

$$\|\psi-\psi_h\|_{0,\Gamma} \lesssim h\,\|\psi\|_{1,\Gamma}.$$

This rate can be improved a little in weaker norms, but is still far worse than the kind of bounds we obtained for the Dirichlet problem with single–layer potentials or for the Neumann problem with double–layer potentials. It must be said, however, that in the last case, continuity was a requirement on the space, since the density of a double layer operator belongs to $H^{1/2}(\Gamma)$, where line discontinuities are forbidden.

Remark. The integral equation

$$\frac{1}{2}\,\psi + \int_\Gamma \partial_{\nu(\,\cdot\,)}\phi(\,\cdot\,,\mathbf{y})\,\psi(\mathbf{y})\,\mathrm{d}\gamma(\mathbf{y}) = \lambda, \qquad \text{on } \Gamma$$

(this would be for an interior Neumann problem) is basically where everything begun for integral equations. In fact, the operator was the Laplace operator and the problem was being set in two dimensions. The name of Ivar Fredholm is strongly related to this effort of dealing with boundary integral equations of the second kind (identity plus compact operator), at a moment where all the functional analysis was still in diapers. The effort of Fredholm, as well as that of Hilbert, the

Riesz brothers, Schauder and many others, on developing abstract mathematical tools to deal with linear operators in abstract spaces was originated in a big part from the effort of solving (showing that it has a solution and trying to get it in some cases) this integral equation as a way to prove existence of solution of boundary value problems when the nice Sobolev–space–and–distribution–theory was still decades away. □

11.3 Direct formulations

We have already mentioned the possibility of using the representation formula

$$u = \mathcal{D}_\Gamma g - \mathcal{S}_\Gamma \lambda, \qquad \text{in } \Omega^+$$

and the integral equation

$$-\tfrac{1}{2}\, g + K_\Gamma\, g = V_\Gamma \lambda$$

as a way of solving the exterior Neumann problem. This problem should be solved in $H^{1/2}(\Gamma)$ but, as before, the principal part of the integral equation (minus one half times the identity operator) is elliptic in $H^0(\Gamma)$. One can devise then a Galerkin method similar to the one for the single–layer representation, but using a $H^{1/2}-$conforming boundary element space, i.e., one with continuity conditions over interfaces of elements. The analytical techniques developed in Section 8 can be used here to show convergence in $H^{1/2}(\Gamma)$ provided that we can use some inverse inequalities, which hold under some severe restrictions on the triangulation.

If one is not that much interested in convergence of the Galerkin approximation of g to this function in the correct norm (the trace norm $H^{1/2}(\Gamma)$), but only in the exterior solution sufficiently far from the obstacle, it is possible to benefit from Aubin–Nitsche estimates in weak norms, which provide improved convergence rates.

Finally, since we know what the normal derivatives of single and double layer operators look like, we can go back to the representation formula

$$u = \mathcal{D}_\Gamma g - \mathcal{S}_\Gamma \lambda, \qquad \text{in } \Omega^+$$

and take the normal derivative from the exterior

$$\lambda = \partial_\nu^+ u = \partial_\nu \mathcal{D}_\Gamma g - \partial_\nu^+ \mathcal{S}_\Gamma \lambda = -W_\Gamma g - (-\tfrac{1}{2}\lambda + K_\Gamma^t \lambda)$$

to obtain the integral equation

$$W_\Gamma g = -\tfrac{1}{2}\lambda - K_\Gamma^t \lambda,$$

which is always solvable but fails to be uniquely solvable when $-k^2$ is a Neumann eigenvalue of the Laplace operator in the interior domain. The same kind of numerical techniques than those used for the double–layer representation apply here.

Remark. I've deliberately omitted any mention to collocation methods in this section. Of course they also apply to this situation, at least formally. In the case of equations of the second kind (for sufficiently smooth obstacles) it is even possible to do a proper analysis of the method, but this analysis takes place more naturally in Hölder spaces than in Sobolev spaces. When the hypersingular operator W_Γ appears in the equation, things become trickier from the analytical point of view and there is still a lot to be done. □

12 Further reading

There are not many books dealing with the mathematical and numerical analysis of boundary element methods. The literature is however much more important in the engineering world, where you will be able to find many details on algorithms, implementation and especially different problems where boundary element techniques apply.

The book

> *Boundary Element Methods* by Goong Chen, Jingmin Zhou, Academic Press, 1992

details the boundary integral formulations for the Laplace, Helmholtz, Navier–Lamé (linear elasticity) and biharmonic (Kirchhoff plate) equations. The Sobolev theory is explained with care in the case of smooth interfaces. The fundamentals of Sobolev theory and finite element theory are carefully explained. There are also some explanations on pseudo–differential operators, a theory that allows for a generalization of the behaviour of all the boundary integral operators for smooth boundaries. The section on numerical analysis is not very long and right now it is not up–to–date.

The whole theory on boundary integral formulations based on elliptic operators (all the equations where the principal part is V_Γ or W_Γ) is explained with an immense care and taste for mathematical detail in

> *Strongly Elliptic Systems and Boundary Integral Equations* by William McLean, Cambridge University Press, 2000.

This is a book of hard mathematics, where you will learn a lot but are asked to have patience. It does not cover numerical analysis.

If you are not afraid of reading maths in German, this is a very good choice:

> *Randelementmethoden. Analyse, Numerik und Implementierung schneller Algorithmen* by Stefan Sauter and Christoph Schwab, Teubner, 2004.

The book covers theoretical aspects, numerical analysis as well as many details on how to approximate the integrals of Galerkin discretizations and how to solve efficiently the large dense linear systems.

Three other books, with an increasing slope towards applications:

> *A Practical Guide to Boundary Element Methods with the Software Library BEMLIB*, by C. Pozrikidis, CRC Press, 2002.

> *Programming the Boundary Element Method : An Introduction for Engineers*, by Gernot Beer, John Wiley & Sons, 2001.

> *Boundary Element Methods for Engineers and Scientists*, by Lothar Gaul, Martin Kögl, Marcus Wagner, Springer, 2003