Lecture on

Boundary Element Methods

Clemens Pechstein[1]

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[1]Institute of Computational Mathematics, Johannes Kepler University Linz

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Chapter 1

Introduction

The boundary element method (BEM) is an approach to solve partial differential equations (PDEs) by appropriately discretized boundary integral equations (BIEs). These integral equations act only on the boundary of the computational domain and are derived using a fundamental solution according to the differential operator under consideration. The solution of the BIE is used to reconstruct the solution of the original PDE in the whole domain. In this introduction we briefly sketch this approach in two examples and we give an overview on the whole lecture.

In the following we consider a simple well-known model problem. Let $\Omega \subset \mathbb{R}^d$ ($d = 2$ or 3) be a domain with "smooth" boundary Γ (we will discuss smoothness later on). Find $u : \overline{\Omega} \to \mathbb{R}$ such that

$$\begin{aligned} -\Delta u &= 0 \quad && \text{in } \Omega\,, \\ u &= g_D && \text{on } \Gamma\,. \end{aligned} \tag{1.1}$$

This is the pure Dirichlet problem for Laplace's equation.

The fundamental solution to the Laplace operator $-\Delta$ is given by

$$U^*(x,\, y) = \begin{cases} -\frac{1}{2\pi} \log|x-y| & \text{for } d = 2\,, \\ \frac{1}{4\pi} \frac{1}{|x-y|} & \text{for } d = 3\,. \end{cases}$$

As a characteristic property of this fundamental solutions we have that

$$-\Delta_x U^*(x,\, y) \;=\; \delta_y(x)$$

in the distributional sense, where δ_y denotes Dirac's delta distribution. We also have that

$$-\Delta_x U^*(x,\, y) \;=\; 0 \quad \forall y \neq x$$

in a strong sense (note that $U^*(x,\, y)$ is C^∞ unless $x = y$).

Example 1.1 (indirect approach) We make the ansatz that the solution u of (1.1) fulfills

$$u(x) \;=\; \int_\Gamma U^*(x,\,y)\,w(y)\,ds_y \quad \text{for } x \in \Omega\,, \tag{1.2}$$

for some (yet unknown) density $w : \Gamma \to \mathbb{R}$. Then u satisfies indeed the homogeneous Laplace equation. Proof:

$$-\Delta u(x) \;=\; -\Delta_x \int_\Gamma U^*(x,\,y) w(y)\,ds_x \;=\; \int_\Gamma \underbrace{-\Delta_x U^*(x,\,y)}_{=0}\, w(y)\,ds_y \;=\; 0\,.$$

Here we could swap integration and differentiation because $x \neq y$. We now define the boundary integral operator

$$(V\,w)(x) \;:=\; \int_\Gamma U^*(x,\,y)\,w(y)\,ds_y \quad \text{for } x \in \Gamma\,.$$

In order to fulfill our Dirichlet boundary conditions, the density $w : \Gamma \to \mathbb{R}$ has to satisfy

$$V\,w \;= g_D \quad \text{on } \Gamma\,. \tag{1.3}$$

This is a boundary integral equation (BIE) of the first kind. Once we have solved this equation, i. e., we have w, formula (1.2) defines the solution u of (1.1).

Example 1.2 (direct approach) Green's second formula reads

$$\int_\Omega -u\,\Delta v + v\,\Delta u\,dx \;=\; \int_\Gamma -u\,\frac{\partial v}{\partial n} + v\,\frac{\partial u}{\partial n}\,ds_x\,.$$

Setting $v(x) := U^*(x,\,y)$ with $y \in \Omega$ we obtain

$$\begin{aligned}\int_\Omega \underbrace{-\Delta_x U^*(x,\,y)}_{=\delta_y(x)}\, u(x)\,dx + \int_\Omega U^*(x,\,y)\,\Delta u(x)\,dx \\ = \;-\int_\Gamma u(x)\,\frac{\partial}{\partial n_x} U^*(x,\,y)\,ds_x + \int_\Gamma U^*(x,\,y)\,\frac{\partial u}{\partial n}(x)\,ds_x\end{aligned}$$

Without worrying about correctness, we interpret the first integral as an evaluation of Dirac's delta distribution and obtain

$$\begin{aligned}u(y) \;=\; &\int_\Omega U^*(x,\,y)\,\underbrace{\big[-\Delta u(x)\big]}_{=0}\,dx - \int_\Gamma \Big[\frac{\partial}{\partial n_x} U^*(x,\,y)\Big]\,\underbrace{u(x)}_{=\gamma_0 u}\,ds_x \\ &+ \int_\Gamma U^*(x,\,y)\,\underbrace{\frac{\partial u}{\partial n}(x)}_{=\gamma_1 u}\,ds_x \qquad \forall y \in \Omega\,.\end{aligned} \tag{1.4}$$

This identity is called *Green's third formula* or *representation formula*. It represents the value of u in the interior of Ω in terms of the so-called *Cauchy data*

$$\begin{pmatrix} \gamma_0 u \\ \gamma_1 u \end{pmatrix} = \begin{pmatrix} u \\ \frac{\partial u}{\partial n} \end{pmatrix} \qquad \text{on } \Gamma\,,$$

i. e., the *trace* of u and the *normal derivative*. By making a careful (non-trivial) transition $y \to \Gamma$, one obtains an equation of the form

$$\underbrace{u(y)}_{=g_D(y)} = -(\widetilde{K} \underbrace{u}_{=g_D})(y) + \Big(V \frac{\partial u}{\partial n}\Big)(y) \qquad \forall y \in \Gamma\,, \tag{1.5}$$

where $\widetilde{K}$ can be represented by an integral operator (more details are given in subsequent chapters), and V is the operator from before. We see that in case of our pure Dirichlet problem, the unknown normal derivative $\partial u/\partial n$ can be determined *directly* via the above BIE that is similar to (1.3).

Other approaches

- The ansatz

$$u(x) = \int_\Gamma \frac{\partial}{\partial n_x} U^*(x,\, y)\, v(y)\, ds_y \quad \text{for } x \in \Omega\,,$$

  for some density $v : \Gamma \to \mathbb{R}$ also fulfills $-\Delta u = 0$, and it leads to a BIE of the second kind.

- Formula (1.5) was something like "$\gamma_0(1.4)$". We can also use "$\gamma_1(1.4)$", which also leads to a BIE of the second kind.

In this lecture we will clarify in which spaces we have to work, and if and in which sense the integral equations are solvable. Secondly, we will discuss numerical methods to solve the discretized equations.

Overview on numerical methods Similarly to the finite volume method (FVM), the finite difference method (FDM), and in particular the finite element method (FEM), we will discretize our BIE

$$B\, v = g$$

(having in mind equations (1.3) or (1.5)) using a mesh of the boundary Γ, consisting of boundary elements Γ_j.

- In the *collocation method* we make the piecewise constant ansatz

$$v_h(x) \;=\; \sum_{j=1}^{n} v_j \, \chi_{\Gamma_j}$$

for our approximate solution v_h, where χ_{Γ_j} denotes the characteristic function. Of course we cannot expect $B\, v_h = g$ on the whole boundary. Instead we chose a set of test points $\{y_j\}_{j=1\ldots n} \subset \Gamma$ and seek for the coefficients $(v_j)_{j=1\ldots n}$ to satisfy

$$(B\, v_h)(y_j) \;=\; g(y_i) \qquad \forall i = 1 \ldots n \,,$$

which leads to a linear system of algebraic equations.

- In the more general *Galerkin* method, a projection method, we fix a space V where the solution v of the BIE is sought (i. e., some function space we did not yet specify). Then we choose a discrete subspace $V_h \subset V$ and seek an approximate solution $v_h \in V_h$ such that

$$\langle B\, v_h,\, w_h \rangle \;=\; \langle g,\, w_h \rangle \qquad \forall w_h \in V_h \,.$$

This is a projection of the continuous equation on V to the discrete space V_h.

Other topics of this lecture include the correct treatment of (mixed) boundary conditions, error estimates, and pros and cons compared to the finite element method. Obviously, a huge advantage is the reduction in dimension: instead of an equation on $\Omega \subset \mathbb{R}^d$, we get an equation on $\Gamma \subset \mathbb{R}^{d-1}$. It will turn out that BEM system matrices are dense, but that they can be approximated by data-sparse matrices and/or that their application to a vector can be done in quasi-linear time. These techniques which we will briefly touch are covered by the keyword *fast BEM*.

Among typical applications of BEM are exterior field problems, screen, and crack problems. We do not cover these problems, but only give some hints how exterior field problems can be treated.

Chapter 2

PDEs, Fundamental solutions, Green's formulae, and a first boundary integral equation

2.1 Notations and definitions

In the following let $\Omega \subset \mathbb{R}^d$ (with $d = 2$ or 3) be a domain (open and connected) with boundary $\Gamma = \partial\Omega$. Very often, Ω will be bounded too. Nevertheless, we will also work with unbounded domains, e. g., with the complement of a bounded domain. If Ω is bounded, we will implicitly assume that it is also simply connected (i. e., any closed curve in Ω can be contracted to a point, where the whole process of contraction occurs in Ω) and that its boundary has only one connected component. However, this restriction is not essential. More important is the restriction to the class of Lipschitz domains that will be defined in the sequel.

Definition 2.1. (a) The set

$$\widetilde{\Omega} := \{x \in \mathbb{R}^d : x_d < \gamma(\widetilde{x}) \quad \text{for } \widetilde{x} = (x_1, \ldots, x_{d-1}) \in \mathbb{R}^{d-1}\}$$

is called a *Lipschitz hypograph* if $\gamma : \mathbb{R}^{d-1} \to \mathbb{R}$ is Lipschitz continuous, i. e., there exists a constant $M > 0$ such that

$$|\gamma(\widetilde{x}) - \gamma(\widetilde{y})| \ \leq \ M\,|\widetilde{x} - \widetilde{y}| \qquad \forall \widetilde{x},\, \widetilde{y} \in \mathbb{R}^{d-1}\,.$$

Note that $\widetilde{\Gamma} := \partial\widetilde{\Omega} = \{x \in \mathbb{R}^d : x_d = \gamma(\widetilde{x}) \text{ for some } \widetilde{x} \in \mathbb{R}^{d-1}\}$.

(b) The open set $\Omega \subset \mathbb{R}^d$ is a *Lipschitz domain* if its boundary Γ is compact and there exist finite families $\{W_j\}$ and $\{\Omega_j\}$ such that

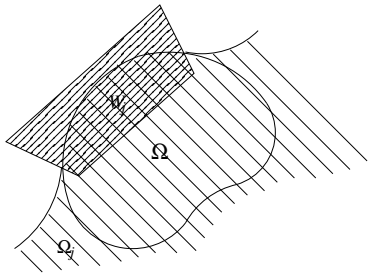


Figure 2.1: Sketch of Definition 2.1.

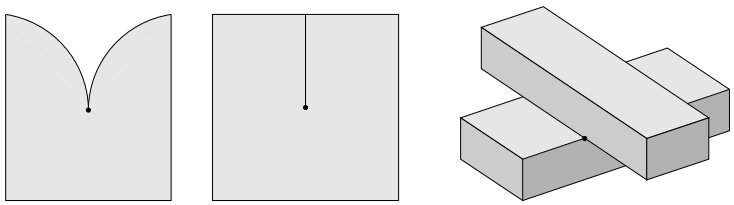


Figure 2.2: Examples of non-Lipschitz domains.

(i) $\{W_i\}$ is a finite open cover of Γ, i. e., $W_j \subset \mathbb{R}^d$ are open sets and $\Gamma \subset \bigcup_j W_j$,

(ii) each Ω_j can be transformed to a Lipschitz hypograph by a rigid motion (a rotation plus a translation),

(iii) $W_j \cap \Omega = W_j \cap \Omega_j$ for all j.

(c) If the parameterizations γ_j of each hypograph Ω_j in the above definition satisfy $\gamma_j \in C^k(\mathbb{R}^{d-1})$ we simply write $\Gamma \in C^k$. If $\gamma_j \in C^{k,1}(\mathbb{R}^{d-1})$ (the k-th derivative Lipschitz) we write $\Gamma \in C^{k,1}$. With this notation, the boundary Γ of a Lipschitz domain fulfills $\Gamma \in C^{0,1}$. If these conditions hold only piecewise (on a finite non-overlapping partition of $\Gamma = \bigcup \overline{\Gamma}_k$) we write $\Gamma \in C^k_{\mathrm{pw}}$ or $\Gamma \in C^{k,1}_{\mathrm{pw}}$.

Many polygons and polyhedra are Lipschitz domains. Some counterexamples are shown in Figure 2.1: in the leftmost domain, the graph fails to be Lipschitz, in the second domain, the boundary fails to be on one side, and in the last domain, the boundary fails to be a graph at all.

Note that Ω is Lipschitz if and only if $\mathbb{R}^d \setminus \overline{\Omega}$ is Lipschitz.

Lemma 2.2. *Let Ω be a Lipschitz domain. Then it has a surface measure (denoted s) and an outward unit normal vector (denoted n) s-almost everywhere on Γ.*

Proof. The proof follows from Rademacher's theorem. □

Notation. We introduce the following differential operators,

- the *gradient* $\nabla u := \begin{pmatrix} \frac{\partial u}{\partial x_1} \\ \vdots \\ \frac{\partial u}{\partial x_d} \end{pmatrix}$ of a scalar field $u : \Omega \to \mathbb{R}$,
- the *divergence* $\operatorname{div} F := \sum_{i=1}^{d} \frac{\partial F_i}{\partial x_i}$ of a vector field $F : \Omega \to \mathbb{R}^d$,
- the *normal derivative* $\frac{\partial u}{\partial n} := \nabla u \cdot n$,
- the *Laplace operator* $\Delta u := \operatorname{div} \nabla u = \sum_{i=1}^{d} \frac{\partial^2 u}{\partial x_i^2}$,
- the *Helmholtz operator* $-\Delta u - \kappa^2 u$ for some $\kappa \in \mathbb{R}$,
- the *Lamé operator* of linearized elasticity $-\mu\,\Delta u - (\lambda + \mu)\nabla \operatorname{div} u$.

In order to indicate the differentiation variable we write ∇_x, Δ_y, etc.

Theorem 2.3 (Gauss)**.** *Let Ω be a bounded Lipschitz domain and let the vector field $F : \overline{\Omega} \to \mathbb{R}^d$ be differentiable. Then*

$$\int_\Omega \mathit{div}\, F \, dx \;=\; \int_\Gamma F \cdot n \, ds \,.$$

In this lecture we will mainly work in the world of Laplace and Poisson. Our standard problem is to find $u : \overline{\Omega} \to \mathbb{R}$ such that

$$\begin{aligned} -\Delta u &= f \quad && \text{in } \Omega \,, \\ u &= g_D && \text{on } \Gamma_D \,, \\ \frac{\partial u}{\partial n} &= g_N && \text{on } \Gamma_N \,, \end{aligned} \tag{2.1}$$

where the Dirichlet boundary Γ_D is a part of Γ, and the Neumann boundary $\Gamma_N = \Gamma \setminus \Gamma_D$. If $\Gamma_N = \Gamma$, we have the compatibility (solvability) condition

$$\int_\Omega f \, dx + \int_\Gamma g_N \, ds \;=\; 0 \,. \tag{2.2}$$

2.2 Fundamental solutions

Definition 2.4. Let $C_0^\infty(\Omega) := \{\varphi \in C^\infty(\Omega) : \operatorname{supp}\varphi \subset\subset \Omega\}$, i. e., the infinitely many times differentiable functions with compact support in Ω. Let $\{\varphi_n\}$ be a sequence in $C_0^\infty(\Omega)$. We write

$$\varphi_n \to 0 \text{ sequentially}$$

if and only if for all $K \subset\subset \Omega$ and for all multi-indices α,

$$\partial^\alpha \varphi_n \to 0 \text{ uniformly on } K\,.$$

We denote by $\mathcal{D}(\Omega)$ the space $C_0^\infty(\Omega)$ equipped with this convergence. This is no metric space, but we can define continuity via the above sequential convergence. We set

$$\mathcal{D}'(\Omega) := \{\ell : \mathcal{D}(\Omega) \to \mathbb{R} : \ell \text{ linear and continuous}\}\,,$$

and denote the evaluation of such linear forms by $\langle \ell,\, \varphi\rangle := \ell(\varphi)$. The continuity says that $\varphi_n \to 0$ sequentially implies $\langle \ell,\, \varphi_n\rangle \to 0$. $\mathcal{D}'(\Omega)$ is called space of *Schwartz distributions* on Ω.

Example 2.5.

- Each function $u \in L^1_{\mathrm{loc}}(\Omega)$ (i. e., $|u|$ is integrable on each compact subset of Ω) defines a distribution $\overline{u} \in \mathcal{D}'(\Omega)$ by

$$\langle \overline{u},\, \varphi\rangle := \int_\Omega u\,\varphi\,dx \qquad \text{for } \varphi \in \mathcal{D}(\Omega)\,.$$

  In the following we identify u and $\overline{u}$. If a distribution $\ell \in \mathcal{D}'(\Omega)$ has a representation by an $L^1_{\mathrm{loc}}(\Omega)$ function, it is called *regular distribution.*

- The *Dirac delta-distribution* for a point $y \in \Omega$ is defined by

$$\delta_y \in \mathcal{D}'(\Omega): \quad \langle \delta_y,\, \varphi\rangle := \varphi(y) \quad \text{for } \varphi \in \mathcal{D}(\Omega)\,.$$

  This distribution is not regular, it cannot be represented by a function.

Definition 2.6. Let L be a scalar elliptic differential operator. Then $U^*(\cdot,\cdot) : \Omega \times \Omega \to \mathbb{R}$ is called *fundamental solution* if

$$L_x U^*(x,\, y) = \delta_y$$

(in the distributional sense).

Fundamental solutions do not necessarily exist for any differential operator. Even if they do, they might be difficult to construct. In the following we discuss a few well-known operators.

Example 2.7. 1. Laplace operator: $L = -\Delta$:

$$U^*(x,\, y) = \begin{cases} \frac{1}{2}(1 - |x-y|) & \text{for } d = 1\,, \\ -\frac{1}{2\pi}\log|x-y| & \text{for } d = 2\,, \\ \frac{1}{4\pi}\frac{1}{|x-y|} & \text{for } d = 3\,. \end{cases}$$

2. Helmholtz operator: $L = -\Delta - \kappa^2 I$ and $d = 3$:

$$U^*(x,\, y) = \frac{e^{\mathrm{i}\kappa|x-y|}}{4\pi|x-y|} = \frac{1}{4\pi|x-y|}\big[\cos(\kappa|x-y|) + \mathrm{i}\,\sin(\kappa|x-y|)\big]\,.$$

3. Further operators: For the Lamé operator and the Stokes system see, e. g., [Steinbach]. For $L\,u = -\mathrm{div}(A\,\nabla u) + 2\,b\cdot\nabla u + c\,u$ see, e. g., [Sauter/Schwab]. Very general elliptic systems are treated in [McLean].

Lemma 2.8. *Let L be strongly elliptic with constant coefficients. Then $U^*(x,\, y)$ is C^∞ in $\mathbb{R}^d \times \mathbb{R}^d \setminus \{(x,x) : x \in \mathbb{R}^d\}$. We have*

$$L_x U^*(x,\, y) = 0 \qquad \forall x \neq y$$

(in the strong sense).

Remark 2.9. For $d = 2$ we can use

$$U_r^*(x,\, y) = \frac{1}{2\pi}\log\frac{r}{|x-y|}$$

as fundamental solution, for all $r > 0$.

In the following we restrict ourselves to $L = -\Delta$.

2.3 Green's formulae

Lemma 2.10. *Let $\Omega \subset \mathbb{R}^d$ be a bounded Lipschitz domain. Then Green's first formula,*

$$\int_\Omega u\,\Delta v\,dx \;=\; -\int_\Omega \nabla u\cdot\nabla v\,dx + \int_\Gamma u\,\frac{\partial v}{\partial n}\,ds \qquad \forall u \in C^1(\overline{\Omega}),\, v \in C^2(\overline{\Omega})$$

and Green's second formula,

$$\int_\Omega u\,\Delta v - v\,\Delta u\,dx = \int_\Gamma u\,\frac{\partial v}{\partial n} - v\frac{\partial u}{\partial n}\,ds \qquad \forall u,\, v \in C^2(\overline{\Omega})$$

hold.

Note that we can relax $C^1(\overline{\Omega})$ and $C^2(\overline{\Omega})$ a bit such that all involved quantities are well defined. Using density arguments we can replace C^k above by H^k; we will treat this in detail in Chapter 4.

We now set $v(x) := U^*(x,\, y)$, do not worry about non-smoothness and obtain *Green's third formula* (also called *representation formula*),

$$\begin{aligned} u(y) \;=\; & -\int_\Omega U^*(x,\, y)\Delta_x u(x)\, dx - \int_\Gamma \frac{\partial}{\partial n_x} U^*(x,\, y)\, u(x)\, ds_x \;+ \\ & + \int_\Gamma U^*(x,\, y)\, \frac{\partial u}{\partial n}(x)\, ds_x \qquad\qquad \forall y \in \Omega\,. \end{aligned} \tag{2.3}$$

A sketch of a proof is found in the introduction. We will provide a careful proof in Chapter 4.

Remark 2.11. 1. In Green's first formula above, we can assume that $u \in H^1(\Omega)$ and $v \in H^2(\Omega)$, such that the traces $\gamma_0 := u_{|\Gamma}$ and $\gamma_1 = \nabla v \cdot n$ are well-defined. If $v \in H^1(\Omega)$ with $\Delta v \in L^2(\Omega)$, one can show that $\frac{\partial v}{\partial n}$ remains well-defined and a further generalization is possible, see Chapter 4.

2. The proof of (2.3) cannot be performed like

$$\int_\Omega u(x)\big[-\Delta_x U^*(x,\, y)\big]dx \;=\; \langle \delta_y,\, u\rangle \;=\; u(y)\,,$$

because $u \neq C_0^\infty(\Omega)$ (u has not necessarily a compact support). Instead we can use Dirac's delta distribution on the entire space $\mathbb{R}^d$, but then we have to formally set $-\Delta u = 0$ on $\mathbb{R}^d \setminus \Omega$, i. e., we loose smoothness. We therefore need a careful treatment which will involve distributions, and which is for now postponed to Chapter 4.

3. Formula (2.3) only holds for $y \in \Omega$. In general, we have

$$\begin{aligned} \sigma(y)\, u(y) \;=\; & -\int_\Omega U^*(x,\, y)\, \Delta_x u(x)\, dx - \int_\Gamma \frac{\partial}{\partial n_x} U^*(x,\, y)\, u(x)\, ds_x \;+ \\ & + \int_\Gamma U^*(x,\, y)\, \frac{\partial u}{\partial n}(x)\, ds_x \qquad\qquad \forall y \in \overline{\Omega}\,, \end{aligned}$$

with

$$\sigma(y) := \begin{cases} 1 & \text{if } y \in \Omega\,, \\ \frac{1}{2\pi}\theta(y) & \text{if } y \in \Gamma,\, d = 2\,, \\ \frac{1}{4\pi}\theta(y) & \text{if } y \in \Gamma,\, d = 3\,, \end{cases} \tag{2.4}$$

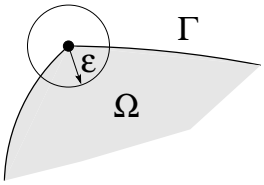


Figure 2.3: Sketch of σ from (2.4).

and

$$\theta(y) := \lim_{\varepsilon \to 0} \frac{1}{\varepsilon^{d-1}} \int\limits_{x \in \Omega:\, |y-x| = \varepsilon} ds$$

For sufficiently smooth Γ (e. g., C^1_{pw}), $\sigma = \frac{1}{2}$ almost everywhere on Γ, see Figure 2.3.

We will now derive a simple boundary integral equation for a boundary value problem of Laplace's equation. For the time being we do not worry about spaces and solvability, and we assume that the representation formula holds. We continue with a numerical method, the collocation method, in Chapter 3. Later on, we will investigate everything more precisely.

2.4 A first boundary integral equation

Consider problem (2.1) with $\Gamma_D = \Gamma$ and $f = 0$, i. e., the pure Dirichlet problem for Laplace's equation. From the representation formula above we obtain

$$\sigma(y)\, u(y) \;=\; -\int_\Gamma \frac{\partial}{\partial n_x} U^*(x,\, y)\, u(x)\, ds_x + \int_\Gamma U^*(x,\, y)\, \frac{\partial u}{\partial n_x}(x)\, ds_x \quad \forall y \in \overline{\Omega}\,.$$

We now restrict this equation to the boundary Γ and observe that then only the known Dirichlet trace $u_{|\Gamma} = \gamma_0 u$ and the unknown Neumann trace $\frac{\partial u}{\partial n} = \gamma_1 u$ appear in the equation. We define the boundary integral operators

$$(V\, w)(y) := \int_\Gamma U^*(x,\, y)\, w(x)\, ds_x \qquad \text{for } y \in \Gamma\,,$$
$$(K\, v)(y) := \int_\Gamma \frac{\partial}{\partial n_x} U^*(x,\, y)\, v(x)\, ds_x \qquad \text{for } y \in \Gamma\,.$$

The operator V is called *single layer potential operator*, and K is called *double layer potential operator*. For smooth functions v and w the integrals are well-defined as a weakly singular surface integrals. With the above equation we get

$$V \frac{\partial u}{\partial n} = \sigma u + K u \,, \tag{2.5}$$

which is a weakly singular boundary integral of the first kind for the unknown Neumann trace $\frac{\partial u}{\partial n}$.

Chapter 3

A simple collocation method

3.1 A pointwise boundary integral equation

We consider the domain Ω with boundary $\Gamma \in C^1$ for simplicity, i. e., $\sigma(y) = \frac{1}{2}$ for all $y \in \Gamma$. In this chapter we treat the mixed boundary value problem of Laplace's equation,

$$\begin{aligned} -\Delta u &= 0 && \text{in } \Omega\,, \\ u &= g_D && \text{on } \Gamma_D\,, \\ \frac{\partial u}{\partial n} &= g_N && \text{on } \Gamma_N = \Gamma \setminus \Gamma_D\,. \end{aligned} \tag{3.1}$$

Splitting the integrals in (2.5) into Dirichlet and Neumann part, and ordering with respect to what is known and what is unknown, we obtain

$$\text{Find } u = u_{|\Gamma_N} \text{ and } t := \frac{\partial u}{\partial n}|_{\Gamma_D}: \tag{3.2}$$

$$\int_{\Gamma_N} \frac{\partial}{\partial n_x} U^*(x,\, y)\, u(x)\, ds_x - \int_{\Gamma_D} U^*(x,\, y)\, t(x)\, ds_x = f_D(y) \quad \forall y \in \Gamma_D\,,$$

$$\frac{1}{2} u(y) + \int_{\Gamma_N} \frac{\partial}{\partial n_x} U^*(x,\, y)\, u(x)\, ds_x - \int_{\Gamma_D} U^*(x,\, y)\, t(x)\, ds_x = f_N(y) \quad \forall y \in \Gamma_N\,,$$

with

$$f_D(y) := -\frac{1}{2} g_D(y) - \int_{\Gamma_D} \frac{\partial}{\partial n_x} U^*(x,\, y)\, g_D(x)\, ds_x + \int_{\Gamma_N} U^*(x,\, y)\, g_N(x)\, ds_x\,,$$

$$f_N(y) := -\int_{\Gamma_D} \frac{\partial}{\partial n_x} U^*(x,\, y)\, g_D(x)\, ds_x + \int_{\Gamma_N} U^*(x,\, y)\, g_N(x)\, ds_x\,.$$

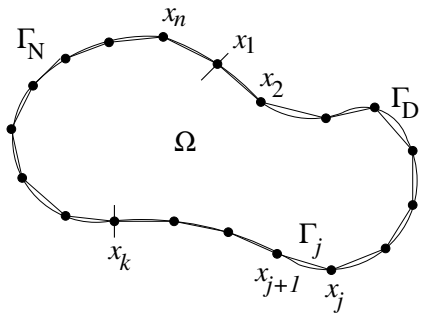


Figure 3.1: Discretization of the boundary of a two-dimensional domain.

3.2 Discretization in two dimensions

Boundary discretization

We introduce nodes $x_1, \ldots, x_n \in \Gamma$ with $x_i \neq x_j$ for $i \neq j$.

Notation. $x_{n+1} := x_1$

$\Gamma_j := \{x_j + t(x_{j+1} - x_j) \in \mathbb{R}^2 : 0 \leq t < 1\}$ (element)

$h_j := |x_{j+1} - x_j|$ (mesh size)

$\Gamma_h := \bigcup_{j=1}^n \Gamma_j$ (approximated boundary)

We assume that both parts Γ_D and Γ_N have only one connected component and that we have chosen our enumeration such that

$$\Gamma_{hD} := \bigcup_{j=1}^{k} \Gamma_j \qquad \text{and} \qquad \Gamma_{hN} := \bigcup_{j=k+1}^{n} \Gamma_j$$

approximate Γ_D and Γ_N, respectively, see Figure 3.1.

Piecewise constant approximation

We approximate the Cauchy data $(u,\, t) = (u_{|\Gamma},\, \frac{\partial u}{\partial n}|_\Gamma)$ by piecewise constant functions,

- $u(x) \approx u_j$ for $x \in \Gamma_j$ and $j = 1, \ldots, n$,

$$u_h(x) := \sum\nolimits_{j=1}^{n} u_j \, \chi_{\Gamma_j}(x) \qquad \text{for } x \in \Gamma_h \,,$$

- $t(x) \approx t_j$ for $x \in \Gamma_j$ and $j = 1, \ldots, n$,

$$t_h(x) := \sum\nolimits_{j=1}^{n} t_j \, \chi_{\Gamma_j}(x) \qquad \text{for } x \in \Gamma_h \,,$$

where χ_{Γ_j} is the characteristic function on Γ_h that equals 1 on Γ_j and 0 elsewhere.

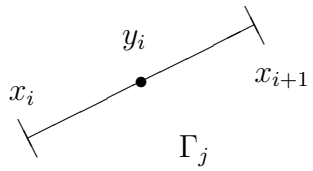
The values $u_1, \ldots, u_k$ (on Γ_{hD}) and $t_{k+1}, \ldots, t_n$ (on Γ_{hN}) are usually approximated from the known boundary data g_D and g_N, e. g.,

$$\begin{aligned} u_j &= \frac{1}{2}\big[g_D(x_j) + g_D(x_{j+1})\big] \qquad \text{for } j = 1, \ldots, k \text{ (on } \Gamma_{hD}), \\ t_j &= \frac{1}{2}\big[g_N(x_j) + g_N(x_{j+1})\big] \qquad \text{for } j = k+1, \ldots, n \text{ (on } \Gamma_{hN}). \end{aligned}$$

Collocation

Our boundary integral equation (3.2) cannot be fulfilled exactly, since this would lead to infinitely many equations for $k + (n - k) = n$ unknowns. Therefore, we choose a set of test points, the *collocation points* $\{y_j\}_{i=1,\ldots,n}$, e. g., chosen to be

$$y_i = \frac{1}{2}(x_i + x_{i+1}).$$



Evaluating (3.2) only at $\{y_i\}_{i=1,\ldots,n}$ we obtain a system of linear equations. With

$$\widetilde{b}_{ij} := \int_{\Gamma_j} \frac{\partial}{\partial n_x} U^*(x, y_i)\, ds_x, \qquad a_{ij} := \int_{\Gamma_j} U^*(x, y_i)\, ds_x,$$

the system reads

$$\forall i = 1, \ldots, k: \sum_{j=k+1}^{n} \widetilde{b}_{ij}\, u_j - \sum_{j=1}^{k} a_{ij}\, t_j = -\frac{1}{2}u_i - \sum_{j=1}^{k} \widetilde{b}_{ij}\, u_j + \sum_{j=k+1}^{n} a_{ij}\, t_j,$$

$$\forall i = k+1, \ldots, n: \frac{1}{2}\, u_j + \sum_{j=k+1}^{n} \widetilde{b}_{ij}\, u_j - \sum_{j=1}^{k} a_{ij}\, t_j = -\sum_{j=1}^{k} \widetilde{b}_{ij}\, u_j + \sum_{j=k+1}^{n} a_{ij}\, t_j.$$

With

$$b_{ij} := \frac{1}{2}\delta_{ij} + \widetilde{b}_{ij},$$

where $\delta_{ij} = 1$ if $i = j$ and else zero (Kronecker delta), the matrices

$$B_D = (b_{ij})_{\substack{1\le i\le n \\ 1\le j\le k}} \qquad B_N = (b_{ij})_{\substack{1\le i\le n \\ k+1\le j\le n}} \qquad A_D = (a_{ij})_{\substack{1\le i\le n \\ 1\le j\le k}} \qquad A_N = (a_{ij})_{\substack{1\le i\le n \\ k+1\le j\le n}}$$

and the vectors

$$u_D = (u_j)_{1\le j\le k} \quad u_N = (u_j)_{k+1\le j\le n} \quad t_D = (t_j)_{1\le j\le k} \quad t_N = (t_j)_{k+1\le j\le n}$$

we can write the system in the compact form

$$\underbrace{\big[B_N\big| - A_D\big]}_{=:C\in\mathbb{R}^{n\times n}} \begin{bmatrix} u_N \\ t_D \end{bmatrix} \;=\; \underbrace{\big[- B_D\big|A_N\big] \begin{bmatrix} u_D \\ t_N \end{bmatrix}}_{=:f\in\mathbb{R}^n} .$$

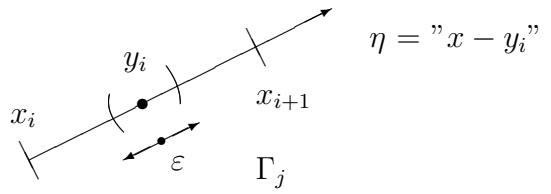
In general, the matrix C is *dense* and *non-symmetric*.

3.3 Computation of matrix entries in two dimensions

1. The diagonal entry a_{ii}

$$a_{ii} \;=\; \int_{\Gamma_i} U^*(x,\, y_i)\, ds_x \;=\; -\frac{1}{2\pi}\int_{\Gamma_i} \log|x-y_i|\, ds_x \;=\; -\frac{1}{2\pi}\int_{-|x_i-y_i|}^{|x_{i+1}-y_i|} \log|\eta|\, d\eta$$

where in the last step we have used the line integral parameterization sketched below.



We treat this as a weakly singular integral, i. e.,

$$\lim_{\varepsilon\to 0}\int_{\Gamma_i\setminus B_\varepsilon(y_i)} \log|x-y_i|\, ds_x$$

where $B_\varepsilon(y_i)$ is the open unit ball with center y_i and radius ε. This means, in the parameterized integral we have to exclude the region $[-\varepsilon,\varepsilon]$. Recall that $h_i = |x_{i+1}-x_i|$ and $y_i = \frac{1}{2}(x_i + x_{i+1})$. Thus,

$$|x_{i+1}-y_i| = |x_i - y_i| = \frac{h_i}{2}\,.$$

The integral with $[-\varepsilon, \varepsilon]$ being excluded equals the sum of the following two integrals,

$$\begin{aligned}\int_{\varepsilon}^{h_i/2} \log|\eta| d\eta &= \eta(\log\eta - 1)\Big|_{\varepsilon}^{h_i/2} = \frac{h_i}{2}\big(\log\frac{h_i}{2} - 1\big) - \varepsilon(\log\varepsilon - 1)\,,\\ \int_{-h_i/2}^{-\varepsilon} \log|\eta| d\eta &= \frac{h_i}{2}\big(\log\frac{h_i}{2} - 1\big) - \varepsilon(\log\varepsilon - 1)\,.\end{aligned}$$

Using de l'Hospital's theorem, one easily finds that

$$\lim_{\varepsilon\to 0} \varepsilon\log\varepsilon = \lim_{\varepsilon\to 0}\frac{\log\varepsilon}{\varepsilon^{-1}} = \frac{\text{“}-\infty\text{”}}{+\infty} = \lim_{\varepsilon\to 0}\frac{\varepsilon^{-1}}{-\varepsilon^{-2}} = \lim_{\varepsilon\to 0} -\varepsilon = 0\,.$$

Hence,

$$a_{ii} = -\frac{1}{2\pi} h_i\big(\log\frac{h_i}{2} - 2\big)\,.$$

2. The diagonal entry $\widetilde{b}_{ii}$

$$\widetilde{b}_{ii} = \int_{\Gamma_i} \frac{\partial}{\partial n_x} U^*(x,\, y_i)\, ds_x = -\frac{1}{2\pi}\int_{\Gamma_i}\frac{\partial}{\partial n_x}\log|x - y_i|\, ds_x$$

Using that $\frac{\partial v}{\partial n} = \nabla v \cdot n$ and $\nabla_x|x-y| = \nabla_x\sqrt{(x-y)\cdot(x-y)} = \frac{(x-y)}{|x-y|}$, we obtain

$$\widetilde{b}_{ii} = -\frac{1}{2\pi}\int_{\Gamma_i}\frac{1}{|x-y_i|}\frac{(x-y_i)}{|x-y_i|}\cdot n(x)\, ds_x$$

However, one easily sees that the normal vector is always perpendicular to the vector $x - y_i$, therefore

$$\widetilde{b}_{ii} = 0\,.$$

3. The off-diagonal entry a_{ij}, $i \neq j$ with x_j, x_{j+1}, y_i not collinear

We introduce a coordinate transformation, see Figure 3.2.

$$\left.\begin{aligned} a &= |z - y_i| \\ \cos\theta &= \frac{|z-y_i|}{|x-y_i|}\end{aligned}\right\} \implies |x - y_i| = \frac{a}{\cos\theta}$$

$$\begin{aligned}\eta &= a\,\tan\theta\\ ds_x = d\eta &\overset{(*)}{=} a\,\frac{d}{d\theta}\big(\tan\theta\big)\,d\theta = \frac{a}{\cos^2\theta}\,d\theta \overset{(**)}{=} a\,(1+\tan^2\theta)\,d\theta\end{aligned}$$

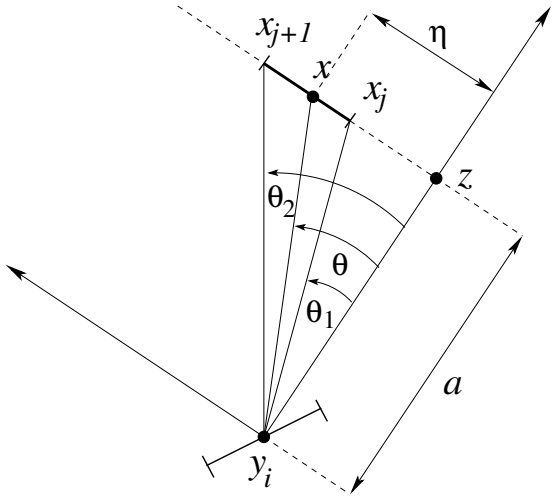
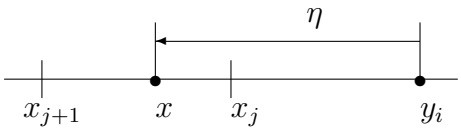


Figure 3.2: Coordinate transformation for Case 3.

$$
\begin{aligned}
a_{ij} &= -\frac{1}{2\pi}\int_{\Gamma_j} \log|x-y_i|\,ds_x \overset{(*)}{=} -\frac{a}{2\pi}\int_{\theta_1}^{\theta_2} \log\Big(\frac{a}{\cos\theta}\Big)\ \overset{\curvearrowleft}{\frac{d}{d\theta}}\ \big(\underbrace{\tan\theta}_{=\frac{\sin\theta}{\cos\theta}}\big)\,d\theta \\
&= -\frac{a}{2\pi}\Big[\log\Big(\frac{a}{\cos\theta}\Big)\,\tan\theta\Big]_{\theta_1}^{\theta_2} + \frac{a}{2\pi}\underbrace{\int_{\theta_1}^{\theta_2}\frac{\cos\theta}{a}\,\frac{(-a)\,(-\sin\theta)}{\cos^2\theta}\,\frac{\sin\theta}{\cos\theta}\,d\theta}_{=\ \int_{\theta_1}^{\theta_2}\tan^2\theta\,d\theta\ \overset{(**)}{=}\ \big[\tan\theta-\theta\big]_{\theta_1}^{\theta_2}} \\
&= -\frac{a}{2\pi}\Big\{\tan\theta\,\Big[\log\Big(\frac{a}{\cos\theta}\Big)-1\Big]+\theta\Big\}_{\theta_1}^{\theta_2}
\end{aligned}
$$

4. The off-diagonal entry a_{ij}, $i \neq j$ with x_j, x_{j+1}, y_i collinear

For simplicity we treat only the case that y_i is on the side of x_j, see the figure below, the other case is of course analogous.



Then,

$$a_{ij} \;=\; -\frac{1}{2\pi}\int_{|x_j-y_i|}^{|x_{j+1}-y_i|} \log|\eta|\,d\eta \;=\; -\frac{1}{2\pi}\Big[\eta\,(\log\eta-1)\Big]_{|x_j-y_i|}^{|x_{j+1}-y_i|}$$

5. The off-diagonal entry $\widetilde{b}_{ij}$, $i \neq j$

Using what we have already obtained in Case 2 we get

$$\widetilde{b}_{ij} \;=\; -\frac{1}{2\pi}\int_{\Gamma_j} \frac{(x-y_i)\cdot n(x)}{|x-y_i|^2}\,ds_x\,.$$

If x_j, x_{j+1}, and y_i are collinear, $n(x) \perp (x-y_i)$ and thus $\widetilde{b}_{ij}=0$. In the other case, we can use the coordinate transformation introduced in Case 3. There, $x-y_i=(a,\,\eta)^T$ and $|x-y_i|=\frac{a}{\cos\theta}$, the normal vector equals $(1,\,0)^T$, and $ds_x=\frac{a}{\cos^2\theta}\,d\theta$. Hence,

$$\widetilde{b}_{ij} \;=\; -\frac{1}{2\pi}\int_{\theta_1}^{\theta_2} \frac{a\cdot 1+\eta\cdot 0}{\frac{a^2}{\cos^2\theta}}\frac{a}{\cos^2\theta}\,d\theta \;=\; -\frac{1}{2\pi}\int_{\theta_0}^{\theta_1} d\theta \;=\; -\frac{1}{2\pi}(\theta_2-\theta_1)\,.$$

Remark 3.1. 1. We see that we can compute the entries of A, B analytically. However, the following numerical issues have to be taken into account: (i) one needs stable evaluations of the formulae, and (ii) the case distinction (e. g., the collinear test) must be done properly. Clearly, in implementations one needs to introduce relative criteria, taking the size of the domain/element into account.

2. In some rare situations, where the above issues cause problems, one may switch to numerical integration.

3. The matrix B represents the operator $\frac{1}{2}I+K$. If we have $\Gamma_D=\Gamma$ and $u_{|\Gamma}=1$, then $\frac{\partial u}{\partial n}=0$ because the solution is constant. Let $\mathbf{1}$ denote the constant function of value 1 on Γ. Then

$$(\frac{1}{2}I+K)\mathbf{1} \;=\; V\,\frac{\partial u}{\partial n} \;=\; 0\,.$$

This means $\mathbf{1}$ is in the kernel of $\frac{1}{2}I+K$. Often this property is also desired in the discrete setting. Let $\mathbb{1} := (1,\ldots,1)^T \in \mathbb{R}^n$. Then we would like to have

$$B\,\mathbb{1}=0$$

i. e., preserve the kernel of $\frac{1}{2}I + K$. This can be achieved by redefining

$$b_{ii} := -\sum_{j=1,\, j\neq i}^{n} b_{ij} \qquad \text{for } i = 1, \ldots, n\,,$$

which is known as the *row sum trick*. The values b_{ii} are then usually close to $\frac{1}{2}$.

Before we move to three-dimensional problems, we shortly summarize what we have obtained so far, and draw a comparison with a standard finite element method.

Summary of the collocation method

- Discretization of the boundary
- Generation of A, B, leading to the system $C \begin{bmatrix} u_N \\ t_D \end{bmatrix} = f$
- Solve the system
- Post-processing (optional), e. g., calculate some values $u(y)$ for $y \in \Omega$ using the representation formula.

Comparison with FEM

Assume that for both the boundary and the finite element method we have a quasi-uniform triangulation such that the mesh sizes fulfill

$$h \leq h_i \leq \widetilde{c}\, h \qquad \forall i$$

with a uniform constant $\widetilde{c} > 0$. Then for the BEM, the number of unknowns behaves as $n = \mathcal{O}(h^{-1})$ and for the FEM, the number of unknowns $N = \mathcal{O}(h^{-2})$. In the following table we assume that a direct solver for the FEM exploits the band structure of the stiffness matrix, and that we have an optimal iterative solver, like multi-level or multi-grid.

		direct		iterative	
2D	unknowns	mem	ops	mem	ops
FEM	$\mathcal{O}(h^{-2})$	$\mathcal{O}(h^{-3})$	$\mathcal{O}(h^{-4})$	$\mathcal{O}(h^{-2})$	$\mathcal{O}(h^{-2})$
BEM	$\mathcal{O}(h^{-1})$	$\mathcal{O}(h^{-2})$	$\mathcal{O}(h^{-3})$	$\mathcal{O}(h^{-2})$	$\geq \mathcal{O}(h^{-2})$?

In the table "mem" indicates the storage amount and "ops" the number of floating point operations. We see a clear advantage of BEM over FEM

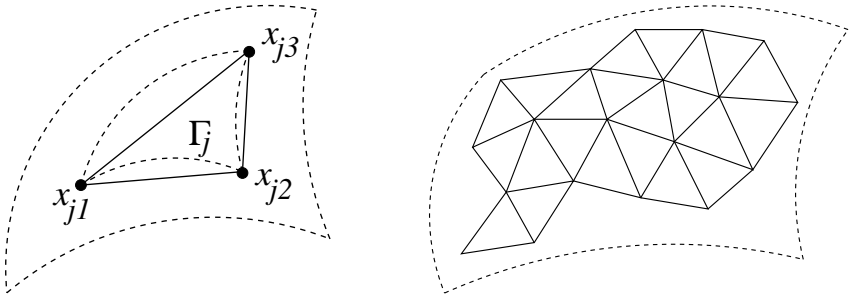


Figure 3.3: *Left:* plane triangular boundary element, *right:* part of a BEM mesh.

when using direct solvers. Since the BEM matrix C is dense, we need $\mathcal{O}(h^{-2})$ memory cells to store it and at least the same complexity to apply it. Using a fast BEM and approximating the matrix in some data-sparse form, the storage and computational complexity can be lowered to $\mathcal{O}(h^{-1}\log^{\alpha}(h^{-1}))$, which then outperforms the FEM, at least asymptotically.

3.4 Three-dimensional problems

Boundary discretization in three dimensions

In the three-dimensional case we approximate the boundary Γ by a triangulation

$$\Gamma_h = \bigcup_{i=1}^{n} \overline{\Gamma}_j$$

where each Γ_j is a plane, regular triangle with its vertices lying on Γ, see Figure 3.3.

Notation. The vertices of the triangles (the nodes of the triangulation) are denoted by x_i. The three nodes of a fixed triangle (element) Γ_j are denoted by x_{j1}, x_{j2}, and x_{j3}. For each triangle Γ_j we define the mesh size $h_i := |\Gamma_j|^{1/2}$.

Again we assume that the elements approximate the Dirichlet and Neumann part separately, and that we have an enumeration of the elements such that

$$\overline{\Gamma}_{hD} = \bigcup_{j=1}^{k} \overline{\Gamma}_j \qquad \text{and} \qquad \overline{\Gamma}_{hN} = \bigcup_{j=k+1}^{n} \overline{\Gamma}_j \,.$$

Piecewise constant approximation

Again, our variables are $(u,\, t) = (u_{|\Gamma},\, \frac{\partial u}{\partial n})$. We choose the approximations

$$\begin{aligned} u_h(x) &= \sum_{j=1}^{n} u_j\, \chi_{\Gamma_j}(x) \qquad \text{for } x \in \Gamma_h \text{ a.e.,} \\ t_h(x) &= \sum_{j=1}^{n} t_j\, \chi_{\Gamma_j}(x) \qquad \text{for } x \in \Gamma_h \text{ a.e.} \end{aligned}$$

The values $u_1, \ldots, u_k$ (on Γ_{hD}) and $t_{k+1}, \ldots, t_n$ (on Γ_{hN}) are usually constructed from the known boundary data g_D, g_N, e. g.,

$$\begin{aligned} u_j &= \frac{1}{3}\big[g_D(x_{j1}) + g_D(x_{j2}) + g_D(x_{j3})\big] \qquad \text{for } j = 1, \ldots, k\,, \\ t_j &= \frac{1}{3}\big[g_N(x_{j1}) + g_N(x_{j2}) + g_N(x_{j3})\big] \qquad \text{for } j = k+1, \ldots, n\,. \end{aligned}$$

Collocation

We choose n collocation points $\{y_i\}_{i=1}^n$, e. g., the center of gravity of each element,

$$y_i := \frac{1}{3}\big(x_{i1} + x_{i2} + x_{i3}\big)\,.$$

Evaluating (3.2) at these collocation points we obtain the linear system

$$\frac{1}{2}u_i + \sum_{j=1}^{n} u_j \underbrace{\int_{\Gamma_j} \frac{\partial}{\partial n_x} U^*(x,\, y)\, ds_x}_{=:\widetilde{b}_{ij}} - \sum_{j=1}^{n} t_j \underbrace{\int_{\Gamma_j} U^*(x,\, y)\, ds_x}_{=:a_{ij}} \;=\; 0\,.$$

In short, with $b_{ij} = \frac{1}{2}\delta_{ij} + \widetilde{b}_{ij}$, this can be written as $B\,u - A\,t = 0$. Splitting the matrices and vectors as before we get

$$\underbrace{\big[B_N \big| -A_D\big]}_{=:C} \begin{bmatrix} u_N \\ t_D \end{bmatrix} \;=\; \underbrace{\big[-B_D \big| A_N\big] \begin{bmatrix} u_D \\ t_N \end{bmatrix}}_{=:f}$$

Computation of the matrix entries a_{ij}, $\widetilde{b}_{ij}$

The integrals

$$a_{ij} \;=\; \frac{1}{4\pi} \int_{\Gamma_j} \frac{1}{|x - y_i|}\, ds_x$$

and

$$\widetilde{b}_{ij} \;=\; \frac{1}{4\pi}\int_{\Gamma_j} \frac{\partial}{\partial n_n}\frac{1}{|x-y_i|}\,ds_x \;=\; -\frac{1}{4\pi}\int_{\Gamma_j} \frac{(x-y_i)\cdot n(x)}{|x-y_i|^3}\,ds_x$$

can be computed analytically and several cases have to be taken into account. As in two dimensions, numerical integration is sometimes chosen as an alternative. Also, $\widetilde{b}_{ii} = 0$ (because $y_i \in \Gamma_i$) but one can use the row sum trick to preserve the kernel of $\frac{1}{2}I + K$.

Comparison with FEM

We assume shape-regular, quasi-uniform triangulations of Ω and Γ. This means in particular for the boundary element mesh that $h \le h_j \le \widetilde{C}\,h$ and that the radius of the largest inscribed circle of each boundary element is comparable to h_j, i. e., the triangles do not degenerate. Then $n = \mathcal{O}(h^{-2})$. For the finite element method the number of unknowns behaves then as $\mathcal{O}(h^{-3})$. Since the BEM system matrix C is dense, we need $\mathcal{O}(h^{-4})$ memory cells to store it. Assuming again that a direct solver for FEM exploits the band structure of the stiffness matrix, and that we have an optimal iterative FEM solver (multi-level or multi-grid), the comparison reads as follows.

		direct		iterative	
3D	unknowns	mem	ops	mem	ops
FEM	$\mathcal{O}(h^{-3})$	$\mathcal{O}(h^{-5})$	$\mathcal{O}(h^{-7})$	$\mathcal{O}(h^{-3})$	$\mathcal{O}(h^{-3})$
BEM	$\mathcal{O}(h^{-2})$	$\mathcal{O}(h^{-4})$	$\mathcal{O}(h^{-6})$	$\mathcal{O}(h^{-4})$	$\ge \mathcal{O}(h^{-4})$?

As in two dimensions, direct solvers for BEM have a better complexity than those for the FEM, however, it is not really satisfactory. Using dense BEM matrices, no iterative method can outperform optimal iterative methods for FEM, because the storage amount is already larger than for FEM. Using fast BEM and good preconditioners, both the storage and computational complexity can be lowered to $\mathcal{O}(h^{-2}\log^{\alpha} h^{-2})$.

Chapter 4

Boundary integral operators

In this chapter we first introduce Sobolev spaces on the computational domain and its boundary and briefly give some important results on these. Then we derive and prove a representation formula for functions in the Sobolev space H^1 that satisfy a Poisson equation in weak sense. As briefly outlined in Remark 2.11, we will do this on the whole space $\mathbb{R}^d$ and allow the function to be discontinuous across the boundary (and only there). This technique is summarized under the keyword *transmission property*. The discontinuity will require the use of some distributional spaces that we will also introduce in the following first section. The representation formula that we derive can be expressed in terms of so-called *volume* and *surface potentials* which involve the fundamental solution. Taking traces of these potentials we obtain boundary integral operators and two boundary integral equations which relate the Cauchy data, i. e., the trace and the normal derivative. Finally, we show some properties of the boundary integral operators.

4.1 Sobolev spaces and distributions

In this section we try to be self-contained at the risk of repeating earlier lectures. The proofs of the following results are omitted. Most of them can be found in standard textbooks, and for all of them proofs or references to proofs are found in [Steinbach].

Recall that Ω is always assumed to be a Lipschitz domain. As stated before, Ω can therefore be the (bounded) interior of its boundary, or its (unbounded) exterior. For the following Sobolev spaces defined on Ω, we can also replace Ω by $\mathbb{R}^d$.

Definition 4.1. (i) We define

$$L^1_{\mathrm{loc}}(\Omega) := \{u : \Omega \to \mathbb{R} : |u| \text{ is integrable over every compact set in } \Omega\}.$$

Given $u \in L^1_{\mathrm{loc}}(\Omega)$, a function $v \in L^1_{\mathrm{loc}}(\Omega)$ is called *weak derivative* of u with respect to x_i if

$$\int_\Omega v\,\varphi\,dx \;=\; -\int_\Omega u\,\frac{\partial\varphi}{\partial x_i}\,dx \qquad \forall\varphi \in C_0^\infty(\Omega)\,.$$

We write $v = \frac{\partial u}{\partial x_i}$. Higher derivatives are defined recursively.

(ii) For $k \in \mathbb{N}_0$ we define

$$H^k(\Omega) := \left\{u \in L^2(\Omega) : \forall\alpha,\, |\alpha| \le k : \partial^\alpha u \in L^2(\Omega)\right\},$$

equipped with the norm

$$\|u\|_{H^k(\Omega)} := \Big(\sum_{|\alpha|\le k} \|\partial^\alpha u\|^2_{L^2(\Omega)}\Big)^{1/2}.$$

(iii) For $s \in \mathbb{R}$ let $\lfloor s\rfloor$ denote the largest integer smaller than s. For $s = \lfloor s\rfloor + \sigma \in \mathbb{R}^+$ with $\sigma \in (0,\,1)$ we define

$$H^s(\Omega) := \left\{u \in H^{\lfloor s\rfloor}(\Omega) : \|u\|_{H^s(\Omega)} < \infty\right\},$$

equipped with the norm

$$\|u\|_{H^s(\Omega)} := \Big(\|u\|^2_{H^{\lfloor s\rfloor}(\Omega)} + \sum_{|\alpha|\le\lfloor s\rfloor} \int_\Omega\int_\Omega \frac{|\partial^\alpha u(x) - \partial^\alpha u(y)|^2}{|x-y|^{d+2\sigma}}\,dx\,dy\Big)^{1/2}.$$

(iv) For $s \in \mathbb{R}^+_0$ we define

$$H^s_0(\Omega) := \overline{C_0^\infty(\Omega)}^{\|\cdot\|_{H^s(\Omega)}} \qquad \text{and} \qquad H^{-s}(\Omega) := \left[H^s_0(\Omega)\right]^*,$$

i. e., $H^s_0(\Omega)$ is the closure of $C_0^\infty(\Omega)$ with respect to the norm $\|\cdot\|_{H^s(\Omega)}$, and $H^{-s}(\Omega)$ is the dual space of $H^s_0(\Omega)$, equipped with the usual dual norm. We will sometimes also use $H^s(\Omega)^*$, the dual of $H^s(\Omega)$. Then, $H^s(\Omega)^* \subset H^{-s}(\Omega)$ for $s \ge 0$.

It can be shown that all of these spaces own an inner product and that they are complete, i. e., they are Hilbert spaces. One can also show that provided Ω is compact then $C^\infty(\overline{\Omega})$ is dense in $H^s(\Omega)$ for all $s \ge 0$. Note that sometimes in the literature, the spaces $H^s(\Omega)$ are defined via the Fourier transform. For Lipschitz domains, however, the definition can be shown to be equivalent to the one above.

Remark 4.2. 1. Recall if Ω is Lipschitz then $\Gamma = \partial\Omega$ has a surface measure (s). Therefore,

$$L^2(\Gamma) := \left\{ u : \Gamma \to \mathbb{R} : \int_\Gamma |u|^2 \, ds < \infty \right\}$$

is well-defined. With the inner product $(u,\, v)_{L^2(\Gamma)} := \int_\Gamma u\, v \, ds$ it can be shown to be a Hilbert space.

2. As an alternative definition, we can also parameterize Γ using J sufficiently smooth and bijective functions $\chi_i : \tau_i \to \Gamma_i$ with a smooth parameter domain $\tau_i \subset \mathbb{R}^{d-1}$, such that $\Gamma = \bigcup_{i=1}^J \Gamma_i$. Then we can define

$$L^2_{\chi_i}(\Gamma_i) := \left\{ u : \Gamma_i \to \mathbb{R} : \widetilde{u} := u \circ \chi_i \in L^2(\tau_i) \right\},$$

equipped with the norm $\|u\|_{L^2_{\chi_i}} := \|\widetilde{u}\|_{L^2(\tau_i)}$. Using suitable partition of unity functions this can be used to give an alternative definition of $L^2(\Gamma)$ which can be shown to be equivalent to the one above. The concept of parameterization and partition of unity would be suitable to define $H^s(\Gamma)$ for $s \geq 0$. However, we will mainly work in $H^{1/2}(\Gamma)$ and use the alternative definition below.

Definition 4.3. (i) For $\sigma \in (0,\, 1)$ we define

$$H^\sigma(\Gamma) := \left\{ u \in L^2(\Gamma) : \|u\|_{H^\sigma(\Gamma)} < \infty \right\}$$

with the Sobolev-Slobodeckij norm

$$\|u\|_{H^\sigma(\Gamma)} := \left(\|u\|^2_{L^2(\Gamma)} + \int_\Gamma \int_\Gamma \frac{|u(x) - u(y)|^2}{|x-y|^{d-1+2\sigma}} \, ds_x \, ds_y \right)^{1/2}.$$

(ii) Note that $\overline{C_0^\infty(\Gamma)}^{\|\cdot\|_{H^\sigma(\Gamma)}} = H^\sigma(\Gamma)$ since Γ is a closed manifold. We define

$$H^{-\sigma}(\Gamma) := \left[H^\sigma(\Gamma) \right]^*.$$

Remark 4.4. 1. For the definition of higher order Sobolev spaces on Γ, we can either use parameterization and partition of unity (see the remark before) or tangential derivatives. These definitions are in general not equivalent, unless the boundary is sufficiently smooth, $\Gamma \in C^{\lfloor s \rfloor, 1}$.

2. For an open sub-manifold $\widetilde{\Gamma} \subset \Gamma$, the space $L^2(\widetilde{\Gamma})$ is well-defined and we can also define $H^\sigma(\widetilde{\Gamma})$ for $\sigma \in (0,\, 1)$ analogous to Definition 4.3. Then, $\overline{C_0^\infty(\widetilde{\Gamma})}^{\|\cdot\|_{H^\sigma(\widetilde{\Gamma})}} = H^\sigma(\widetilde{\Gamma})$ if $\sigma \in [0,\, \frac{1}{2}]$, otherwise the spaces differ from each other.

Theorem 4.5 (Trace theorem)**.** *The trace operator*

$$\gamma_0 : C^\infty(\overline{\Omega}) \to C^\infty(\Gamma) : u \mapsto u_{|\Gamma}$$

has a unique extension to a continuous linear operator

$$\gamma_0 : H^1(\Omega) \to H^{1/2}(\Gamma)\,,$$

i. e., there exists a constant $c_T > 0$ such that

$$\|\gamma_0 u\|_{H^{1/2}(\Gamma)} \;\leq\; c_T\; \|u\|_{H^1(\Omega)} \qquad \forall u \in H^1(\Omega)\,.$$

Furthermore, there exists a continuous linear operator

$$\mathcal{E} : H^{1/2}(\Gamma) \to H^1(\Omega) \qquad \textit{with} \qquad \gamma_0 \mathcal{E} w = w \quad \forall w \in H^{1/2}(\Gamma)\,,$$

i. e., there exists a constant $c_{IT} > 0$ such that

$$\|\mathcal{E} w\|_{H^1(\Omega)} \;\leq\; c_{IT}\; \|w\|_{H^{1/2}(\Gamma)} \qquad \forall w \in H^{1/2}(\Gamma)\,.$$

The operator $\mathcal{E}$ is often called extension operator *and is obviously a* right inverse *of γ_0.*

Remark 4.6. The above lemma basically states that $H^{1/2}(\Gamma)$ is the trace space of $H^1(\Omega)$. For higher order Sobolev spaces we have the following result. If $\Gamma \in C^{k-1,1}$ then

$$\gamma_0 : H^s(\Omega) \to H^{s-1/2}(\Gamma) \qquad \forall s \in (\tfrac{1}{2},\, k]\,.$$

If Γ is the boundary of a Lipschitz domain the same holds even for $s \in (\frac{1}{2},\, \frac{3}{2})$.

The next lemma characterizes $H^1_0(\Omega)$ to consist of the H^1-functions with vanishing trace (which is a-priori not clear).

Lemma 4.7. *(i)* $H^1_0(\Omega) \;=\; \big\{u \in H^1(\Omega) : \gamma_0 u = 0\big\}$.

(ii) The norm

$$|\!|\!| u |\!|\!|_{H^{1/2}(\Gamma)} := \inf_{\substack{\widetilde{u} \in H^1(\Omega) \\ \gamma_0 \widetilde{u} = u}} \|\widetilde{u}\|_{H^1(\Omega)}$$

is well-defined and equivalent to $\|\cdot\|_{H^{1/2}(\Gamma)}$.

The second part of the above lemma states that the norm of the minimal extension is equivalent to the $H^{1/2}$ norm. Indeed the *minimum* is attained. The operator $\mathbb{E}$ in the trace theorem does not necessarily give this minimum. For convenience, if it is clear from the context, we may sometimes write $u_{|\Gamma}$ or even u instead of $\gamma_0 u$.

Finally, we introduce some distributional spaces. In the following definitions the domain Ω can be replaced by its complement $\mathbb{R}^d \setminus \overline{\Omega}$ or by $\mathbb{R}^d$.

Definition 4.8. (i) Recall that $\mathcal{D}(\Omega)$ is the space $C_0^\infty(\Omega)$ equipped with the sequential convergence, where

$$\varphi_n \to 0 \text{ sequentially } \iff \forall K \subset\subset \Omega\ \forall \alpha : \partial^\alpha \varphi_n \to 0 \text{ uniformly in } K\,.$$

$\mathcal{D}'(\Omega)$ is the dual of $\mathcal{D}(\Omega)$, where the definition of the continuity (which is necessary for defining the dual space) is not based on a norm but on the sequential convergence only.

(ii) We define $\mathcal{E}(\Omega)$ to be the space $C^\infty(\Omega)$ equipped with the sequential convergence (defined exactly as above).

(iii) We define the Schwartz space of *rapidly decreasing functions*

$$\mathcal{S}(\mathbb{R}^d) := \big\{\varphi \in C^\infty(\Omega) : \sup_{x\in\mathbb{R}^d} |x^\alpha\,(\partial^\beta\varphi)(x)| < \infty \quad \forall \text{ multi-indices } \alpha,\, \beta\big\}\,.$$

Above, for a multi-index $\alpha = (\alpha_1, \ldots, \alpha_d)$ we have used the notation $x^\alpha = x_1^{\alpha_1}\, x_2^{\alpha_2} \cdots x_d^{\alpha_d}$. Functions in the above Schwartz space and their derivatives decrease faster than any polynomial. We equip $\mathcal{S}(\mathbb{R}^d)$ with the following sequential convergence,

$$\varphi_n \to 0 \text{ sequentially } \iff \forall \alpha,\, \beta : x^\alpha(\partial^\beta\varphi_n) \to 0 \text{ uniformly in } \mathbb{R}^d\,.$$

With this convergence, we can define the dual $\mathcal{S}'(\mathbb{R}^d)$, which is called the space of *temperate distributions*.

Example 4.9. Whereas it is easy to imagine functions in $\mathcal{D}(\Omega)$ and functions which lie only in $\mathcal{E}(\Omega)$ (not having compact support), it is not a-priori clear if there exist functions that lie in $\mathcal{S}(\mathbb{R}^d)$ but not in $\mathcal{D}(\mathbb{R}^d)$. However,

$$\varphi(x) := e^{-|x|^2} \qquad \Longrightarrow \qquad \varphi \in \mathcal{S}(\mathbb{R}^d)\,.$$

Lemma 4.10. *The following statements hold.*
$\mathcal{D}(\mathbb{R}^d) \subset \mathcal{S}(\mathbb{R}^d) \subset \mathcal{E}(\mathbb{R}^d)$
$\mathcal{E}'(\mathbb{R}^d) \subset \mathcal{S}'(\mathbb{R}^d) \subset \mathcal{D}'(\mathbb{R}^d)$
$\mathcal{S}(\mathbb{R}^d) \subset H^s(\mathbb{R}^d) \qquad \forall s \geq 0$

Note, that *any* derivative of a distribution is again a distribution. Assume that $u \in \mathcal{D}'(\Omega)$, then we can define $\frac{\partial u}{\partial x_i}$ by

$$\langle \frac{\partial u}{\partial x_i},\, \varphi\rangle := -\langle u,\, \frac{\partial \varphi}{\partial x_i}\rangle \qquad \text{for } \varphi \in \mathcal{D}(\Omega)\,.$$

If u is a regular distribution, the distributional derivative coincides with the weak derivative. This concept works similarly for $\mathcal{E}'(\Omega)$ and $\mathcal{S}'(\mathbb{R}^d)$.

4.2 Green's identities revisited

In this section we first derive Green's first identity for $H^2(\Omega)$. Then we introduce a generalization of the normal derivative, which allows us to have Green's first identity in the larger space $H^1(\Omega)$.

First, recall that for a function $u \in H^2(\Omega)$, its normal derivative is well-defined in the sense that

$$\frac{\partial u}{\partial n} \;=\; \underbrace{(\gamma_0 \nabla u)}_{\in H^{1/2}(\Gamma)^d} \cdot n \,.$$

Depending on the smoothness of the boundary this function is piecewise smooth. In any case we can integrate it because due to Cauchy-Schwarz,

$$\int_\Gamma \frac{\partial u}{\partial n}\, ds \;\leq\; \int_\Gamma |(\gamma_0 \nabla u)| \underbrace{|n|}_{=1}\, ds \;<\; \infty \,.$$

Lemma 4.11. *For $u \in H^2(\Omega)$ and $v \in H^1(\Omega)$ we have Green's first formula,*

$$\int_\Omega \nabla u \cdot \nabla v \, dx \;=\; \int_\Omega (-\Delta u)\, v \, dx + \int_\Gamma \frac{\partial u}{\partial n}\, v \, ds \,.$$

Proof. With the same arguments as above the boundary integral in the assertion of the lemma is well-defined. First, we note that the formula holds for u, $v \in C^\infty(\overline{\Omega})$. Secondly, all expressions are well-defined and continuous with respect to $\|u\|_{H^2(\Omega)}$ and $\|v\|_{H^1(\Omega)}$. For instance, $\int_\Omega \nabla u \cdot \nabla v \, dx$ is linear and continuous in both u and v, as

$$\int_\Omega \nabla u \cdot \nabla v \, dx \;\leq\; \|\nabla u\|_{L^2(\Omega)} \, \|\nabla v\|_{L^2(\Omega)} \;\leq\; \|u\|_{H^2(\Omega)} \, \|v\|_{H^1(\Omega)}$$

implies that if u or v converges to zero, also the expression converges to zero. Finally, since $C^\infty(\overline{\Omega})$ is dense in $H^s(\Omega)$ the closuring principle implies the identity: u and v can be approximated by sequences u_n, $v_n \in C^\infty(\overline{\Omega})$ and the identity holds as well for the limit. □

It can be shown that for $u \in H^2(\Omega)$, $\frac{\partial u}{\partial n} \in H^{-1/2}(\Gamma)$. The next lemma states that we can generalize the definition of the normal derivative to less regular functions such that Green's first identity still holds.

Lemma 4.12. *Suppose that $u \in H^1(\Omega)$ and $\Delta u \in L^2(\Omega)$. Then there exists a unique linear and continuous form $g \in H^{-1/2}(\Gamma)$ such that*

$$\int_\Omega \nabla u \cdot \nabla v \, dx \;=\; \int_\Omega (-\Delta u)\, v \, dx + \langle g,\, \gamma_0 v \rangle \qquad \forall v \in H^1(\Omega) \,.$$

Moreover

$$\|g\|_{H^{-1/2}(\Gamma)} \;\leq\; c_{IT}\left\{|u|_{H^1(\Omega)} + \|\Delta u\|_{L^2(\Omega)}\right\}.$$

Proof. First, recall that $\langle\cdot,\,\cdot\rangle$ above denotes the dual pairing between $H^{-1/2}(\Gamma)$ and $H^{1/2}(\Gamma)$. Sometimes we will write $\langle\cdot,\,\cdot\rangle_\Gamma$ in order to emphasize the manifold under consideration. Note also that $\Delta u \in L^2(\Omega)$ means that the distributional Laplacian of u is in $L^2(\Omega)$. By the trace theorem we have $\gamma_0\mathcal{E}w = w$ for all $w \in H^{1/2}(\Gamma)$. We define $g \in H^{-1/2}(\Gamma)$ by

$$\langle g,\, w\rangle = \int_\Omega \nabla u\cdot\nabla(\mathcal{E}w)\,dx + \int_\Omega (\Delta u)\,\mathcal{E}w\,dx \qquad \text{for } w \in H^{1/2}(\Gamma)\,.$$

Obviously, g is well-defined and really in $H^{-1/2}(\Gamma)$. We first show that this g fulfills the identity stated in the lemma. In a second step we will show that g is unique.

Let $v \in H^1(\Omega)$ and set $v_0 := v - \mathcal{E}\gamma_0 v$. Then, by the trace theorem, $\gamma_0 v_0 = 0$ and thus, $v_0 \in H^1_0(\Omega)$ due to Lemma 4.7. Since $C_0^\infty(\Omega)$ is dense in $H^1_0(\Omega)$, we can approximate v_0 by a sequence $(\varphi_n) \in C_0^\infty(\Omega)$ such that $\varphi_n \to v_0$ in the H^1-norm. Using this sequence we can conclude from the definition of the distributional derivatives of u that

$$\int_\Omega \nabla u\cdot\nabla v_0\,dx = \lim_{n\to\infty}\int_\Omega \nabla u\cdot\nabla\varphi_n\,dx = \lim_{n\to\infty}\int_\Omega (-\Delta u)\,\varphi_n\,dx = \int_\Omega (-\Delta u)\,v_0\,dx\,.$$

From this identity and the definition of g we can conclude that

$$\begin{aligned}
\int_\Omega \nabla u\cdot\nabla v\,dx \;&=\; \int_\Omega \nabla u\cdot\nabla(v_0 + \mathcal{E}\gamma_0 v)\,dx\\
&=\; \int_\Omega \nabla u\cdot\nabla v_0\,dx + \int_\Omega \nabla u\cdot\nabla(\mathcal{E}\gamma_0 v)\,dx\\
&=\; \int_\Omega (-\Delta u)\,v_0\,dx + \langle g,\,\gamma_0 v\rangle - \int_\Omega (\Delta u)\,\mathcal{E}\gamma_0 v\,dx\\
&=\; \int_\Omega (-\Delta u)\,v\,dx + \langle g,\,\gamma_0 v\rangle\,.
\end{aligned}$$

Assume now that $g_1,\, g_2 \in H^{-1/2}(\Gamma)$ meet the requirements of the lemma. Then the above identities imply that

$$\langle g_2 - g_1,\,\gamma_0 v\rangle \;=\; 0 \qquad \forall v \in H^1(\Omega)\,.$$

However, $\gamma_0 : H^1(\Omega) \to H^{1/2}(\Gamma)$ is surjective. Hence,

$$\langle g_2 - g_1,\, w\rangle \;=\; 0 \quad \forall w \in H^{1/2}(\Gamma) \qquad\Longrightarrow\qquad g_2 \;=\; g_1\,,$$

which means that g is unique.

Finally, we show that g is bounded in terms of u. The definition of g, the trace theorem, and the Cauchy-Schwarz inequality yield

$$\begin{aligned}
\|g\|_{H^{-1/2}(\Gamma)} &= \sup_{v\in H^{1/2}(\Gamma)\setminus\{0\}} \frac{|\langle g,\, v\rangle|}{\|v\|_{H^{1/2}(\Gamma)}} \\
&\leq \sup_{v\in H^{1/2}(\Gamma)\setminus\{0\}} \frac{1}{c_{IT}^{-1}\,\|\mathcal{E}v\|_{H^1(\Omega)}} \Big| \int_\Omega \nabla u\cdot\nabla(\mathcal{E}v)\,dx + \int_\Omega \Delta u(\mathcal{E}v)\,dx\Big| \\
&\leq \sup_{v\in H^{1/2}(\Gamma)\setminus\{0\}} \frac{c_{IT}}{\|\mathcal{E}v\|_{H^1(\Omega)}} \Big\{ |u|_{H^1(\Omega)}\,|\mathcal{E}v|_{H^1(\Omega)} + \|\nabla u\|_{L^2(\Omega)}\,\|\mathcal{E}v\|_{L^2(\Omega)}\Big\}\,.
\end{aligned}$$

Since $|\mathcal{E}v|_{H^1(\Omega)} \leq \|\mathcal{E}v\|_{H^1(\Omega)}$ and $\|\mathcal{E}v\|_{L^2(\Omega)} \leq \|\mathcal{E}v\|_{H^1(\Omega)}$ the denominator finally cancels and we obtain the desired bound for $\|g\|_{H^{-1/2}(\Gamma)}$. □

Corollary 4.13. *Let $u \in H^1(\Omega)$ and $f \in H^1(\Omega)^*$ such that $-\Delta u = f$ weakly in Ω, i. e.,*

$$\int_\Omega \nabla u\cdot\nabla\varphi\,dx \;=\; \langle f,\,\varphi\rangle \qquad \forall\varphi\in D(\Omega)\,.$$

Then there exists a unique linear form $g \in H^{-1/2}(\Gamma)$ such that

$$\int_\Omega \nabla u\cdot\nabla v\,dx \;=\; \langle f,\,v\rangle_\Omega + \langle g,\,v\rangle_\Gamma \qquad \forall v\in H^1(\Omega)\,.$$

Moreover,

$$\|g\|_{H^{-1/2}(\Gamma)} \;\leq\; c_{IT}\Big\{|u|_{H^1(\Omega)} + \|f\|_{H^1(\Omega)^*}\Big\}$$

Proof. The proof follows the line of the proof of Lemma 4.12, except that we replace $\int_\Omega(\Delta u)\,\mathcal{E}v\,dx$ by $-\langle f,\,\mathcal{E}v\rangle$ and we use the above assumptions as well as the fact that the linear form f is continuous. □

Note that g in Lemma 4.12 depends on u and on Δu. In Corollary 4.13 it depends on u and on f which is somehow $-\Delta u$. Since the identities generalize Green's first identity, we write

$$\gamma_1 u := \; g\,,$$

being aware that we can only use this operator when $\Delta u \in L^2(\Omega)$ or if u fulfills a weak Poisson equation. Occasionally, we may also write $\frac{\partial u}{\partial n} := g$. With the definitions of g and the bounds in terms of u, Δu, and f, we see that the *operator* γ_1 is linear and continuous. The following examples illustrate this generalized normal derivative.

Example 4.14. 1. We consider a pure Dirichlet problem with $f \in L^2(\Omega)$. Starting from the classical formulation

$$-\Delta u \;=\; f \quad \text{in } \Omega, \qquad u \;=\; 0 \quad \text{on } \Gamma$$

we derive as usual that we wish to find $u \in H^1_0(\Omega)$ satisfying

$$-\Delta u \;=\; f \qquad \text{weakly in } \Omega\,.$$

The normal derivative $\gamma_1 u$ is then characterized by the identity

$$\langle \gamma_1 u,\, w\rangle \;=\; \int_\Omega \nabla u \cdot \nabla(\mathcal{E} w)\, dx - \int_\Omega f\,(\mathcal{E} w)\, dx \qquad \text{for } w \in H^{1/2}(\Gamma)\,,$$

and it is independent of the choice of the extension $\mathcal{E}$ as long it fulfills the requirements from the trace theorem.

2. We now consider a pure Neumann problem with $f \in L^2(\Omega)$ and $g_N \in H^{-1/2}(\Gamma)$. Staring from the classical formulation

$$-\Delta u \;=\; f \quad \text{in } \Omega, \qquad \frac{\partial u}{\partial n} \;=\; g_N \quad \text{on } \Gamma$$

we look for a function $u \in H^1(\Omega)$ that satisfies

$$-\Delta u \;=\; f \qquad \text{weakly in } \Omega\,.$$

Due to Lemma 4.12, u has a normal derivative $\gamma_1 u \in H^{-1/2}(\Gamma)$ defined by

$$\langle \gamma_1 u,\, \gamma_0 v\rangle \;=\; \int_\Omega \nabla u \cdot \nabla v\, dx - \int_\Omega f\, v\, dx \qquad \forall v \in H^1(\Omega)\,.$$

Requiring that $\gamma_1 u = g_N$ in the sense of $H^{-1/2}(\Gamma)$ this yields to the equation

$$\int_\Omega \nabla u \cdot \nabla v\, dx \;=\; \int_\Omega f\, v\, dx + \langle g_N,\, v\rangle \qquad \forall v \in H^1(\Omega)\,,$$

which is the usual variational formulation for the pure Neumann problem.

3. Later on we will mostly consider the case $f = 0$, for which Corollary 4.13 is not needed. *For advanced readers only:* assume that $f \in H^1(\Omega)^*$ is defined by

$$\langle f,\, v\rangle := \int_\Omega f_1\, v\, dx + \langle f_2,\, \gamma_0 v\rangle_\Gamma \qquad \text{for } v \in H^1(\Omega)\,,$$

with $f_1 \in L^2(\Omega)$ and $f_2 \in H^{-1/2}(\Gamma)$. Then

$$\langle g,\, w\rangle = \int_\Omega \nabla u \cdot \nabla(\mathcal{E}w)\, dx - \int_\Omega f_1\, \mathcal{E}w\, dx - \langle f_2,\, w\rangle \qquad \forall w \in H^{1/2}(\Gamma)\,,$$

which implies the Green type identity

$$\int_\Omega \nabla u \cdot \nabla v\, dx \;=\; \int_\Omega f_1\, v\, dx + \langle f_2 + g,\, \gamma_0 v\rangle_\Gamma \qquad \forall v \in H^1(\Omega)\,.$$

In that sense g equals to what is needed to *complete* Green's identity.

4.3 The transmission property

In this subsection we derive the prerequisites for the representation formula, Green's third identity.

Assume first that Ω is bounded and define by $\Omega^{\rm ext} := \mathbb{R}^d \setminus \overline{\Omega}$ its complement, also called the *exterior domain*. Recall, that since Ω is Lipschitz also $\Omega^{\rm ext}$ is Lipschitz, that the Sobolev spaces $H^s(\Omega^{\rm ext})$ are well-defined and that $H^{1/2}(\Gamma)$ is the trace space of $H^1(\Omega^{\rm ext})$ as well. In order to emphasize expressions related to Ω, the *interior* of Γ, we write

$$\Omega^{\rm int} := \Omega, \qquad \gamma_0^{\rm int} := \gamma_0, \qquad \gamma_1^{\rm int} := \gamma_1\,.$$

When applying the trace theorem, Lemma 4.12, and Corollary 4.13 on $\Omega^{\rm ext}$ we obtain trace operators $\gamma_0^{\rm ext}$ and $\gamma_1^{\rm ext}$. To this end we consider a function $u \in H^1(\Omega^{\rm int} \cup \Omega^{\rm ext})$, where

$$H^1(\Omega^{\rm int} \cup \Omega^{\rm ext}) := \{u \in L^2(\mathbb{R}^d) : u_{|\Omega^{\rm int}} \in H^1(\Omega^{\rm int}),\, u_{|\Omega^{\rm ext}} \in H^1(\Omega^{\rm ext})\}\,.$$

Moreover, assume that

$$\begin{aligned} -\Delta u &= f^{\rm int} \qquad \text{weakly in } \Omega^{\rm int}\,,\\ -\Delta u &= f^{\rm ext} \qquad \text{weakly in } \Omega^{\rm ext}\,, \end{aligned} \tag{4.1}$$

for some linear forms $f^{\rm int} \in H^1(\Omega^{\rm int})^*$ and $f^{\rm ext} \in H^1(\Omega^{\rm ext})^*$. Then, by slightly modifying Corollary 4.13, we have

$$\begin{aligned} \int_{\Omega^{\rm int}} \nabla u \cdot \nabla v\, dx &= \langle f^{\rm int},\, v\rangle + \langle \gamma_1^{\rm int} u,\, \gamma_0^{\rm int} v\rangle \qquad \forall v \in H^1(\Omega^{\rm int})\,,\\ \int_{\Omega^{\rm ext}} \nabla u \cdot \nabla v\, dx &= \langle f^{\rm ext},\, v\rangle - \langle \gamma_1^{\rm ext} u,\, \gamma_0^{\rm ext} v\rangle \qquad \forall v \in H^1(\Omega^{\rm ext})\,. \end{aligned} \tag{4.2}$$

Note the sign flip in the second line. Here, $\gamma_1^{\rm ext} u$ generalizes $\frac{\partial u}{\partial n}$ with n being the *outward* unit normal vector to Γ, i. e., *inward* with respect to $\Omega^{\rm ext}$.

Definition 4.15. Suppose that $u \in H^1(\Omega^{\text{int}} \cup \Omega^{\text{ext}})$ such that (4.1) holds. Then we define

$$\begin{aligned} f \in H^1(\mathbb{R}^d)^* : \ \langle f,\, v\rangle \ &= \ \langle f^{\text{int}},\, v_{|\Omega^{\text{int}}}\rangle + \langle f^{\text{ext}},\, v_{|\Omega^{\text{ext}}}\rangle \qquad \text{for } v \in H^1(\mathbb{R}^d)\,, \\ [\gamma_0 u] &:= \ \gamma_0^{\text{ext}} u - \gamma_0^{\text{int}} u \quad \in H^{1/2}(\Gamma)\,, \\ [\gamma_1 u] &:= \ \gamma_1^{\text{ext}} u - \gamma_1^{\text{int}} u \quad \in H^{-1/2}(\Gamma)\,. \end{aligned}$$

We refer to $[\gamma_0 u]$ and $[\gamma_1 u]$ as the *jump* of the trace and the normal derivative, respectively. If $[\gamma_0 v] = 0$ (which is the case if $v \in H^1(\mathbb{R}^d)$) we have $\gamma_0 v = \gamma_0^{\text{int}} v = \gamma_0^{\text{ext}} v$.

Using the above definitions we can conclude from (4.2) that

$$\int_{\Omega^{\text{int}}} \nabla u \cdot \nabla v \, dx + \int_{\Omega^{\text{ext}}} \nabla u \cdot \nabla v \, dx \ = \ \langle f,\, v\rangle - \langle [\gamma_1 u],\, \gamma_0\, v\rangle \qquad \forall v \in H^1(\mathbb{R}^d)\,.$$

With the next definition and lemma we slowly approach the representation formula.

Definition 4.16. We define the adjoint trace operators

$$\begin{aligned} \gamma_0^* : H^{-1/2}(\Gamma) \to \mathcal{E}'(\mathbb{R}^d) : \qquad & \langle \gamma_0^* w,\, \varphi\rangle := \langle w,\, \gamma_0 \varphi\rangle \qquad \text{for } \varphi \in \mathcal{E}(\mathbb{R}^d)\,, \\ \gamma_1^* : H^{1/2}(\Gamma) \to \mathcal{E}'(\mathbb{R}^d) : \qquad & \langle \gamma_1^* v,\, \varphi\rangle := \langle \gamma_1 \varphi,\, v\rangle \qquad \text{for } \varphi \in \mathcal{E}(\mathbb{R}^d)\,. \end{aligned}$$

Note further that a function $u \in H^1(\Omega^{\text{int}} \cup \Omega^{\text{ext}})$ can be seen as a distribution in $\mathcal{D}'(\mathbb{R}^d)$ and also in $\mathcal{S}'(\mathbb{R}^d)$. Hence, its distributional Laplacian Δu is in $\mathcal{D}'(\mathbb{R}^d)$ and also in $\mathcal{D}'(\mathbb{R}^d)$, and it fulfills

$$\langle \Delta u,\, \varphi\rangle \ = \ \langle u,\, \Delta\varphi\rangle \qquad \forall \varphi \in \mathcal{D}(\mathbb{R}^d) \text{ or } \mathcal{S}(\mathbb{R}^d)\,.$$

Lemma 4.17. *Assume that $u \in H^1(\Omega^{\text{int}} \cup \Omega^{\text{ext}})$ fulfills (4.1). Then*

$$\langle -\Delta u,\, \varphi\rangle \ = \ \langle f,\, \varphi\rangle + \langle \gamma_1^*[\gamma_0 u],\, \varphi\rangle - \langle \gamma_0^*[\gamma_1 u],\, \varphi\rangle \qquad \forall \varphi \in \mathcal{D}(\mathbb{R}^d)\,.$$

In short:

$$-\Delta u \ = \ f + \gamma_1^*[\gamma_0 u] - \gamma_0^*[\gamma_1 u] \qquad \text{in } \mathcal{D}'(\mathbb{R}^d)\,.$$

Proof. Consider $\varphi \in \mathcal{D}(\mathbb{R}^d)$. In the following we use the distributional definition of $-\Delta u$ and the fact that the distribution u is defined by integrating the piecewise H^1-function u against the test function over Ω^{int} and Ω^{ext} separately.

$$\langle -\Delta u,\, \varphi\rangle \ = \ \langle u,\, -\Delta\varphi\rangle \ = \ \int_{\Omega^{\text{int}}} u(-\Delta\varphi)\, dx + \int_{\Omega^{\text{ext}}} u(-\Delta\varphi)\, dx\,.$$

For both terms we use Lemma 4.11 (Green's first identity) and formula (4.2),

$$\begin{aligned}
&\langle -\Delta u,\, \varphi\rangle \\
&\quad = \int_{\Omega^{\mathrm{int}}} \nabla u \cdot \nabla v \, dx - \langle \gamma_1 \varphi,\, \gamma_0^{\mathrm{int}} u\rangle + \int_{\Omega^{\mathrm{ext}}} \nabla u \cdot \nabla v \, dx + \langle \gamma_1 \varphi,\, \gamma_0^{\mathrm{ext}} u\rangle \\
&\quad = \langle f^{\mathrm{int}},\, \varphi\rangle + \langle \gamma_1^{\mathrm{int}} u,\, \gamma_0 \varphi\rangle - \langle \gamma_1 \varphi,\, \gamma_0^{\mathrm{int}} u\rangle + \\
&\qquad + \langle f^{\mathrm{ext}},\, \varphi\rangle - \langle \gamma_1^{\mathrm{ext}} u,\, \gamma_0 \varphi\rangle + \langle \gamma_1 \varphi,\, \gamma_0^{\mathrm{ext}} u\rangle \\
&\quad = \langle f,\, \varphi\rangle - \underbrace{\langle [\gamma_1 u],\, \gamma_0 \varphi\rangle}_{= \langle \gamma_0^* [\gamma_1 u], \varphi\rangle} + \underbrace{\langle \gamma_1 \varphi,\, [\gamma_0 u]\rangle}_{= \langle \gamma_1^* [\gamma_0 u], \varphi\rangle} .
\end{aligned}$$

In the last steps we just used the definitions of f, the trace jumps, and the adjoint trace operators. □

We will now convolute the distributional equation obtained in Lemma 4.17 with the fundamental solution, in order to obtain u instead of $-\Delta u$ on the left hand side.

4.4 Volume and surface potentials, Green's third identity

We define the *Newton potential*

$$(G\,\varphi)(x) := \int_{\mathbb{R}^d} U^*(x,\, y)\, \varphi(y)\, dy \qquad \text{for } \varphi \in \mathcal{S}(\mathbb{R}^d)\,.$$

The integral above is understood as a weakly singular integral: if we would just integrate over a bounded set, the integral is well-defined as a weakly singular one (at least for the fundamental solution we consider), and one can also show that the resulting function is continuous. Since the test function φ is rapidly decreasing, the integral over the whole set $\mathbb{R}^d$ is also well-defined. Moreover since our fundamental solutions fulfill $U^*(x,\, y) = U^*(x - y, 0)$, we can conclude that $G\varphi \in C^1(\mathbb{R}^d)$:

$$\begin{aligned}
\frac{\partial}{\partial x_i}(G\varphi)(x) &= \frac{\partial}{\partial x_i} \int_{\mathbb{R}^d} U^*(x - y,\, 0)\, \varphi(y)\, dy \;= \\
&= \frac{\partial}{\partial x_i} \int_{\mathbb{R}^d} U^*(z, 0)\, \varphi(x - z)\, dz \;= \\
&= -\int_{\mathbb{R}^d} U^*(z, 0)\, \frac{\partial \varphi}{\partial x_i}(x - z)\, dz \;=\; \big(G \frac{\partial \varphi}{\partial x_i}\big)(x)\,,
\end{aligned}$$

where we have substituted z for $x - y$. Applying this argument recursively yields that $G\varphi \in C^\infty(\mathbb{R}^d)$. One can also show that $G\varphi$ itself is rapidly decreasing. Summarizing,

$$G : \mathcal{S}(\mathbb{R}^d) \to \mathcal{S}(\mathbb{R}^d)\,.$$

We define the more general Newton potential

$$G : \mathcal{S}'(\mathbb{R}^d) \to \mathcal{S}'(\mathbb{R}^d) : \quad \langle G\psi,\, \varphi\rangle := \langle \psi,\, G\varphi\rangle \quad \text{for } \psi \in \mathcal{S}'(\mathbb{R}^d),\, \varphi \in \mathcal{S}(\mathbb{R}^d)\,.$$

Lemma 4.18. *Let $u \in \mathcal{S}'(\mathbb{R}^d)$. Then*

$$-\Delta G u \;=\; G(-\Delta u) \;=\; u\,.$$

Proof. Let $\varphi \in \mathcal{S}(\mathbb{R}^d)$.

$$\begin{aligned}\langle -\Delta G u,\, \varphi\rangle \;&=\; \langle Gu,\, -\Delta\varphi\rangle \;=\; \langle u,\, G(-\Delta\varphi)\rangle \;= \\ &=\; \Big\langle u(x),\, \int_{\mathbb{R}^d} U^*(x,\, y)\,(-\Delta_y\varphi)(y)\,dy\Big\rangle_x\end{aligned}$$

We now interpret the inner integral as a distributional evaluation of $U^*(x,\, y)$ for a fixed x. Using the distributional Laplacian, the symmetry of the fundamental solution, and the fact that $-\Delta_y U^*(y,\, x) = \delta_x(y)$, we obtain

$$\langle -\Delta G u,\, \varphi\rangle \;=\; \Big\langle u(x),\, \underbrace{\big\langle -\Delta_y \underbrace{U^*(x,\, y)}_{=U^*(y,\,x)},\, \varphi(y)\big\rangle_y}_{=\,\langle \delta_x,\,\varphi\rangle \,=\, \varphi(x)} \Big\rangle_x \;=\; \langle u,\, \varphi\rangle\,.$$

The proof of the second assertion works analogously, one just has to exploit that $\delta_y(x) = \delta_x(y)$. □

Exercise. Prove the second assertion of Lemma 4.18.

Lemma 4.19. *If the function $u \in H^1(\Omega^{\text{int}} \cup \Omega^{\text{ext}})$ has compact support in $\mathbb{R}^d$ and (4.1) holds, then*

$$u \in \mathcal{S}'(\mathbb{R}^d) \qquad \textit{and} \qquad f \in \mathcal{S}'(\mathbb{R}^d)\,.$$

Proof. Let $\varphi \in \mathcal{S}(\mathbb{R}^d)$ and assume that u is supported on $K \subset\subset \mathbb{R}^d$. Then

$$\langle u,\, \varphi\rangle \;=\; \int_{\mathbb{R}^d} u\,\varphi\,dx \;=\; \int_K u\,\varphi\,dx \;<\; \infty$$

because u and φ are square-integrable over K. Obviously $\langle u,\, \varphi\rangle$ is linear in φ. Furthermore, $\langle u,\, \varphi_n\rangle$ converges to zero if φ_n converges sequentially to zero,

which is already seen from the fact that $\varphi_n \in C^\infty(\overline{K})$ converges uniformly to zero. Thus, u is well-defined as a temperate distribution. Secondly, since $\mathcal{S}(\mathbb{R}^d)$ is dense in $H^1(\mathbb{R}^d)$,

$$\langle f,\, \varphi\rangle \;=\; \langle f^{\mathrm{int}},\; \underbrace{\varphi_{|\Omega^{\mathrm{int}}}}_{\in H^1(\Omega^{\mathrm{int}})} \rangle + \langle f^{\mathrm{ext}},\; \underbrace{\varphi_{|\Omega^{\mathrm{ext}}}}_{\in H^1(\Omega^{\mathrm{ext}})} \rangle \;<\; \infty\,,$$

and so f is well-defined as a temperate distribution too. □

Theorem 4.20. *Let $u \in H^1(\Omega^{\mathrm{int}} \cup \Omega^{\mathrm{ext}})$ have compact support in $\mathbb{R}^d$ and let* (4.1) *hold. Then the abstract representation formula*

$$u \;=\; Gf + G\gamma_1^*[\gamma_0 u] - G\gamma_0^*[\gamma_1 u]$$

holds in the sense of $\mathcal{S}'(\mathbb{R}^d)$.

Proof. Thanks to Lemma 4.19, $u,\ f \in \mathcal{S}'(\mathbb{R}^d)$. Since $\mathcal{E}'(\mathbb{R}^d) \subset \mathcal{S}'(\mathbb{R}^d)$, also $\gamma_1^*[\gamma_0 u],\ \gamma_0^*[\gamma_1 u] \in \mathcal{S}'(\mathbb{R}^d)$. Under the assumption of the compact support the statement of Lemma 4.17 also holds for test functions in $\mathcal{S}(\mathbb{R}^d)$ (the proof is analogous). Hence,

$$-\Delta u \;=\; f + \gamma_1^*[\gamma_0 u] - \gamma_0^*[\gamma_1 u] \qquad \text{in } \mathcal{S}'(\mathbb{R}^d)\,.$$

Applying G to the whole equation, Lemma 4.18 implies the assertion. □

We will now define two surface potentials and decode the statement of the above theorem.

Definition 4.21. We define the *single layer potential*

$$\widetilde{V} := G\gamma_0^* : \quad H^{-1/2}(\Gamma) \to \mathcal{S}'(\mathbb{R}^d)\,,$$

and the *double layer potential*

$$\widetilde{W} := G\gamma_1^* : \quad H^{1/2}(\Gamma) \to \mathcal{S}'(\mathbb{R}^d)\,.$$

For $\varphi \in \mathcal{S}(\mathbb{R}^d)$ and w sufficiently smooth we have

$$\langle \widetilde{V}w,\, \varphi\rangle_{\mathcal{S}'\times\mathcal{S}} \;=\; \langle w,\, \gamma_0 G\varphi\rangle_{H^{-1/2}\times H^{1/2}} \;=\; \int_\Gamma w(x)\,(\gamma_0 G\varphi)(x)\,ds_x \;=$$
$$=\; \int_\Gamma w(x) \int_{\mathbb{R}^d} U^*(x,\, y)\,\varphi(y)\,dy\,ds_x \;=\; \int_{\mathbb{R}^d}\int_\Gamma U^*(x,\, y)\,w(x)\,ds_x\,\varphi(y)\,dy\,,$$

i. e., we have the integral representation

$$(\widetilde{V}w)(y) \;=\; \int_\Gamma U^*(x,\, y)\,w(x)\,ds_x\,,$$

provided that this integral is well-defined. We discuss this in more detail in Lemma 4.25 below. A similar representation can be derived for the double layer potential operator. There, however, the story is more complicated and it will be made clear with Lemma 4.26 and Lemma 4.27 below.

It is immediate from the definitions of $\widetilde{V}$ and $\widetilde{W}$, and from the properties of G that

$$-\Delta Gf \;=f\,,\qquad -\Delta\widetilde{V}w \;=\; \gamma_0^* w,\qquad -\Delta\widetilde{W}v \;=\; \gamma_1^* w\,.$$

Having a closer look to the definitions of the adjoint trace operators we find that the distributions $\gamma_0^* w$, $\gamma_1^* v$ act only on the traces of their test functions, not on the values away from Γ. We can write

$$-\Delta\widetilde{V}w \;=\; 0,\quad -\Delta\widetilde{W}v \;=\; 0,\qquad \text{in } \Omega^{\text{int}}\cup\Omega^{\text{ext}}=\mathbb{R}^d\setminus\Gamma\,,$$

see also the proof of Lemma 4.23 below. With Theorem 4.20 we have that (4.1) implies that

$$u \;=\; Gf+\widetilde{W}[\gamma_0 u]+\widetilde{V}[\gamma_1 u]\qquad \text{in } \mathcal{S}'(\mathbb{R}^d)\,.$$

We also call this equation *Green's third identity*. The two identities above imply that Green's third identity is consistent: the *represented* function indeed fulfills Poisson's equation in Ω^{int} and Ω^{ext}. If we are only interested in Laplace's equation in $\Omega=\Omega^{\text{int}}$, we can formally set $f^{\text{int}}=f^{\text{ext}}=0$, $u_{|\Omega^{\text{ext}}}=0$ and obtain

$$u \;=\; -\widetilde{W}\gamma_0^{\text{int}}u+\widetilde{V}\gamma_1^{\text{int}}u\qquad \text{in } \mathcal{E}'(\Omega)\,. \tag{4.3}$$

In order to obtain boundary integral equations we will apply trace operators γ_0^{int}, γ_1^{int} to (4.3). Before we can do that we must ensure that both surface potentials are really in H^1.

Lemma 4.22. *Let $\zeta\in C_0^\infty(\mathbb{R}^d)$ be a function which equals 1 in a neighborhood of Ω^{int}. Then*

$$\begin{aligned}&\zeta\widetilde{V}: H^{-1/2}(\Gamma)\to H^1(\mathbb{R}^d)\,,\\ &\zeta\widetilde{W}: H^{1/2}(\Gamma)\to H^1(\Omega^{\text{int}}\cup\Omega^{\text{ext}})\end{aligned}$$

are continuous linear operators. Note that $\widetilde{V}$ is continuous *across Γ. This is in general* not *the case for $\widetilde{W}$. Moreover, $\widetilde{V}$, $\widetilde{W}$ are C^∞ in $\mathbb{R}^d\setminus\Gamma$.*

Proof. It is rather easy to see that $\gamma_0^* : H^{-1/2}(\Gamma) \to H^1(\mathbb{R}^d)^*$ by exploiting that $\mathcal{S}(\mathbb{R}^d)$ is dense in $H^1(\mathbb{R}^d)$. Therefore, the proof is reduced to showing that $\zeta G : H^1(\mathbb{R}^d)^* \to H^1(\mathbb{R}^d)$, which can be done, e. g., using the Fourier transform as in [Steinbach]. For the double layer potential, it turns out that $\gamma_1^* : H^{1/2}(\Gamma) \to H^1(\Omega^{\text{int}} \cup \Omega^{\text{ext}})$ only, which finally results in the discontinuity. An alternative prove can be found in [McLean]. □

The following lemma clarifies in which sense the surface potentials are (dis)continuous.

Lemma 4.23. *The operators*

$$\gamma_0^{\text{int}}\widetilde{V} : H^{-1/2}(\Gamma) \to H^{1/2}(\Gamma)\,, \qquad \gamma_1^{\text{int}}\widetilde{V} : H^{-1/2}(\Gamma) \to H^{-1/2}(\Gamma)\,,$$
$$\gamma_0^{\text{int}}\widetilde{W} : H^{1/2}(\Gamma) \to H^{1/2}(\Gamma)\,, \qquad \gamma_1^{\text{int}}\widetilde{W} : H^{1/2}(\Gamma) \to H^{-1/2}(\Gamma)$$

and the corresponding ones with the exterior traces are linear and continuous. The following jump relations hold,

$$[\gamma_0\widetilde{V}w] = 0\,, \qquad [\gamma_1\widetilde{V}w] = -w \qquad \forall w \in H^{-1/2}(\Gamma)\,,$$
$$[\gamma_0\widetilde{W}v] = v\,, \qquad [\gamma_1\widetilde{W}v] = 0 \qquad \forall v \in H^{1/2}(\Gamma)\,.$$

Proof. The traces $\gamma_0^{\text{int}}\widetilde{V}w$, $\gamma_0^{\text{int}}\widetilde{W}v$ (and also the exterior ones) are well-defined in $H^{1/2}(\Gamma)$ due to Lemma 4.22 and the trace theorem. Recall that

$$-\Delta\widetilde{V}w = \gamma_0^* w\,, \qquad -\Delta\widetilde{W}v = \gamma_1^* v \qquad \text{in } \mathcal{E}'(\mathbb{R}^d)\,.$$

Also,

$$\left.\begin{aligned} \langle\gamma_0^* w, \varphi\rangle &= \langle w, \underbrace{\gamma_0\varphi}_{=0}\rangle = 0 \\ \langle\gamma_1^* w, \varphi\rangle &= \langle w, \underbrace{\gamma_1\varphi}_{=0}\rangle = 0 \end{aligned}\right\} \qquad \forall\varphi \in \mathcal{D}(\Omega^{\text{int}}) \subset \mathcal{E}(\mathbb{R}^d)\,,$$

because φ has compact support. The same holds of course for $\varphi \in \mathcal{D}(\Omega^{\text{ext}})$. Therefore, each of $\widetilde{V}w$ and $\widetilde{W}v$ satisfy the weak Laplace equation in Ω^{int} and Ω^{ext}, and so their trace γ_1^{int} and γ_1^{ext} are well-defined in $H^{-1/2}(\Gamma)$.

The jump relation $[\gamma_0\widetilde{V}w] = 0$ follows immediately from Lemma 4.22. We prove now that $[\gamma_1\widetilde{V}w] = -w$. A proof of the two other relations can be found in [McLean]. Let $\zeta \in \mathcal{D}(\mathbb{R}^d)$ with $\zeta_{|U} = 1$ where U is a bounded domain such that $\Omega^{\text{int}} \subset\subset U$. Then Lemma 4.17 implies that

$$\langle -\Delta u, \varphi\rangle = 0 - \langle\gamma_0^*[\gamma_1 u], \varphi\rangle = -\langle[\gamma_1 u], \gamma_0\varphi\rangle \qquad \forall\varphi \in \mathcal{D}(U)\,.$$

Since $-\Delta G\gamma_0^* = \gamma_0^*$ we have

$$\langle -\Delta u,\, \varphi\rangle \;=\; \langle \gamma_0^* w,\, \varphi\rangle \;=\; \langle w,\, \gamma_0\varphi\rangle \qquad \forall \varphi \in \mathcal{D}(U)\,.$$

Since $C^\infty(\Gamma)$ is dense in $H^{1/2}(\Gamma)$ the two identities imply that $[\gamma_1 u] = -w$. □

Next we discuss integral representations of the traces of $\widetilde{V}$ and $\widetilde{W}$.

4.5 Boundary integral operators and their properties

Definition 4.24. We define the *single layer potential operator*

$$V : H^{-1/2}(\Gamma) \to H^{1/2}(\Gamma) : \quad V := \gamma_0 \widetilde{V}\,.$$

Lemma 4.25. *For $w \in H^{-1/2}(\Gamma) \cap L^\infty(\Gamma)$ we have the representation*

$$(V\,w)(x) \;=\; \int_\Gamma U^*(x,\, y)\, w(y)\, ds_y \qquad \forall x \in \Gamma$$

as a weakly singular surface integral.

Proof. Following the paragraph after Definition 4.21 and using that $U^*(x,\, y) = U^*(y,\, x)$ we obtain that for all $\varphi \in \mathcal{S}(\mathbb{R}^d)$,

$$\begin{aligned}
\langle \widetilde{V} w,\, \varphi\rangle \;&=\; \int_\Gamma w(y) \underbrace{\int_{\mathbb{R}^d} U^*(x,\, y)\, \varphi(x)\, dx}_{\in \mathcal{S}(\mathbb{R}^d)}\, ds_y \\
&=\; \int_\Gamma w(y) \lim_{\widetilde{x}\to x} \int_{\mathbb{R}^d} U^*(\widetilde{x},\, y)\, \varphi(x)\, dx\, ds_y \\
&=\; \int_{\mathbb{R}^d} \varphi(x) \Big[\underbrace{\lim_{\widetilde{x}\to x} \int_\Gamma U^*(\widetilde{x},\, y)\, w(y)\, ds_y}_{\in H^1(K)\ \forall K \subset\subset \mathbb{R}^d} \Big]\, dx\,.
\end{aligned}$$

The last line must be interpreted as follows. The function inside the limit is continuous provided that $\widetilde{x} \notin \Gamma$. Thanks to Lemma 4.22 the limit for $\widetilde{x} \to x \in \Gamma$ exists at least the sense of $H^{1/2}(\Gamma)$. Following, e. g., [Sauter/Schwab] it is even $C(\Gamma)$. We now show that excluding a ball of radius ε around the singularity in the integral in the assertion of the lemma, we converge to the

same term as $\varepsilon \to 0$. To this end, let $x \in \Gamma$ and $\varepsilon > 0$ be fixed and choose $\widetilde{x} \in \Omega$ with $|x - \widetilde{x}| < \varepsilon$. In then suffices to show that

$$\begin{aligned}
&\left| \int_\Gamma U^*(\widetilde{x},\, y)\, w(y)\, ds_y - \int_{y\in\Gamma:\ |x-y|>\varepsilon} U^*(x,\, y)\, w(y)\, ds_y \right| \\
&\leq \underbrace{\left| \int_{\substack{y\in\Gamma:\\ |x-y|>\varepsilon}} \big[U^*(\widetilde{x},\, y) - U^*(x,\, y)\big]\, w(y)\, ds_y \right|}_{=:\ (\mathrm{I})} + \underbrace{\left| \int_{\substack{y\in\Gamma:\\ |x-y|\leq\varepsilon}} U^*(\widetilde{x},\, y)\, w(y)\, ds_y \right|}_{=:\ (\mathrm{II})}
\end{aligned}$$

converges to zero as $\varepsilon \to 0$ and $\widetilde{x} \to x$. Since everything is continuous in the first term, we get that

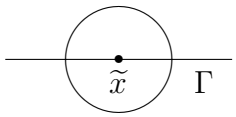
$$\lim_{\widetilde{x}\to x} (\mathrm{I}) \;=\; 0\,.$$

The remaining term can be estimated as follows.

$$(\mathrm{II}) \;\leq\; \|w\|_{L^\infty(\Gamma\cap B_\varepsilon(x))} \int_{\Gamma\cap B_\varepsilon(x)} |U^*(\widetilde{x},\, y)|\, ds_y \;\leq\; \|w\|_{L^\infty(\Gamma)} \int_{\Gamma\cap B_{2\varepsilon}(\widetilde{x})} |U^*(\widetilde{x},\, y)|\, ds_y\,.$$

In case of our fundamental solutions, the integral on the right hand side can be shown to converge to zero as $\varepsilon \to 0$. Here we surrender a precise proof but only present a plausible argument.

For $d = 2$, we consider the case that $\widetilde{x} = x$ and that Γ is a straight line.



Then we have

$$\begin{aligned}
(\mathrm{II}) \;&\leq\; \frac{1}{2\pi} \int_{y\in\Gamma:|y-\widetilde{x}|<2\varepsilon} \big|\log|y-\widetilde{x}|\,\big|\, ds_y \;=\; \frac{1}{2\pi} \int_{-2\varepsilon}^{2\varepsilon} \big|\log|z|\,\big|\, dz \\
&=\; -\frac{1}{\pi} \int_0^{2\varepsilon} \log|z|\, dz \;=\; -\frac{2\varepsilon}{\pi}\big(\log(2\varepsilon) - 1\big) \;\stackrel{\varepsilon\to 0}{\longrightarrow}\; 0\,,
\end{aligned}$$

where we have used the anti-derivative of the logarithm and de l'Hospital in the last step. Thus, if $\varepsilon \to 0$ and $\widetilde{x} \to x$, then $(\mathrm{I}) + (\mathrm{II}) \to 0$.

For $d = 3$, we consider the case that $\widetilde{x} = x$ and that Γ is a plane, i. e., the intersection of Γ and $B_{2\varepsilon}(\widetilde{x})$ is a disc. Introducing polar coordinates we obtain

$$(\mathrm{II}) \;\leq\; \frac{1}{4\pi} \int_{y\in\Gamma:|y-\widetilde{x}|<2\varepsilon} \frac{1}{|y-\widetilde{x}|}\, ds_y \;=\; \frac{1}{4\pi} \int_0^{2\pi} \int_0^{2\varepsilon} \frac{1}{r}\, r\, dr\, d\phi \;=\; \varepsilon \;\to\; 0\,.$$

□

The integral representation in Lemma 4.25 will help us when discretizing boundary integral equations. There, we will discretize the trace space $H^{1/2}(\Gamma)$ with continuous piecewise affine linear functions (the trace of typical finite element functions on Ω), and the space $H^{-1/2}(\Gamma)$, which is the space containing normal derivatives, with piecewise constant functions. These are for sure in $L^\infty(\Gamma)$.

Lemma 4.26. *For $w \in H^{-1/2}(\Gamma) \cap L^\infty(\Gamma)$ we have the representation*

$$\langle \gamma_1^{\rm int} \widetilde{V}\, w,\, v\rangle \;=\; \langle \sigma\, w + K'\, w,\, v\rangle \qquad \forall v \in H^{1/2}(\Gamma)\,,$$

with σ defined according to (2.4), i. e., $\sigma = \frac{1}{2}$ almost everywhere, and

$$(K'w)(x) := \lim_{\varepsilon\to 0} \int\limits_{y\in\Gamma:|y-x|\geq\varepsilon} \frac{\partial}{\partial n_x} U^*(x,\, y)\, w(y)\, ds_y \qquad \text{for } x \in \Gamma\,.$$

Proof. Note first that $K'w := \gamma_1^{\rm int}\widetilde{V}\, w - \sigma w$ is well-defined in $H^{-1/2}(\Gamma)$, i. e., it remains to show that $K'w$ obeys the above integral representation. Due to the fact that $C^\infty(\Gamma)$ is dense in $H^{1/2}(\Gamma)$ it suffices to show the identity for $v = \gamma_0^{\rm int}\varphi$ with $\varphi \in C^\infty(\overline{\Omega})$. Set $u := \widetilde{V}\, w$. Then the definition of $\gamma_1^{\rm int}$ (cf. Lemma 4.12) and Lemma 4.22 imply that

$$\begin{aligned}
\langle \gamma_1^{\rm int} u,\, \gamma_0^{\rm int}\varphi\rangle \;&=\; \int_\Omega \nabla u\cdot\nabla\varphi\, dx \;+\; 0 \\
&=\; \int_\Omega \nabla_x \underbrace{\left[\int_\Gamma \underbrace{U^*(y,\, x)}_{=U^*(x,\,y)}\, w(y)\, ds_y\right]}_{\in C^\infty(\Omega)} \cdot \nabla_x\varphi(x)\, dx \\
&=\; \int_\Omega \nabla_x \left[\lim_{\varepsilon\to 0} \int\limits_{y\in\Gamma:|x-y|\geq\varepsilon} U^*(x,\, y)\, w(y)\, ds_y\right] \cdot \nabla_x\varphi(x)\, dx \\
&=\; \int_\Gamma w(y) \lim_{\varepsilon\to 0} \int_{x\in\Omega:|x-y|\geq\varepsilon} \nabla_x U^*(x,\, y)\cdot\nabla_x\varphi(x)\, dx\, ds_y\,.
\end{aligned}$$

Recall that $\varphi \in C^\infty(\overline{\Omega})$ and $U^*(\cdot,\, y) \in C^\infty(\overline{\Omega}\setminus\overline{B_\varepsilon(y)})$. Hence we can use

Green's identity on $\Omega \setminus \overline{B_\varepsilon(y)}$.

$$\int\limits_{\Omega\setminus\overline{B_\varepsilon(y)}} \nabla_x U^*(x,\,y)\cdot\nabla_x\varphi(x)\,dx \;=\; \int\limits_{\Omega\setminus\overline{B_\varepsilon(y)}} \underbrace{-\Delta_x U^*(x,\,y)}_{=0}\,\varphi(x)\,dx \;+$$
$$+\;\underbrace{\int\limits_{\Gamma\setminus\overline{B_\varepsilon(y)}} \frac{\partial}{\partial n_x}U^*(x,\,y)\,\varphi(x)\,ds_x}_{=:\,(\mathrm{I})} + \underbrace{\int\limits_{\partial B_\varepsilon(y)\cap\Omega} \frac{\partial}{\partial n_x}U^*(x,\,y)\big[\varphi(x)-\varphi(y)\big]\,ds_x}_{=:\,(\mathrm{II})} \;+$$
$$+\;\underbrace{\varphi(y)\int_{\partial B_\varepsilon(y)\cap\Omega}\frac{\partial}{\partial n_x}U^*(x,\,y)\,ds_x}_{=:\,(\mathrm{III})}\,,$$

where we have artificially introduced the last term by subtracting and adding $\varphi(y)$. The term (I) will lead to the operator K'. For the second term we have

$$(\mathrm{II}) \;\le\; \underbrace{\max_{x\in\partial B_\varepsilon(y)\cap\Omega}|\varphi(x)-\varphi(y)|}_{\stackrel{\varepsilon\to0}{\longrightarrow}\,0}\;\underbrace{\int_{\partial B_\varepsilon(y)\cap\Omega}\Big|\frac{\partial}{\partial n_x}U^*(x,\,y)\Big|\,ds_x}_{=:\,(\mathrm{IIa})}\,.$$

A side computation shows that

$$d=2:\nabla_x U^*(x,\,y) = -\frac{1}{2\pi}\nabla_x\log|x-y| = -\frac{1}{2\pi}\frac{1}{|x-y|}\frac{x-y}{|x-y|}\,,$$
$$d=3:\nabla_x U^*(x,\,y) = \frac{1}{4\pi}\nabla_x\frac{1}{|x-y|} = -\frac{1}{4\pi}\frac{1}{|x-y|^2}\frac{x-y}{|x-y|}\,.$$

Using that $n_x=\frac{y-x}{|x-y|}$ for $x\in\partial B_\varepsilon(y)\cap\Omega$ (the normal vector must be outward to $\Omega\setminus\overline{B_\varepsilon(y)}$), this implies $\frac{\partial}{\partial n_x}U^*(x,\,y)=\frac{1}{2\pi(d-1)}\frac{1}{|x-y|^{d-1}}$. Hence,

$$(\mathrm{IIa}) \;\le \int\limits_{x\in\Omega:|x-y|=\varepsilon}\frac{1}{2\pi(d-1)}\underbrace{\frac{1}{|x-y|^{d-1}}}_{=\varepsilon^{d-1}}\,ds_x \;=\; 1\,,$$

and so $(\mathrm{II})\to 0$ as $\varepsilon\to 0$. For the remaining term we obtain

$$\begin{aligned}(\mathrm{III}) \;&=\; \varphi(y)\int_{\partial B_\varepsilon(y)\cap\Omega}\frac{1}{2\pi(d-1)}\,\frac{1}{|x-y|^{d-1}}\,ds_x\\ &=\; \varphi(y)\,\frac{1}{2\pi(d-1)}\,\frac{1}{\varepsilon^{d-1}}\int_{x\in\Omega:|x-y|=\varepsilon}ds_x \;\stackrel{\varepsilon\to0}{\longrightarrow}\; \sigma(y)\,\varphi(y)\,.\end{aligned}$$

Collecting all the terms the assertion follows with $\varepsilon\to 0$. □

Lemma 4.27. *For $v \in H^{1/2}(\Gamma) \cap L^\infty(\Gamma)$ we have the representation*

$$(\gamma_0^{\rm int}\widetilde{W}\, v)(x) \;=\; \big(-1+\sigma(x)\big)\, v(x) + (K\, v)(x) \qquad \text{for } x \in \Gamma\,,$$

with $\sigma(x)$ defined as before and

$$(K\, v)(x) \;=\; \lim_{\varepsilon\to 0} \int_{y\in\Gamma:|y-x|\geq\varepsilon} \Big[\frac{\partial}{\partial n_y} U^*(x,\, y)\Big] v(y)\, ds_y \qquad \text{for } x \in \Gamma\,.$$

Proof. The proof is similar to the one before. □

Exercise. Show that $K : H^{1/2}(\Gamma) \to H^{1/2}(\Gamma)$ and $K' : H^{-1/2}(\Gamma) \to H^{-1/2}(\Gamma)$ are adjoint to each other, i. e.,

$$\langle w,\, K\, v\rangle \;=\; \langle K' w,\, v\rangle \qquad \forall v \in H^{1/2}(\Gamma),\; w \in H^{-1/2}(\Gamma)\,.$$

We call K the *double layer potential operator* and K' the *adjoint double layer potential operator*.

Lemma 4.28. *The hypersingular (boundary integral) operator*

$$D := -\gamma_1^{\rm int}\widetilde{W} : H^{1/2}(\Gamma) \to H^{-1/2}(\Gamma)$$

has the following representation for $v \in H^{1/2}(\Gamma) \cap C(\Gamma)$,

$$(D\, v)(x) \;=\; -\int_\Gamma \frac{\partial}{\partial n_x}\frac{\partial}{\partial n_y}\Big\{U^*(x,\, y)\big[v(y)-v(x)\big]\Big\}\, ds_y \qquad \text{for } x \in \Gamma\,,$$

to be understood as a Cauchy principal value integral.

Proof. We give only a sketch of a proof. First we show that a straightforward technique fails. For $\widetilde{x} \in \Omega$, we have

$$(\widetilde{W}\, v)(\widetilde{x}) \;=\; \frac{1}{2\pi(d-1)} \lim_{\varepsilon\to 0} \int_{\Gamma\setminus B_\varepsilon(\widetilde{x})} \frac{(\widetilde{x}-y)\cdot n_y}{|\widetilde{x}-y|^d}\, v(y)\, ds_y\,.$$

In order to obtain $(D\, v)(x)$ we have form $n_x \cdot \nabla$ of the expression and send $\widetilde{x}$ to x. Exchanging formally the limits $\widetilde{x} \to x$ and $\varepsilon \to 0$ and computing the normal derivative we obtain

$$(D_\varepsilon v)(x) \;=\; \frac{1}{2\pi(d-1)} \int\limits_{\Gamma\setminus B_\varepsilon(x)} \Big[-\frac{n_x\cdot n_y}{|x-y|^d} + d\frac{(x-y)\cdot n_x\,(x-y)\cdot n_y}{|x-y|^{d+2}}\Big] v(y)\, ds_y\,.$$

However the limit $\varepsilon \to 0$ of this integral does *not* exist.

As a trick, we apply Green's third identity (4.3) from page 38 to the constant function $u = \mathbf{1}$ on Ω. Then we get that

$$\mathbf{1} \;=\; -\widetilde{W}\,\mathbf{1} + 0 \qquad \Longrightarrow \qquad \nabla_{\widetilde{x}}(\widetilde{W}\,\mathbf{1})(\widetilde{x}) = 0 \quad \forall \widetilde{x} \in \Omega\,.$$

Here and in the following $\mathbf{1}$ denotes the constant either on Γ or on Ω (which one should be always clear from the context).
Since $(D\,v)(x) = -\lim\limits_{\Omega \ni \widetilde{x} \to x} n_x \cdot \nabla_{\widetilde{x}}(\widetilde{W}\,v)(\widetilde{x})$ for smooth functions v, we have

$$D\,\mathbf{1} \;=\; 0\,.$$

Thus we can write

$$\begin{aligned}(D\,v)(x) \;&=\; \lim_{\Omega \ni \widetilde{x} \to x} n_x \cdot \nabla_{\widetilde{x}} \int_\Gamma \frac{\partial}{\partial n_y} \Big\{ U^*(x,\,y) \big[\underbrace{v(x)}_{\text{const w.r.t. } \widetilde{x},\,y} - v(y) \big] \Big\}\, ds_y \\ &=\; -\int_\Gamma \frac{\partial}{\partial n_x} \frac{\partial}{\partial n_y} \Big\{ U^*(x,\,y) \big[v(x) - v(y) \big] \Big\}\, ds_y\,,\end{aligned}$$

where we omit details for the last part. □

We also discuss an alternative representation of the hypersingular operator which is often used in implementations. First, let $d = 2$. For $\widetilde{v} \in C^1(\overline{\Omega})$ define

$$\operatorname{curl} \widetilde{v} := \begin{pmatrix} \frac{\partial \widetilde{v}}{\partial x_2} \\ -\frac{\partial \widetilde{v}}{\partial x_1} \end{pmatrix}.$$

Let $\Gamma \in C^1_{\mathrm{pw}}$ with the smooth boundary parts $\{\Gamma_k\}$. For $v \in C^1(\Gamma_k)$ we can find an extension $\widetilde{v} \in C^1(\overline{\Omega})$ such that $\widetilde{v}|_{\Gamma_k} = v$. Then we define

$$\operatorname{curl}_{\Gamma_k} v(x) := n(x) \cdot \operatorname{curl} \widetilde{v}(x) \qquad \text{for } x \in \Gamma_k\,.$$

We show that the definition of $\operatorname{curl}_{\Gamma_k} v$ is independent of the extension. Let $\Gamma_k = \{y_k(t) : t \in (t_k,\, t_{k+1})\}$. Then $ds_y = |y_k'(t)|\,dt$ and $n(x) = \frac{1}{|y_k'(t)|}\big(y_{k,2}'(t) \mid -y_{k,1}'(t)\big)^T$ in case of positive orientation. We obtain

$$\begin{aligned}\int_{\Gamma_k} \operatorname{curl}_{\Gamma_k} v\, ds_y \;&=\; \int_{t_k}^{t_{k+1}} \frac{1}{|y_k'(t)|} \Big[y_{k,2}'(t) \frac{\partial \widetilde{v}}{\partial x_2}\big(y_k(t)\big) + y_{k,1}'(t) \frac{\partial \widetilde{v}}{\partial x_1}\big(y_k(t)\big) \Big] |y_k'(t)|\,dt \\ &=\; \int_{t_k}^{t_{k+1}} \frac{d}{dt} v\big(y_k(t)\big)\,dt\,.\end{aligned}$$

Since we can make the pieces Γ_k arbitrary small, this means that $\operatorname{curl}_{\Gamma_k}$ is a tangential derivative. Finally, for $v \in C^1_{\mathrm{pw}}(\Gamma)$ (with respect to the partition into the Γ_k) we define

$$\operatorname{curl}_\Gamma v(x) := \operatorname{curl}_{\Gamma_k} v(x) \qquad \text{for } x \in \Gamma_k\,.$$

Lemma 4.29. *For $d = 2$, $\Gamma \in C^1_{\mathrm{pw}}$ and u, $v \in H^{1/2}(\Gamma) \cap C(\Gamma) \cap C^1_{\mathrm{pw}}(\Gamma)$, we have*

$$\langle D\,u,\, v\rangle_\Gamma \;=\; -\frac{1}{2\pi}\int_\Gamma \operatorname{curl}_\Gamma v(x) \int_\Gamma \log|x-y| \operatorname{curl}_\Gamma u(y)\, ds_y\, ds_x\,,$$

with weakly singular integrals.

The proof that can be found in [Steinbach] is based on the following integration by parts formula,

$$\int_\Gamma v(y) \operatorname{curl}_\Gamma w(y)\, ds_y \;=\; -\int_\Gamma \operatorname{curl}_\Gamma v(y)\, w(y)\, ds_y + \underbrace{\sum_k v\big(y_k(t)\big)\, w\big(y_k(t)\big)\Big|_{t_k}^{t_{k+1}}}_{=0 \text{ if } v\in C(\Gamma)}\,.$$

For $d = 3$ we define the surface-curl of $v \in C^1_{\mathrm{pw}}(\Gamma)$ analogously to the case $d = 2$, but we have to set

$$\operatorname{curl}_{\Gamma_k} v(x) := n(x) \times \nabla \widetilde{v}(x) \qquad \text{for } x \in \Gamma_k\,,$$

for an arbitrary extension $\widetilde{v} \in C^1(\overline{\Omega})$ of v. Note that this is now a vectorial quantity. However, $\operatorname{curl}_\Gamma v \perp n$, so we can view it as a two-dimensional quantity. For almost each $x \in \Gamma$, $\operatorname{curl}_\Gamma v(x)$ is a rotated projection of $\nabla\widetilde{v}$ to the *tangent plane* to x. We see (and one can prove) that the definition is independent of the particular choice of the extension.

Lemma 4.30. *For $d = 3$, $\Gamma \in C^1_{\mathrm{pw}}$ and u, $v \in H^{1/2}(\Gamma) \cup C(\Gamma) \cup C^1_{\mathrm{pw}}(\Gamma)$ we have*

$$\langle D\,u,\, v\rangle_\Gamma \;=\; \frac{1}{4\pi}\int_\Gamma\int_\Gamma \frac{\operatorname{curl}_\Gamma v(x) \cdot \operatorname{curl}_\Gamma u(y)}{|x-y|}\, ds_y\, ds_x\,,$$

with weakly singular integrals.

For a proof see [Steinbach].

Remark 4.31. In short we can write

$$\langle D\,u,\, v\rangle \;=\; \langle \operatorname{curl}_\Gamma u,\, V \operatorname{curl}_\Gamma v\rangle\,.$$

This form is often used in implementations of the Galerkin boundary method.

Exercise. Show that V and D are self-adjoint operators, i. e.,

$$\begin{aligned} \langle w,\, V\,v\rangle &= \langle v,\, V\,w\rangle && \forall v,\, w \in H^{-1/2}(\Gamma)\,,\\ \langle D\,v,\, w\rangle &= \langle D\,w,\, v\rangle && \forall v,\, w \in H^{1/2}(\Gamma)\,. \end{aligned}$$

Consider now the weak equation

$$-\Delta u \;=\; 0 \qquad \text{in } \Omega = \Omega^{\text{int}}\,. \tag{4.4}$$

Then with (4.3) and the previous results we get

$$\begin{aligned}
\gamma_0^{\text{int}} u \;&=\; \underbrace{-\gamma_0^{\text{int}}\widetilde{W}}_{=(1-\sigma)I-K}\,\gamma_0^{\text{int}} u + \underbrace{\gamma_0^{\text{int}}\widetilde{V}}_{=V}\gamma_1^{\text{int}} u && \text{in } H^{1/2}(\Gamma)\,,\\
\gamma_1^{\text{int}} u \;&=\; \underbrace{-\gamma_1^{\text{int}}\widetilde{W}}_{=D}\gamma_0^{\text{int}} u + \underbrace{\gamma_1^{\text{int}}\widetilde{V}}_{=\sigma I+K'}\,\gamma_1^{\text{int}} u && \text{in } H^{-1/2}(\Gamma)\,.
\end{aligned}$$

These are two integral equations relating $\gamma_0^{\text{int}} u$ and $\gamma_1^{\text{int}} u$ (the Cauchy data). Recall that $\sigma = \frac{1}{2}$ almost everywhere. Summarizing,

$$\begin{pmatrix} \gamma_0^{\text{int}} u \\ \gamma_1^{\text{int}} u \end{pmatrix} \;=\; \underbrace{\begin{pmatrix} \frac{1}{2}I - K & V \\ D & \frac{1}{2}I - K' \end{pmatrix}}_{=:\mathcal{C}} \begin{pmatrix} \gamma_0^{\text{int}} u \\ \gamma_1^{\text{int}} u \end{pmatrix}, \tag{4.5}$$

with the block operator $\mathcal{C}$ named after *Calderón*.

Lemma 4.32. *The Calderón operator $\mathcal{C}$ is a projection, i. e., $\mathcal{C}^2 = \mathcal{C}$.*

Proof. We fix $(\varphi,\, \psi) \in H^{1/2}(\Gamma)\times H^{-1/2}(\Gamma)$. Then the function $u := \widetilde{V}\psi + \widetilde{W}\varphi$ fulfills $-\Delta u = 0$ weakly in Ω, is in $H^1(\Omega)$, and

$$\left\{ \begin{array}{rcl} \gamma_0^{\text{int}} u &=& V\,\psi + \frac{1}{2}\varphi - K\,\varphi \\ \gamma_1^{\text{int}} u &=& \frac{1}{2}\psi + K'\psi + D\,\varphi \end{array} \right\} \quad\Longleftrightarrow\quad \begin{pmatrix} \gamma_0^{\text{int}} u \\ \gamma_1^{\text{int}} u \end{pmatrix} \;=\; \mathcal{C}\begin{pmatrix} \varphi \\ \psi \end{pmatrix}.$$

But also $\begin{pmatrix} \gamma_0^{\text{int}} u \\ \gamma_1^{\text{int}} u \end{pmatrix} = \mathcal{C}\begin{pmatrix} \gamma_0^{\text{int}} u \\ \gamma_1^{\text{int}} u \end{pmatrix}$ and so $\mathcal{C}\begin{pmatrix} \varphi \\ \psi \end{pmatrix} = \mathcal{C}^2\begin{pmatrix} \varphi \\ \psi \end{pmatrix}$. □

Remark 4.33. 1. Owing to Lemma 4.32, $\mathcal{C}$ is called *Calderón's projector.* From the projection properties we get the algebraic identities

$$\begin{aligned} V\,D \;&=\; (\tfrac{1}{2}I + K)(\tfrac{1}{2}I - K')\,, & V\,K' \;&=\; K\,V\,,\\ D\,V \;&=\; (\tfrac{1}{2}I + K')(\tfrac{1}{2}I - K)\,, & K'\,D \;&=\; D\,K\,. \end{aligned}$$

2. If replace the right hand side in (4.4) by f^{int}, we have to add

$$\begin{pmatrix} N_0 f \\ N_1 f \end{pmatrix} := \begin{pmatrix} \gamma_0^{\text{int}} G\,f \\ \gamma_1^{\text{int}} G\,f \end{pmatrix}$$

to the right hand side of (4.5), where $\langle f, \varphi\rangle := \langle f^{\text{int}}, \varphi_{|\Omega^{\text{int}}}\rangle$ for $\varphi \in \mathcal{D}(\mathbb{R}^d)$. If f^{int} is an integrable function we get the weakly singular integral representations

$$\begin{aligned}(N_0 f)(x) &= \int_\Omega U^*(x, y)\, f^{\text{int}}(y)\, dy\,,\\ (N_1 f)(x) &= \int_\Omega \frac{\partial}{\partial n_x} U^*(x, y)\, f^{\text{int}}(y)\, dy\,.\end{aligned}$$

In general, these domain integrals are of course costly. Only for some functions f^{int} these integrals may be computed analytically or approximated using smoothness or a special structure of f^{int}.

Exercise. Show the algebraic identities in the remark above.

Before discretizing the two BIEs, we study further properties of the boundary integral operators, among them the ellipticity of the single layer potential operator V, which makes the Lax-Milgram lemma applicable.

4.5.1 The ellipticity of V and D

We first consider the ellipticity of V and give a proof thereof via the single layer potential $\widetilde{V}$ on $\mathbb{R}^d$.

Fix $w \in H^{-1/2}(\Gamma)$. Then $u := \widetilde{V} w$ solves

$$\begin{aligned}-\Delta u &= 0 \qquad && \text{weakly in } \Omega^{\text{int}}\,,\\ \gamma_0^{\text{int}} u &= Vw \qquad && \text{on } \Gamma\,,\end{aligned}$$

and we know from Lemma 4.22 that $u \in H^1(\Omega^{\text{int}})$. Moreover, from Lemma 4.12 we get that

$$\|\gamma_1^{\text{int}} u\|_{H^{-1/2}(\Gamma)} \;\le\; c_{IT}^{\text{int}} \Big(\int_{\Omega^{\text{int}}} |\nabla u|^2\, dx \Big)^{1/2}, \tag{4.6}$$

where c_{IT}^{int} is the constant in the interior trace inequality. We will use this inequality for the following ellipticity proof. There it is of essential importance that the *energy*

$$\int_{\Omega^{\text{int}}} |\nabla \widetilde{V} w|^2\, dx$$

is finite, and this is for sure true since $\widetilde{V} w \in H^1(\Omega^{\text{int}})$. However, if we integrate over the exterior domain Ω^{ext}, this energy could go to infinity. Nevertheless, assuming that it is finite, we get that

$$\|\gamma_1^{\text{ext}} u\|_{H^{-1/2}(\Gamma)} \;\le\; c_{IT}^{\text{ext}} \Big(\int_{\Omega^{\text{ext}}} |\nabla u|^2\, dx \Big)^{1/2},$$

where c_{IT}^{ext} is the constant in the exterior trace inequality. The following lemma shows the ellipticity of V under the assumption of finite energy.

Lemma 4.34. *Define the subspace*

$$H := \{w \in H^{-1/2}(\Gamma) : \|\nabla \widetilde{V} w\|_{L^2(\mathbb{R}^d)} < \infty\}\,.$$

Then the single layer potential operator V is H-elliptic, i. e., there exists a constant $c_V > 0$ such that

$$\langle w,\, Vw\rangle \;\geq\; c_V\, \|w\|^2_{H^{-1/2}(\Gamma)} \qquad \forall w \in H\,.$$

Proof. With the definitions of γ_1^{int} and γ_1^{ext} we obtain for $u = \widetilde{V} w$ that

$$\begin{aligned}
\int_{\Omega^{\text{int}}} \nabla u \cdot \nabla v\, dx &= \langle \gamma_1^{\text{int}} u,\, \gamma_0^{\text{int}} v\rangle\,,\\
\int_{\Omega^{\text{ext}}} \nabla u \cdot \nabla v\, dx &= -\langle \gamma_1^{\text{ext}} u,\, \gamma_0^{\text{ext}} v\rangle\,,
\end{aligned}$$

for all $v \in H^1(\mathbb{R}^d)$, cf. Lemma 4.12. As a matter of fact the same formula holds true if we replace v by u even though $u \notin H^1(\mathbb{R}^d)$. This can be seen from the proof of Lemma 4.12: the extension $\mathcal{E}\gamma_0 u$ can be chosen such that it vanishes outside a ball $U \supset \Omega^{\text{int}}$ such that still $\|\mathcal{E}\gamma_0 u\|_{H^1(\mathbb{R}^d)} \leq c_{IT}^{\text{ext}} \|\gamma_0 u\|_{H^{1/2}(\Gamma)}$. The fact that $w \in H$ ensures that $|u|_{H^1(\mathbb{R}^d)} < \infty$. From all this and from the jump relations from Lemma 4.23 we can conclude that

$$\int_{\mathbb{R}^d} |\nabla u|^2 \;=\; -\langle [\gamma_1 u],\, \gamma_0 u\rangle \;=\; \langle w,\, \gamma_0 u\rangle \;=\; \langle w,\, V\, w\rangle\,.$$

The expression on the left hand side is often refered to as the *total energy*. Using the two inequalities in the paragraph preceding this lemma, we get

$$\begin{aligned}
\langle w,\, V\, w\rangle &= \int_{\Omega^{\text{int}}} |\nabla u|^2\, dx + \int_{\Omega^{\text{ext}}} |\nabla u|^2\, dx\\
&\geq (c_{IT}^{\text{int}})^{-2}\, \|\gamma_1^{\text{int}} u\|^2_{H^{-1/2}(\Gamma)} + (c_{IT}^{\text{ext}})^{-2}\, \|\gamma_1^{\text{ext}} u\|^2_{H^{-1/2}(\Gamma)}\,.
\end{aligned}$$

From the jump relations we can conclude that

$$\begin{aligned}
\|w\|^2_{H^{-1/2}(\Gamma)} &= \|\gamma_1^{\text{int}} u - \gamma_1^{\text{ext}} u\|^2_{H^{-1/2}(\Gamma)} \;\leq\; 2\Big[\|\gamma_1^{\text{int}} u\|^2_{H^{-1/2}(\Gamma)} + \|\gamma_1^{\text{ext}} u\|^2_{H^{-1/2}(\Gamma)}\Big]\\
&\leq \frac{2}{\min\{(c_{IT}^{\text{int}})^{-2},\, (c_{IT}^{\text{ext}})^{-2}\}}\, \langle w,\, Vw\rangle \;=\; \underbrace{2\, \max(c_{IT}^{\text{int}},\, c_{IT}^{\text{ext}})^2}_{=c_V^{-1}} \langle w,\, Vw\rangle\,,
\end{aligned}$$

which shows the ellipticity. □

The next lemma shows that the subspace H is not empty, in fact it is rather large.

Lemma 4.35. *Define the subspace*

$$H_*^{-1/2}(\Gamma) := \left\{ w \in H^{-1/2}(\Gamma) : \langle w,\, 1\rangle = 0 \right\}.$$

Then

(i) For all subsets $K \subset\subset \mathbb{R}^d$ we have that $\widetilde{V}w \in H^1(K)$.

(ii) If $d = 2$ and $w \in H_*^{-1/2}(\Gamma)$ we have $\widetilde{V}w \in H$, i. e., $\|\nabla \widetilde{V}w\|_{L^2(\mathbb{R}^d)} < \infty$. If $d = 3$ this holds for all $w \in H^{-1/2}(\Gamma)$.

Proof. (i) follows immediately from Lemma 4.22. A proof of (ii) can be found in [Steinbach] and it involves the concrete fundamental solutions and their decay behaviour as $|x| \to \infty$. □

This implies that V is $H^{-1/2}(\Gamma)$-elliptic for $d = 3$ and $H_*^{-1/2}(\Gamma)$-elliptic for $d = 2$. In order to see what happens on the "rest" of $H^{-1/2}(\Gamma)$ we do the following construction. We seek $t \in H^{-1/2}(\Gamma)$ such that

$$\langle t,\, Vw\rangle_\Gamma \;=\; 0 \qquad \forall w \in H_*^{-1/2}(\Gamma)$$

and normalize the solution such that $\langle t,\, \mathbf{1}\rangle_\Gamma = 1$. It turns out that we can decompose $t = \widetilde{t} + \alpha\mathbf{1}$ with $\widetilde{t} \in H_*^{-1/2}(\Gamma)$ and $\alpha \in \mathbb{R}$, and that this decomposition is unique: from

$$1 \;=\; \langle t,\, \mathbf{1}\rangle_\Gamma \;=\; \underbrace{\langle \widetilde{t},\, \mathbf{1}\rangle}_{=0} + \alpha\, \langle \mathbf{1},\, \mathbf{1}\rangle_\Gamma$$

we get that $\alpha = |\Gamma|^{-1}$. Hence, we search $\widetilde{t} \in H_*^{-1/2}(\Gamma)$:

$$\langle \widetilde{t},\, Vw\rangle \;=\; -|\Gamma|^{-1}\, \langle \mathbf{1},\, Vw\rangle \qquad \forall w \in H_*^{-1/2}(\Gamma)\,.$$

Due to the Lax-Milgram lemma (see Lemma 4.40 below) this variational equation is uniquely solvable. We define the *natural density*

$$w_{\mathrm{eq}} := \widetilde{t} + |\Gamma|^{-1}\, \mathbf{1}\,.$$

Note that this functional depends only on Γ. We summarize

- $\langle V w_{\mathrm{eq}},\, w\rangle = 0$ for all $w \in H_*^{-1/2}(\Gamma)$,
- $\langle w_{\mathrm{eq}},\, \mathbf{1}\rangle = 1$.

Exercise. Show that $V\, w_{\mathrm{eq}}$ is constant and compute $\langle w_{\mathrm{eq}},\, V w_{\mathrm{eq}}\rangle$. Show also that for $w \in H^{-1/2}(\Gamma)$ there exists the unique decomposition

$$w \;=\; \widetilde{w} + \beta\, w_{\mathrm{eq}} \qquad \text{with } \widetilde{w} \in H_*^{-1/2}(\Gamma) \text{ and } \beta \in \mathbb{R}\,.$$

If V is elliptic on the one-dimensional space spanned by the natural density w_{eq}, we have a chance to conclude the full ellipticity. The next lemma (here presented without a proof) gives a sufficient condition.

Lemma 4.36. *If $d = 2$ and $\operatorname{diam}(\Omega) < 1$ then $\langle w_{\mathrm{eq}},\, V w_{\mathrm{eq}}\rangle > 0$.*

A proof can be found in [HsiaoWendland]. The constant $\lambda := \langle w_{\mathrm{eq}},\, V w_{\mathrm{eq}}\rangle$ depends only on Γ. Sometimes one makes use of the *logarithmic capacity* $\operatorname{cap}_\Gamma := e^{-2\pi\lambda}$. Lemma 4.36 states that this capacity is less than one.

Corollary 4.37. *If $d = 2$ and $\operatorname{diam}(\Omega) < 1$ then V is $H^{-1/2}(\Gamma)$-elliptic. The same holds for $d = 3$ without any restriction on Ω.*

Proof. The three-dimensional case follows immediately from Lemma 4.34 and Lemma 4.35. For $d = 2$ let $w \in H^{-1/2}(\Gamma)$. We know that $w = \widetilde{w} + \beta\, w_{\mathrm{eq}}$ with $\widetilde{w} \in H_*^{-1/2}(\Gamma)$ and $\beta \in \mathbb{R}$. Hence, by an elementary inequality,

$$\|w\|^2_{H^{-1/2}(\Gamma)} \;\leq\; 2\Big[\|\widetilde{w}\|^2_{H^{-1/2}(\Gamma)} + \beta^2\, \|w_{\mathrm{eq}}\|^2_{H^{-1/2}(\Gamma)}\Big]\,.$$

Recall that $\langle w_{\mathrm{eq}},\, V\widetilde{w}\rangle = 0$ (i. e., the decomposition is orthogonal with respect to the V-form) and that V is self-adjoint. Thus, we can conclude from Lemma 4.34 and Lemma 4.35 that

$$\begin{aligned}
\langle w,\, Vw\rangle \;&=\; \langle \widetilde{w},\, V\widetilde{w}\rangle + 2\beta\, \underbrace{\langle w_{\mathrm{eq}},\, V\widetilde{w}\rangle}_{=0} + \beta^2\, \langle w_{\mathrm{eq}},\, V w_{\mathrm{eq}}\rangle \\
&\geq\; c_V\, \|\widetilde{w}\|^2_{H^{-1/2}(\Gamma)} + \langle w_{\mathrm{eq}},\, V w_{\mathrm{eq}}\rangle\, \beta^2 \\
&\geq \min\left\{c_V,\, \frac{\langle w_{\mathrm{eq}},\, V w_{\mathrm{eq}}\rangle}{\|w_{\mathrm{eq}}\|^2_{H^{-1/2}(\Gamma)}}\right\} \Big[\|\widetilde{w}\|^2_{H^{-1/2}(\Gamma)} + \beta^2\, \|w_{\mathrm{eq}}\|^2_{H^{-1/2}(\Gamma)}\Big] \\
&\geq \widetilde{c}_V\, \|w\|^2_{H^{-1/2}(\Gamma)}\,,
\end{aligned}$$

with $\widetilde{c}_V := \frac{1}{2}\min\left\{c_V,\, \frac{\langle w_{\mathrm{eq}}, V w_{\mathrm{eq}}\rangle}{\|w_{\mathrm{eq}}\|^2_{H^{-1/2}(\Gamma)}}\right\}$. □

In the following we assume that if $d = 2$ then $\operatorname{diam}(\Omega) < 1$ such that V is always elliptic.

Remark 4.38. 1. In order to ensure that the condition $\operatorname{diam}(\Omega) < 1$ is satisfied, a simple coordinate scaling suffices,

$$\widehat{x} := \frac{1}{2\operatorname{diam}(\Omega)}\, x\,.$$

2. Why do we need this condition for $d = 2$ at all? The reason is the logarithm appearing in the fundamental solution. Assume that Ω is such that V is $H^{-1/2}(\Gamma)$-elliptic. With a scalar parameter $H > 0$ we define new coordinates

$$\widehat{x} := H\, x\,,$$

then $ds_{\widehat{x}} = H^2\, ds_x$. Let $\widehat{\Gamma}$ denote the transformed boundary, and for $w \in H^{-1/2}(\Gamma)$, let $\widehat{w}(\widehat{x}) := w(\widehat{x}/H)$. If w is smooth we have

$$\begin{aligned}
(Vw)(x) &= -\frac{1}{2\pi}\int_\Gamma \log|x-y|\, w(y) ds_y \\
&= -\frac{1}{2\pi}\int_{\widehat{\Gamma}} \log\big(H^{-1}|x-y|\big)\, \widehat{w}(\widehat{y}) H^{-2}\, ds_{\widehat{y}} \\
&= \underbrace{-\frac{H^{-2}}{2\pi}\int_{\widehat{\Gamma}} \log|x-y|\, \widehat{w}(\widehat{y})\, ds_{\widehat{y}}}_{=H^{-2}\,(\widehat{V}\widehat{w})(\widehat{x})} + \frac{H^{-2}}{2\pi}\log(H)\int_{\widehat{\Gamma}} \widehat{w}(\widehat{y})\, ds_{\widehat{y}}\,.
\end{aligned}$$

We easily show that

$$\begin{aligned}
\langle \widehat{w},\, \widehat{V}\widehat{w}\rangle_{\widehat{\Gamma}} &= \int_\Gamma w(x)\Big\{H^2\,(Vw)(x) - \frac{\log(H)}{2\pi}\int_{\widehat{\Gamma}} \widehat{w}(\widehat{y})\, ds_{\widehat{y}}\Big\} H^2\, ds_x \\
&= H^4\Big\{\langle w,\, Vw\rangle_\Gamma - \frac{\log(H)}{2\pi}\Big(\int_{\widehat{\Gamma}} \widehat{w}(\widehat{y})\, ds_{\widehat{y}}\Big)^2\Big\}\,.
\end{aligned}$$

We see that by choosing H sufficiently large, we can make the additive term large enough such that $\langle \widehat{w},\, \widehat{V}\widehat{w}\rangle_{\widehat{\Gamma}}$ gets negative for $\int_{\widehat{\Gamma}} \widehat{w}\, ds \neq 0$ which is if and only if $\widehat{w} \notin H_*^{-1/2}(\widehat{\Gamma})$.

3. In order to compute the natural density (or an approximation thereof), we can first solve

$$V\widetilde{w}_{\mathrm{eq}} \;=\; 1 \qquad \text{in } H^{1/2}(\Gamma)\,,$$

and then set $w_{\mathrm{eq}} := \frac{1}{\langle \widetilde{w}_{\mathrm{eq}},\, 1\rangle_\Gamma}\, \widetilde{w}_{\mathrm{eq}}$.

The next lemma discusses the ellipticity properties of the hypersingular operator. Therefor, we need to define the subspace

$$\begin{aligned}
H_*^{1/2}(\Gamma) &:= \big\{v \in H^{1/2}(\Gamma) : \langle w_{\mathrm{eq}},\, v\rangle = 0\big\} \\
&= \big\{v \in H^{1/2}(\Gamma) : \langle V^{-1}\mathbf{1},\, v\rangle = 0\big\}\,.
\end{aligned}$$

Lemma 4.39. *The hypersingular operator D is $H_*^{1/2}(\Gamma)$-elliptic, i. e., there exists a constant $c_D > 0$ such that*

$$\langle D\,v,\, v\rangle \;\geq\; c_D\,\|v\|^2_{H^{1/2}(\Gamma)} \qquad \forall v \in H_*^{1/2}(\Gamma)\,.$$

Moreover, $D\,\mathbf{1} = 0$ and there exists a constant $\widetilde{c}_D > 0$ with

$$\langle D\,v,\, v\rangle \;\geq\; \widetilde{c}_D\,|v|^2_{H^{1/2}(\Gamma)} \qquad \forall v \in H^{1/2}(\Gamma)\,.$$

In the context of elliptic operators (like V and D) we can make use of the following well-known lemma.

Lemma 4.40 (Lax-Milgram)**.** *Let X be a Hilbert space and let $A : X \to X^*$ be linear, bounded, and elliptic, i. e., there exist constants $\overline{c}_A$, $\underline{c}_A > 0$ such that*

$$\left.\begin{aligned} \langle A\,v,\, v\rangle &\;\geq\; \underline{c}_A\,\|v\|^2_X \\ \|A\,v\|_{X^*} &\;\leq\; \overline{c}_A\,\|v\|_X \end{aligned}\right\} \qquad \forall v \in X\,.$$

Then, for all $f \in X^*$, the problem

$$\text{find } u \in X: \quad A\,u \;=\; f \qquad \text{in } X^*$$

has a unique solution and

$$\|u\|_X \;\leq\; \frac{1}{\underline{c}_A}\,\|f\|_{X^*}\,.$$

For a proof see, e. g., the lecture on numerical methods for partial differential equations. Note that the lemma states that $A^{-1} : X^* \to X$ is well-defined (obviously linear) and continuous.

We can summarize that the single layer potential operator V induces a norm $\|w\|_V := \sqrt{\langle w,\, Vw\rangle}$ on $H^{-1/2}(\Gamma)$, and $\|v\|_{V^{-1}} := \sqrt{\langle V^{-1}v,\, v\rangle}$ on $H^{1/2}(\Gamma)$, whereas the hypersingular operator induces a semi-norm $|v|_D := \sqrt{\langle D\,v,\, v\rangle}$ on $H^{1/2}(\Gamma)$.

It is straightforward to show that V is an isomorphism between $H_*^{-1/2}(\Gamma)$ and $H_*^{1/2}(\Gamma)$.

4.5.2 Properties of K and K'

If Γ is a smooth surface, then K and K' are compact operators. This is, however, not anymore true for a general Lipschitz domain. We only remark that the operators $\frac{1}{2}I \pm K$, $\frac{1}{2}I \pm K'$ can be shown to be contractions, at least in the subspaces $H_*^{1/2}(\Gamma)$ and $H_*^{-1/2}(\Gamma)$. Therefore, Banach's fixed point theorem guarantees the (unique) solvability of equations involving one these operators, see also [Steinbach].

4.5.3 Mapping properties

The operators V, K, K', and D are so-called *pseudo-differential operators* of integer order: for $s \in [-\frac{1}{2}, \frac{1}{2}]$ the mappings

$$\begin{aligned} V &: H^{-1/2+s}(\Gamma) \to H^{1/2+s}(\Gamma)\,, \\ K &: H^{1/2+s}(\Gamma) \to H^{1/2+s}(\Gamma)\,, \\ K' &: H^{-1/2+s}(\Gamma) \to H^{-1/2+s}(\Gamma)\,, \\ D &: H^{1/2+s}(\Gamma) \to H^{-1/2+s}(\Gamma) \end{aligned}$$

are continuous. Hence, K and K' are pseudo differential operators of order 0, V is of order $+1$ (a smoothing operator), and D is of order -1 (a differential type operator). A proof is found in [Costabel].

4.6 Boundary integral equations

4.6.1 The Dirichlet boundary value problem

Consider the classical formulation of a pure Dirichlet problem: for a given function g on Γ find $t = \frac{\partial u}{\partial n}$ where

$$\begin{aligned} -\Delta u &= 0 \qquad \text{in } \Omega\,, \\ u &= g \qquad \text{on } \Gamma\,. \end{aligned}$$

Translated into an abstract framework we wish to find $t \in H^{-1/2}(\Gamma)$ such that

$$V\,t \;=\; (\tfrac{1}{2}I + K)g \qquad \text{in } H^{1/2}(\Gamma)\,. \tag{4.7}$$

As we have seen before, $V : H^{-1/2}(\Gamma) \to H^{1/2}(\Gamma)$ is self-adjoint, linear, bounded, and elliptic. The spaces $H^{\pm 1/2}(\Gamma)$ are reflexive (i. e., the dual of the dual is the original space), and so $(\frac{1}{2}I + K)g$ is really in the dual of $H^{-1/2}(\Gamma)$. Due to the Lax-Milgram lemma, equation (4.7) is uniquely solvable and

$$\|t\|_{H^{-1/2}(\Gamma)} \;\le\; \frac{1}{\widetilde{c}_V}\,\|(\tfrac{1}{2}I + K)g\|_{H^{1/2}(\Gamma)} \;\le\; C\,\|g\|_{H^{1/2}(\Gamma)}\,,$$

where in the last step we have used the boundedness of $\frac{1}{2}I + K$. In other words, t depends continuously on the data g.

4.6.2 The Steklov-Poincaré operator

In the above setting we can write $t = V^{-1}(\frac{1}{2}I + K)g$ and define the *Steklov-Poincaré operator*

$$S := V^{-1}(\tfrac{1}{2}I + K)\,.$$

Obviously, this operator is linear and bounded. Since $t = S\,g$ above, S is also called *Dirichlet-to-Neumann map*. Using the second Calderón equation in (4.5), we find that

$$t \;=\; D\,g + (\tfrac{1}{2}I + K')t\,,$$

and so

$$S \;=\; D + (\tfrac{1}{2}I + K')V^{-1}(\tfrac{1}{2}I + K)\,.$$

This shows that S is self-adjoint. It can also be shown that S has the same ellipticity properties as D, i. e., it induces a semi-norm on $H^{1/2}(\Gamma)$.

4.6.3 The Neumann boundary value problem

Using the second equation in (4.5) the Neumann boundary value problem can be written the following way. Given $t \in H^{-1/2}(\Gamma)$, find $g \in H^{1/2}(\Gamma)$:

$$D\,g \;=\; (\tfrac{1}{2}I - K')t$$

Since D is only semi-elliptic and $\ker(D) = \operatorname{span}\{\mathbf{1}\}$, we obtain the solvability condition $(\frac{1}{2}I - K')t \in \operatorname{range}(D)$ which can be shown to be equivalent to

$$\langle t,\, 1\rangle_\Gamma = 0\,.$$

The above equation is then solvable up to a constant. As a regularization one can use

$$\langle \widetilde{D}\,u,\, v\rangle \;=\; \langle D\,u,\, v\rangle + \alpha\,\langle w_{\mathrm{eq}},\, u\rangle\,\langle w_{\mathrm{eq}},\, v\rangle$$

with a positive regularization parameter α. We can also replace w_{eq} above by $\mathbf{1}$. In both cases, $\widetilde{D}$ is bounded and elliptic on the whole of $H^{1/2}(\Gamma)$ and therefore invertible. The unique solution g of $\widetilde{D}\,g = (\frac{1}{2}I - K')t$ also solves $D\,g = (\frac{1}{2}I - K')t$, provided that $\langle t,\, 1\rangle_\Gamma = 0$.

4.6.4 Exterior problems

For simplicity consider first the exterior Dirichlet problem. For a given function g on Γ, find $t = \frac{\partial u}{\partial n}$ such that

$$\begin{aligned} -\Delta u \;&=\; 0 \quad \text{in } \Omega^{\mathrm{ext}} \\ \gamma_0^{\mathrm{ext}} u \;&=\; g \quad \text{on } \Gamma\,. \end{aligned}$$

If we pose this equation in $H^1(\Omega^{\text{ext}})$ we face two problems. First, the surface potentials $\widetilde{V}$ and $\widetilde{W}$ are in general *not* in $H^1(\Omega^{\text{ext}})$ (cf. Lemma 4.22) and so it will be difficult to represent the solution. Secondly, solutions in $H^1(\Omega^{\text{ext}})$ decay very fast, usually not like solutions of physical problems (e. g., acoustic or electromagnetic waves propagation). For $d = 3$ a typical *radiation condition* for Laplace's equation is

$$|u(x)| \;=\; \mathcal{O}(|x|^{-1}) \qquad \text{as } |x| \to \infty\,.$$

Enlarging the space to

$$\begin{aligned} H^1_*(\Omega^{\text{ext}}) = \{u \in \mathcal{D}'(\Omega^{\text{ext}}) :\; & -\Delta u = 0 \text{ weakly in } \Omega^{\text{ext}}\,, \\ & u \in H^1(U) \quad \forall U \subset\subset \Omega^{\text{ext}} \text{ and} \\ & |u(x)| = \mathcal{O}(|x|^{-1}) \text{ as } |x| \to \infty\} \end{aligned}$$

we can derive the same tools (e. g., Green's third identity), and obtain the boundary integral equations

$$\begin{pmatrix} \gamma_0^{\text{ext}} u \\ \gamma_1^{\text{ext}} u \end{pmatrix} \;=\; \begin{pmatrix} \frac{1}{2} I + K & -V \\ -D & \frac{1}{2} I - K' \end{pmatrix} \begin{pmatrix} \gamma_0^{\text{ext}} u \\ \gamma_1^{\text{ext}} u \end{pmatrix}\,.$$

Note that there is only a sign-flip in V and D compared to an interior problem. We see that with the radiation condition above, the treatment of exterior problems is analogous to interior ones. A precise treatment of radiation conditions can be found in [McLean].

4.6.5 Mixed boundary value problems

Let Γ_D and Γ_N be disjoint non-trivial parts of Γ such that $\Gamma = \overline{\Gamma_D \cup \Gamma_N}$. Given g_D on Γ_D and g_N on Γ_N find u with

$$\begin{aligned} -\Delta u &= 0 && \text{in } \Omega\,, \\ u &= g_D && \text{on } \Gamma_D\,, \\ \frac{\partial u}{\partial n} &= g_N && \text{on } \Gamma_N\,. \end{aligned}$$

Translating this classical formulation to a variational framework, we should clarify in which spaces the traces $\gamma_0^{\text{int}} u_{|\Gamma_N}$ and $\gamma_1^{\text{int}} u_{|\Gamma_D}$ have to lie. To this end we fix an extension $\widetilde{u} \in H^1(\Omega)$ with $u_{|\Gamma_D} = g_D$ and homogenize the problem: we wish to find $u - \widetilde{u} =: u_0 \in H^1_D(\Omega)$ such that

$$\int_\Omega \nabla u_0 \cdot \nabla v \, dx \;=\; \int_{\Gamma_N} g_N \, v \, dx - \int_\Omega \nabla \widetilde{u} \cdot \nabla v \, dx \qquad \forall v \in H^1_D(\Omega)\,,$$

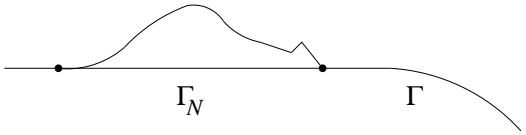


Figure 4.1: Illustration of the space $\widetilde{H}^{1/2}(\Gamma_N)$.

where $H^1_D(\Omega) = \{v \in H^1(\Omega) : v_{|\Gamma_D} = 0\}$. We find that $\gamma_0^{\text{int}} u_0$, $\gamma_0^{\text{int}} v \in H^{1/2}(\Gamma)$ and they vanish on Γ_D. In order to characterize this property we introduce the space

$$\widetilde{H}^{1/2}(\Gamma_N) := \overline{C_0^\infty(\Gamma_N)}^{\|\cdot\|_{H^{1/2}(\Gamma)}},$$

which can easily be shown to be a subspace of $H^{1/2}(\Gamma_N)$. More precisely $\widetilde{H}^{1/2}(\Gamma_N)$ contains all functions from $H^{1/2}(\Gamma_N)$ that can be extended by zero to Γ such that the resulting function is still in $H^{1/2}(\Gamma)$ (see Figure 4.1). We set

$$H^{-1/2}(\Gamma_N) := \widetilde{H}^{1/2}(\Gamma_N)^*, \qquad \widetilde{H}^{-1/2}(\Gamma_N) := H^{1/2}(\Gamma_N)^*,$$

and repeat the same definitions replacing Γ_N by Γ_D. Note that

$$\widetilde{H}^{1/2}(\Gamma_N) \overset{\neq}{\subset} H^{1/2}(\Gamma_N), \qquad H^{-1/2}(\Gamma_N) \overset{\neq}{\supset} \widetilde{H}^{-1/2}(\Gamma_N).$$

We find that in the homogenized variational formulation above, $\gamma_0^{\text{int}} u_0$, $\gamma_0^{\text{int}} v \in \widetilde{H}^{1/2}(\Gamma_N)$. Thus we can assume

$$g_N \in H^{-1/2}(\Gamma_N) \;=\; \widetilde{H}^{1/2}(\Gamma_N)^*,$$

and replace the integral over Γ_N by the corresponding duality product. Furthermore, we construct the following extensions

$$\begin{aligned}
&\widetilde{g}_D \in H^{1/2}(\Gamma): && (\widetilde{g}_D)_{|\Gamma_D} &&= g_D, \\
&\widetilde{g}_N \in H^{-1/2}(\Gamma): && \langle \widetilde{g}_N, v\rangle_\Gamma &&= \langle g_N, v\rangle_{\Gamma_N} \qquad \forall v \in \widetilde{H}^{1/2}(\Gamma_N),
\end{aligned}$$

and set

$$\begin{aligned}
u_0 &:= \gamma_0^{\text{int}} u - \widetilde{g}_D \qquad \in \widetilde{H}^{1/2}(\Gamma_N), \\
t_0 &:= \gamma_1^{\text{int}} u - \widetilde{g}_N \qquad \in \widetilde{H}^{-1/2}(\Gamma_D).
\end{aligned}$$

Then we obtain the following system from Calderón's equations,

$$\begin{pmatrix} V & -K \\ K' & D \end{pmatrix} \begin{pmatrix} t_0 \\ u_0 \end{pmatrix} = \begin{pmatrix} -V & \frac{1}{2}I + K \\ \frac{1}{2}I - K' & -D \end{pmatrix} \begin{pmatrix} \widetilde{g}_N \\ \widetilde{g}_D \end{pmatrix}.$$

This system can be shown to be block-skew symmetric and coercive, i. e., Lax-Milgram ensures the existence of a unique solution. Multiplying the last line by -1, we obtain a block-symmetric and indefinite system, a saddle-point problem. Such systems are well-treated in the lecture on numerical methods for continuum mechanics.

Chapter 5

Galerkin BEM

5.1 Abstract projection methods

Let X and Y be reflexive Hilbert spaces and let $A : X \to Y^*$ be a linear, bounded, and bijective operator. For $f \in Y^*$ given we consider the operator equation

$$\text{find } u \in X : \quad A\,u \;=\; f \qquad \text{in } Y^*\,,$$

which is equivalent to the variational formulation

$$\text{find } u \in X : \quad \langle A\,u,\, v\rangle \;=\; \langle f,\, v\rangle \qquad \forall v \in Y\,.$$

In order to define a projection method we consider finite dimensional subspaces $X_h \subset X$ and $Y_h \subset Y$ with the following bases,

$$X_h \;=\; \operatorname{span}\{\varphi_i\}_{i=1}^{n_h}\,, \qquad Y_h \;=\; \operatorname{span}\{\psi_i\}_{i=1}^{n_h}\,.$$

We now restrict the above variational formulation to these subspaces.

$$\text{Find } u_h \in X_h : \quad \langle A\,u_h,\, v_h\rangle \;= \langle f,\, v_h\rangle \qquad \forall v_h \in Y_h\,.$$

Apparently, the resulting residual $f - A\,u_h \in Y^*$ is then orthogonal to Y_h with respect to the duality-product. In that sense we have projected the residual to the complement of Y_h. Due to linearity it is sufficient that the variational equation holds for the basis functions ψ_i only. Since $u_h = \sum_{i=1}^{n_h} u_j\,\varphi_j$ for some coefficients $\{u_j\}$ this yields the system

$$\sum_{j=1}^{n_h} u_j \underbrace{\langle A,\, \varphi_j,\, \psi_i\rangle}_{=:[A_h]_{ij}} \;=\; \underbrace{\langle f,\, \psi\rangle}_{=:[\underline{f}_h]_i}\,,$$

which is linear in the coefficients u_j. With $\underline{u}_h = [u_j]_{j=1}^{n_h}$ we get the matrix-vector form

$$A_h \, \underline{u}_h \;=\; \underline{f}_h \, .$$

Here, X_h is called *trial space*, and Y_h the *test space*. Most of the time, $Y = X$ and $Y_h = X_h$. Then we speak of a *Galerkin method*. If X_h and Y_h differ from each other, we speak in general of a *Galerkin-Petrov method*. If $Y^* = X$ and if we choose $\psi_i = A\,\varphi_i$ we obtain a *least-squares* method, being equivalent to minimize $\|A\,u_h - f\|_X^2$ for $u_h \in X_h$.

The following two examples illustrate Galerkin methods for two of the boundary integral equations we have discussed before.

Example 5.1 (Dirichlet problem)**.** For a fixed $g \in H^{1/2}(\Gamma)$, consider the equation

$$\text{find } t \in H^{-1/2}(\Gamma): \quad V\,t \;=\; (\tfrac{1}{2}I + K)g$$

($X := Y := H^{-1/2}(\Gamma)$, $A := V$, and $f := (\frac{1}{2}I + K)g$). If we fix $X_h = \operatorname{span}\{\varphi_i\}_{i=1}^{n_h}$ we obtain the linear system

$$V_h \, \underline{t}_h \;=\; \underline{r}_h \, ,$$

with $[V_h]_{ij} = \langle \varphi_j, V\varphi_i \rangle$ and $[\underline{r}_h]_i = \langle \varphi_i, (\frac{1}{2}I + K)g \rangle$.

Example 5.2 (Neumann problem)**.** For a fixed $t \in H^{-1/2}(\Gamma)$, consider the equation

$$\widetilde{D}\,u \;=\; (\tfrac{1}{2}I - K')t$$

($X := Y := H^{1/2}(\Gamma)$, $A = \widetilde{D}$, and $f := (\frac{1}{2}I - K')t$). If we fix $X_h = \operatorname{span}\{\varphi_i\}_{i=1}^{n_h}$ we obtain the linear system

$$\widetilde{D}_h \, \underline{u}_h \;=\; \underline{r}_h \, ,$$

with $[\widetilde{D}_h]_{ij} = \langle \widetilde{D}\,\varphi_j, \varphi_i \rangle$ and $[\underline{r}_h]_i = \langle (\frac{1}{2}I - K')t, \varphi_i \rangle$. Here, $\widetilde{D}$ is a suitable regularization of D, see Section 4.6.3.

The next example draws a connection to the collocation method discussed in Chapter 3.

Example 5.3 (Collocation method)**.** Suppose that $X \subset C(\Gamma)$ and $Y^* \subset C(\Gamma)$, and that $\delta_y \in Y$ for arbitrary points $y \in \Gamma$. Let $X_h = \operatorname{span}\{\varphi_i\}_{i=1}^{n_h}$. For a fixed set of collocation points $\{y_i\}_{i=1}^{n_h}$ we define the basis for Y_h to be

$$\psi_i := \delta_{y_i} \, .$$

The problem of the collocation method is that we need the variables and expressions under consideration to be continuous. For $d = 2$ or 3 and $\Gamma \in C^1$ we have the regularity result $u \in H^2(\Omega) \subset C(\overline{\Omega})$ only for suitable boundary data. Here we see that the collocation method is limited, and indeed only little theory is known.

In the following we treat Galerkin methods only. There we have the following important result.

Lemma 5.4 (Céa)**.** *Let the operator $A : X \to X^*$ be linear, bounded, and elliptic and fix $f \in X^*$ and $X_h \subset X$. Let furthermore $u \in X$ and $u_h \in X_h$ be such that*

$$\begin{aligned} \langle A\,u,\, v\rangle &= \langle f,\, v\rangle \qquad \forall v \in X\,, \\ \langle A\,u_h,\, v_h\rangle &= \langle f,\, v_h\rangle \qquad \forall v_h \in X_h\,. \end{aligned}$$

Then we have the estimates

$$\|u_h\|_X \;\leq\; \frac{1}{\underline{c}_A}\,\|f\|_{X^*}\,,$$

and

$$\|u - u_h\|_X \;\leq\; \frac{\overline{c}_A}{\underline{c}_A} \inf_{v_h \in X_h} \|u - v_h\|_X\,.$$

The proof is based on the result of the Lax-Milgram lemma and the *Galerkin orthogonality*

$$\langle A(u - u_h),\, v_h\rangle \;=\; 0 \qquad \forall v_h \in V_h\,,$$

see, e. g., the lecture on numerical methods for partial differential equations.

5.2 Trial spaces

Suppose first that Ω is polygonal (polyhedral if $d = 3$), i. e.,

$$\Gamma \;=\; \bigcup_{j=1}^{J} \overline{\Gamma}_j\,,$$

where Γ_j are line segments (plane polygons if $d = 3$).

Consider a family $\{\Gamma_h\}_{h\in\Theta}$ of regular meshes

$$\Gamma_h = \bigcup_{i=1}^{n_h^{\mathrm{el}}} \overline{\tau}_{h,i}\,,$$

where the *elements* $\tau_{h,i}$ are line segments (plane triangles if $d = 3$). Since we will only treat one mesh at the time, we simply write $\tau_i := \tau_{h,i}$. Let $\{x_j\}_{j=1}^{n_h^{\mathrm{nd}}}$ be the *nodes* of the mesh. Note that due to our assumption that Ω is polygonal (polyhedral) we have $\Gamma_h = \Gamma$.

For each element we define the *local mesh size*

$$h_i := |\tau_i|^{1/(d-1)}, \qquad \text{and set} \qquad h := \max_{i=1}^{n_h^{\mathrm{el}}},$$

where $|\tau_i|$ denotes the length (area) of the element. We assume *shape regularity* (i. e., for $d = 3$ the radius ρ_i of the largest inscribed circle in τ_i fulfills $\rho_i > c\, h_i$ with a uniform constant $c > 0$) and a *quasi-uniform* mesh:

$$h_i \;\geq\; c\, h \qquad \forall i = 1, \ldots, n_h^{\mathrm{el}}.$$

Now we can define the *basis functions*

$$\varphi_i^0 \;:=\; \chi_{\tau_i} \qquad \text{for } i = 1, \ldots, n_h^{\mathrm{el}},$$

$$\varphi_j^1 \;:=\; \left\{ \begin{array}{ll} 1 & \text{if } x = x_j \\ 0 & \text{if } x = x_k,\ k \neq j \\ \text{continuous p.w. affine linear elsewhere} & \end{array} \right\} \qquad \text{for } j = 1, \ldots, n_h^{\mathrm{nd}},$$

where χ_{τ_i} is the characteristic function, and we define the spaces

$$\begin{aligned} S_h^0(\Gamma) &:= \operatorname{span}\{\varphi_i^0\}_{i=1}^{n_h^{\mathrm{el}}} && \text{(p.w. constant, discontinuous)}, \\ S_h^1(\Gamma) &:= \operatorname{span}\{\varphi_j^1\}_{j=1}^{n_h^{\mathrm{nd}}} && \text{(p.w. affine linear, continuous)}. \end{aligned}$$

Like in the FEM, the basis functions can be constructed via reference elements. Via an affine linear transformation, each element τ_i can be mapped to the reference element $\widehat{\tau}$ (the interval $(0, 1)$ for $d = 2$, and the well-known reference triangle for $d = 3$), cf. Figure 5.1. The shape functions on the reference element read

$$\left\{ \begin{array}{l} \widehat{\varphi}_0^1(\xi) = 1 - \xi \\ \widehat{\varphi}_1^1(\xi) = \xi \end{array} \right\} \qquad \left\{ \begin{array}{l} \widehat{\varphi}_0^1(\xi) = 1 - \xi_1 - \xi_2 \\ \widehat{\varphi}_1^1(\xi) = \xi_1 \\ \widehat{\varphi}_2^1(\xi) = \xi_2 \end{array} \right\}$$

for the interval and the triangle, respectively. We remark that using suitable transformations the spaces $S_h^0(\Gamma)$, $S_h^1(\Gamma)$ can also be defined for curved boundaries.

In the following we briefly discuss the approximation properties of these spaces; for more details see, e g., [Steinbach].

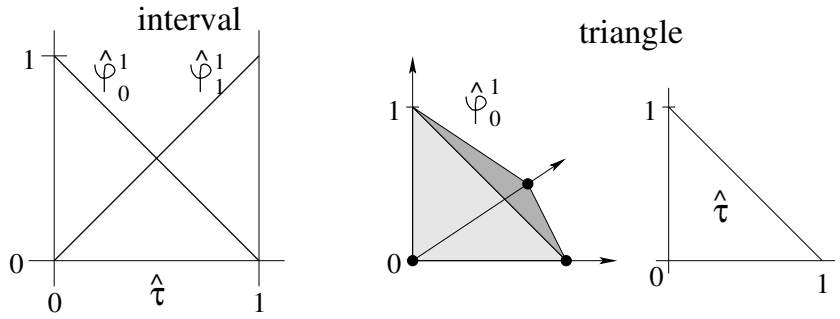


Figure 5.1: Reference elements, sketches of affine linear basis functions.

Lemma 5.5 (approximation by $S_h^0(\Gamma)$)**.** *Let $\sigma \in [-1, 0]$, $s \in [\sigma, 1]$ and $t \in H^s(\Gamma)$. Then*

$$\inf_{w_h \in S_h^0(\Gamma)} \|t - w_h\|_{H^\sigma(\Gamma)} \;\leq\; c\, h^{s-\sigma}\, \|t\|_{H^s(\Gamma)}\,,$$

where the norm on the right hand side can be replaced by the seminorm $|t|_{H^s(\Gamma)}$ if $s > 0$. The same holds if replace Γ by a part $\widetilde{\Gamma} \subset \Gamma$.

Lemma 5.6 (approximation by $S_h^1(\Gamma)$)**.** *Let $\sigma \in [0, 1]$, $s \in [\sigma, 2]$ and $u \in H^s(\Gamma)$. Then*

$$\inf_{v_h \in S_h^1(\Gamma)} \|u - v_h\|_{H^\sigma(\Gamma)} \;\leq\; c\, h^{s-\sigma}\, \|u\|_{H^s(\Gamma)}\,,$$

where the norm on the right hand side can be replaced by the seminorm $|u|_{H^s(\Gamma)}$ if $s > 0$.

5.3 Error estimates for the Dirichlet BVP

First, we discuss the error in the normal derivative. Therefor we need to define

$$H^s_{\mathrm{pw}}(\Gamma) := \left\{ v \in L^2(\Gamma) : v_{|\Gamma_j} \in H^s(\Gamma_j) \quad \forall j = 1, \ldots, J \right\},$$

where Γ_j are the smooth edges (faces) of the polygon (polyhedron) Γ, equipped with the norm

$$\|t\|_{H^s_{\mathrm{pw}}(\Gamma)} := \Big(\sum_{j=1}^{J} \|t\|^2_{H^s(\Gamma_j)} \Big)^{1/2}.$$

Analogously we can define the seminorm $|t|_{H^s_{\mathrm{pw}}(\Gamma)}$. We need this because the normal vector is discontinuous and so is the normal derivative $t = \gamma_1^{\mathrm{int}} u$.

Let now $t \in H^{-1/2}(\Gamma)$ and $t_h \in S_h^0(\Gamma)$ fulfill

$$\begin{aligned} \langle w, V\,t\rangle &= \langle w, (\tfrac{1}{2}I + K)g\rangle \qquad \forall w \in H^{-1/2}(\Gamma)\,, \\ \langle w_h, V\,t_h\rangle &= \langle w_h, (\tfrac{1}{2}I + K)g\rangle \qquad \forall w_h \in S_h^0(\Gamma)\,. \end{aligned} \tag{5.1}$$

Then Céa's lemma implies that

$$\|t - t_h\|_{H^{-1/2}(\Gamma)} \;\leq\; c \inf_{w_h \in S_h^0(\Gamma)} \|t - w_h\|_{H^{-1/2}(\Gamma)}\,.$$

From Lemma 5.5 we can conclude that

$$\|t - t_h\|_{H^{-1/2}(\Gamma)} \;\leq\; c\,h^{s+\frac{1}{2}}\,\|t\|_{H^s_{\mathrm{pw}}} \qquad \text{for } s \in [-\tfrac{1}{2},\,1]\,, \tag{5.2}$$

of course assumed that the normal derivative of the solution fulfills this regularity. In the optimal case, if $t \in H^1_{\mathrm{pw}}(\Gamma)$, we obtain the convergence rate $\mathcal{O}(h^{3/2})$ as $h \to 0$.

Remark 5.7. We have the following regularity result for the Dirichlet problem due to [Dauge]. Let Ω be convex and let ω denote the largest angle between the parts Γ_i. Then

$$g \in H^{3/2+\sigma}(\Gamma) \quad\Longrightarrow\quad u \in H^{2+\sigma}(\Omega) \qquad \text{for } \sigma \in \big(-\tfrac{1}{2},\,\min\big\{\tfrac{3}{2},\,\tfrac{\pi}{\omega} - 1\big\}\big)\,.$$

We see that if $\omega < \frac{2}{3}\pi$ and $g \in H^2(\Gamma)$, then $u \in H^{5/2}(\Omega)$ which implies that $\nabla u \in [H^{3/2}(\Omega)]^d$. It can be shown that $\gamma_0 : H^{3/2}(\Omega) \to H^1_{\mathrm{pw}}(\Gamma)$ for polygonal (polyhedral) Lipschitz domains. Thus, we can expect that $t \in \gamma_1^{\mathrm{int}} u = (\gamma_0 \nabla u)\cdot n \in H^s_{\mathrm{pw}}(\Gamma)$ for $s \in [-\frac{1}{2}, 1]$, and we obtain the optimal convergence rate $\mathcal{O}(h^{3/2})$ for the assumptions on g and Γ above.

Finally, we discuss the error in the *interior* of Ω. Let t, t_h solve (5.1) and let $u \in H^1(\Omega)$ be harmonic such that $\gamma_0^{\mathrm{int}} u = g$ and $\gamma_1^{\mathrm{int}} u = t$, i. e.,

$$u \;=\; \widetilde{V}\,t - \widetilde{W}\,g\,.$$

Due to Lemma 4.22 we know that $u_{|\Omega} \in C^\infty(\Omega)$ (note that $u \notin C^\infty(\overline{\Omega})$, but only $u \in H^1(\Omega)$). We set

$$u_h := \;\widetilde{V}\,t_h - \widetilde{W}\,g\,,$$

i. e., the harmonic function such that $\gamma_0^{\mathrm{int}} u_h = g$ and $\gamma_1^{\mathrm{int}} u_h = t_h$. Also $u_{h|\Omega} \in C^\infty(\Omega)$. Hence, for a point $\widetilde{x} \in \Omega$, we can investigate the error

$$|u(\widetilde{x}) - u_h(\widetilde{x})| \;=\; |\widetilde{V}(t - t_h)(\widetilde{x})|\,.$$

Recall that for smooth functions we have

$$\widetilde{V}(t-t_h)(\widetilde{x}) \;=\; \int_\Gamma U^*(\widetilde{x},\, y)\,\big[t(y)-t_h(y)\big]\,ds_y\,.$$

Assume now that $t,\ t_h \in H^\sigma(\Gamma)$ for some σ (e. g., $\sigma = -\frac{1}{2}$). Then, since $U^*(\widetilde{x},\,\cdot) \in C^\infty(\Gamma) \subset H^{-\sigma}(\Gamma)$, we get by duality that

$$|u(\widetilde{x}) - u_h(\widetilde{x})| \;\le\; \|U^*(\widetilde{x},\,\cdot)\|_{H^{-\sigma}(\Gamma)}\,\|t-t_h\|_{H^\sigma(\Gamma)}\,.$$

Due to a result by Aubin and Nitsche (see e. g., [Steinbach]), the statement of Lemma 5.5 holds also for $\sigma \in [-2,\,-\frac{1}{2}]$, $s \in [-\frac{1}{2},\,1]$. Thus, we can choose $\sigma = -2$ and obtain

$$|u(\widetilde{x}) - u_h(\widetilde{x})| \;\le\; c\,h^{2+s}\,\|U^*(\widetilde{x},\,\cdot)\|_{H^2(\Gamma)}\,\|t\|_{H^s_{\rm pw}(\Gamma)}\,,$$

where again $\|t\|_{H^s_{\rm pw}(\Gamma)}$ may be replaced by the corresponding seminorm if $s > 0$. This means, for our Lipschitz polygon (polyhedron) we get the optimal convergence rate $\mathcal{O}(h^3)$.

Remark 5.8. We can also give a bound for the H^1-error using variational techniques (see, e. g., [Steinbach]). Let u_h be defined as above, then

$$\|u-u_h\|_{H^1(\Omega)} \;\le\; c\,\|t-t_h\|_{H^{-1/2}(\Gamma)} \;\le\; c\,h^{s+\frac{1}{2}}\,\|t\|_{H^s_{\rm pw}(\Gamma)}$$

for $s \in [-\frac{1}{2},\,1]$. Thus, the optimal convergence rate is $\mathcal{O}(h^{3/2})$. This is in contrast to the FEM where we obtain only a rate of $\mathcal{O}(h)$ for linear elements!

5.4 Computation of matrix entries

In principle the computation of the matrix entries

$$\begin{aligned}[V_h]_{ij} \;&=\; \langle \varphi_j^0,\, V\varphi_i^0\rangle_\Gamma \qquad\qquad \text{for } i,\,j = 1,\ldots,n_h^{\rm el}\\ &=\; \int_{\tau_i}\int_{\tau_j} U^*(x,\,y)\,ds_x\,ds_y\end{aligned}$$

is very similar to what we have seen in Chapter 3. The double integrals can be computed analytically where $[V_h]_{ij}$ involves a weakly singular surface integral if $i = j$ or if $\tau_i,\ \tau_j$ touch each other. For details we refer to [Rjasanow/Steinbach] and [Sauter/Schwab]. The following boundary element matrices are also often needed:

$$\left.\begin{aligned}[K_h]_{ik} \;&=\; \langle \varphi_i^0,\, K\,\varphi_k^1\rangle_\Gamma\\ [M_h]_{ik} \;&=\; \langle \varphi_i^0,\, \varphi_k^1\rangle_\Gamma\end{aligned}\right\} \qquad \text{for } i = 1,\ldots,n_h^{\rm el},\ k = 1,\ldots,n_h^{\rm nd}\,.$$

We can make use of these in our Dirichlet problem when we represent the Dirichlet data by a continuous piecewise affine linear function. The matrix M_h is a mass matrix; note that it does *not* equal the identity matrix. However, in contrast to the other boundary element matrices, the mass matrix M_h is sparse. The operator $\frac{1}{2}I+K$ is then obviously discretized by $\frac{1}{2}M_h+K_h$.

For other boundary value problems, we need the matrix

$$\begin{aligned}[D_h]_{k\ell} &= \langle D\,\varphi_\ell^1,\,\varphi_k^1\rangle_\Gamma \qquad\qquad \text{for } k,\,\ell = 1,\,\ldots,\,n_h^{\mathrm{nd}} \\ &= \langle \underbrace{\operatorname{curl}_\Gamma \varphi_\ell^1}_{\in S_h^0(\Gamma)},\, V\, \underbrace{\operatorname{curl}_\Gamma \varphi_k^1}_{\in S_h^0(\Gamma)}\rangle_\Gamma\,,\end{aligned}$$

where we have used Lemmas 4.29 and 4.30; the fact that $\operatorname{curl}_\Gamma \varphi_k^1 \in S_h^0(\Gamma)$ is easily seen. Let $w_h \in S_h^1(\Gamma)$ with the coefficient vector $\underline{w}_h \in \mathbb{R}^{n_h^{\mathrm{el}}}$ (we write $\underline{w}_h \leftrightarrow w_h$), and let $\underline{v}_h \leftrightarrow v_h \in S_h^1(\Gamma)$. Then it turns out that there exists a sparse matrix C_h such that

$$w_h \;=\; \operatorname{curl}_\Gamma v_h \quad\Longleftrightarrow\quad \underline{w}_h \;=\; C_h\,\underline{v}_h\,.$$

Thus,

$$D_h \;=\; C_h^\top V_h\, C_h\,.$$

The adjoint of K' corresponds of course to $K_h^\top$. We see that we basically need to compute entries of V_h and K_h in order to discretize the BVPs discussed in Section 4.6.

Exercise. Give an explicit description of the matrix C_h.

5.5 The conditioning of V_h

In this section we briefly investigate the spectral condition number of V_h. The condition number of a typical FEM stiffness matrix is $\mathcal{O}(h^{-2})$ as $h \to 0$. The next lemma shows that $\kappa(V_h) = \mathcal{O}(h^{-1})$ only.

Lemma 5.9. *Let $w_h \in S_h^0(\Gamma)$ with $w_h \leftrightarrow \underline{w}_h \in \mathbb{R}^{n_h^{el}}$. Then there exist constants $c_1,\, c_2 > 0$ such that*

$$c_1\, h^d\, \|\underline{w}_h\|_{\ell^2}^2 \;\le\; (V_h\,\underline{w}_h,\,\underline{w}_h)_{\ell^2} \;\le\; c_2\, h^{d-1}\, \|\underline{w}_h\|_{\ell^2}^2\,.$$

Hence the spectral condition number of V_h fulfills

$$\kappa(V_h) \;=\; \mathcal{O}(h^{-1})\,.$$

Proof. Surprisingly, the following proof is not based on the actual entries of V_h. Instead we use boundedness and ellipticity of the single layer potential operator V and properties of the spaces $H^{-1/2}(\Gamma)$ and $S_h^0(\Gamma)$. First, we observe that

$$(V_h\,\underline{w}_h,\,\underline{w}_h) \;=\; \langle w_h,\,V\,w_h\rangle\,.$$

Upper bound: Using the fact that

$$\begin{aligned}\|w_h\|_{H^{-1/2}(\Gamma)} \;&=\; \sup_{v\in H^{1/2}(\Gamma)} \frac{\langle w_h,\,v\rangle}{\|v\|_{H^{1/2}(\Gamma)}} \;\le\; \sup_{v\in H^{1/2}(\Gamma)} \frac{(w_h,\,v)_{L^2(\Gamma)}}{\|v\|_{L^2(\Gamma)}} \\ &\le\; \sup_{v\in L^2(\Gamma)} \frac{(w_h,\,v)_{L^2(\Gamma)}}{\|v\|_{L^2(\Gamma)}} \;\le\; \|w_h\|_{L^2(\Gamma)}\end{aligned}$$

and the boundedness of V we obtain

$$\begin{aligned}\langle w_h,\,V\,w_h\rangle \;&\le\; c\,\|w_h\|^2_{H^{-1/2}(\Gamma)} \;\le\; c\,\|w_h\|^2_{L^2(\Gamma)} \\ &=\; c\sum_{i=1}^{n_h^{\mathrm{el}}} w_i^2 \underbrace{|\tau_i|}_{=h_i^{d-1}\le h^{d-1}} \;\le\; c\,h^{d-1}\,\|\underline{w}_h\|^2_{\ell^2}\,,\end{aligned}$$

where in the last steps we have used the definitions of h_i and h.

Lower bound: Matters are more complicated here. In fact we need some tools.

(i) We define the *space of local bubble functions*

$$S_h^B(\Gamma) := \;\mathrm{span}\{\varphi_i^B\}_{i=1}^{n_h^{\mathrm{el}}} \quad\subset H^{1/2}(\Gamma)$$

with the basis functions φ_i^B defined via the reference element and

$$\varphi^B(\xi) := \;\begin{cases}\xi(1-\xi) & \text{if } d=2\,,\\ \xi_1\,\xi_2\,(1-\xi_1-\xi_2) & \text{if } d=3\,.\end{cases}$$

(ii) We have the *inverse inequality*

$$\|v_h\|_{H^{1/2}(\Gamma)} \;\le\; c\,h^{-1/2}\,\|v_h\|_{L^2(\Gamma)} \qquad \forall v_h\in S_h^B(\Gamma)\,.$$

This inequality can e. g. be obtained from an interpolation of corresponding estimates of the L^2- and the H^1-norm.

(iii) We define the L^2-*projection* $Q_h^B : L^2(\Gamma)\to S_h^B(\Gamma)$ by the relation

$$\int_{\tau_i}(Q_h^B w)\,ds_x \;=\; \int_{\tau_i} w\,ds_x \qquad \forall i=1,\dots,n_h^{\mathrm{el}} \quad \text{for } w\in L^2(\Gamma)\,.$$

(iv) We have the *stability estimate*

$$\|Q_h^B w\|_{L^2(\Gamma)} \;\leq\; \sqrt{2}\,\|w\|_{L^2(\Gamma)} \qquad \forall w \in L^2(\Gamma)\,,$$

cf. [Steinbach].

With the help of the above tools we can conclude that

$$\begin{aligned}\|w_h\|_{H^{-1/2}(\Gamma)} \;&=\; \sup_{v\in H^{1/2}(\Gamma)} \frac{\langle w_h,\, v\rangle}{\|v\|_{H^{1/2}(\Gamma)}} \;\geq\; \frac{\langle w_h,\, Q_h^B w_h\rangle}{\|Q_h^B w_h\|_{H^{1/2}(\Gamma)}} \\ &\overset{(iii)}{=} \frac{\int_\Gamma (w_h)^2\,ds}{\|Q_h^B w_h\|_{H^{-1/2}(\Gamma)}} \overset{(ii),(iv)}{\geq} \widetilde{c}\,h^{1/2}\,\frac{\|w_h\|^2_{L^2(\Gamma)}}{\|w_h\|_{L^2(\Gamma)}}\end{aligned}$$

where in the penultimate step we have used that w_h is piecewise constant (thus $w_h \in L^2(\Gamma)$), and so

$$\langle w_h,\, Q_h^B w_h\rangle \;=\; \int_\Gamma w_h\,(Q_h^B w_h)\,ds \;=\; \sum_{i=1}^{n_h^{\mathrm{el}}} w_{h|\tau_i} \underbrace{\int_{\tau_i} Q_h^B w_h\,ds}_{=\int_{\tau_i} w_h\,ds} \;=\; \int_\Gamma (w_h)^2\,ds\,.$$

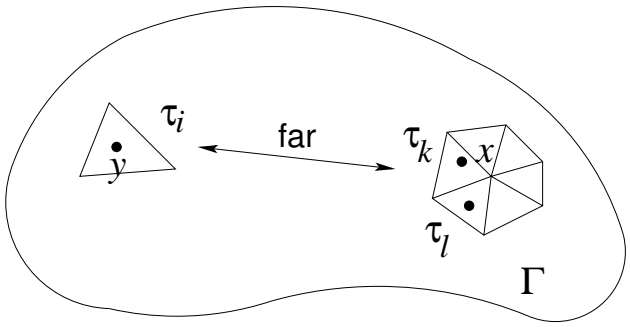
This concludes the proof. □

Chapter 6

Fast BEM

6.1 Motivation

We have seen that the crucial problem is the *storage* of the matrices V_h, K_h, etc. For a quasi-uniform mesh we need $\mathcal{O}(h^{2(d-1)})$ memory where we have only $\mathcal{O}(h^{d-1})$ unknowns. The basic idea of fast boundary element methods is to *approximate* the matrices with less storage amount. Here we give a motivation why this can be possible. Let Γ be the boundary of a three-dimensional domain, let τ_i, τ_k, τ_ℓ, etc. be elements, where τ_i is *far* away from τ_k and all the remaining elements touch τ_k, see the figure below.



With our definition of V_h we have

$$[V_h]_{ik} \;=\; \int_{\tau_i}\int_{\tau_k} \frac{1}{4\pi}\,\frac{1}{|x-y|}\,ds_x\,ds_y\,.$$

Since $1/|x-y|$ decays very fast if $|x-y|$ becomes large, we can write $|x-y| \approx |x_i^* - x_k^*|$ where x_i^* and x_k^* are the centers of τ_i and τ_k, respectively. Thus the double integral is approximated by a constant. For an element τ_ℓ touching τ_k, we have

$$[V_h]_{i\ell} \;\approx\; [V_h]_{ik}$$

because the difference $|x_i^* - x_k^*| \approx |x_i^* - x_\ell^*|$. In the figure above we can approximate *six* double integrals (six entries of the matrix) by *one* constant, which leads to a reduced storage amount. Using some tricks one can generalize this concept.

Among many fast BEM approaches are

- *wavelets* (here one constructs a special basis which leads to a sparse representation),
- the *fast multipole method* (using taylor expansion one can realize at least a fast application of the matrices),
- hierarchical matrices and data-sparse approximation

For more details see e. g., [Steinbach] and [Bebendorf]. We will follow the last approach. There the main tricks are

- low-rank matrices, and
- hierarchical clustering.

The hierarchical matrices were introduced by Hackbusch and Khoromskij. The data-sparse approximation that we will discuss is named adaptive cross approximation (ACA) and was introduced by Bebendorf and Rjasanow. Other techniques and references can be found in [Bebendorf], [Steinbach], and also online at `www.hlib.org`.

6.2 Low-rank matrices

For a matrix $A \in \mathbb{R}^{m\times n}$ we define

$$\operatorname{range}(A) := \{A\,y : y \in \mathbb{R}^n\}\,, \qquad \operatorname{rank}(A) := \dim(\operatorname{range}(A))\,.$$

Lemma 6.1. *(i)* $\operatorname{rank}(A) \le \min(m,\, n) \quad \forall A \in \mathbb{R}^{m\times n}$

(ii) $\operatorname{rank}(A\,B) \le \min(\operatorname{rank}(A),\, \operatorname{rank}(B)) \quad \forall A \in \mathbb{R}^{m\times p}\,,\ B \in \mathbb{R}^{p\times n}$

(iii) $\operatorname{rank}(A+B) \le \operatorname{rank}(A) + \operatorname{rank}(B) \quad \forall A,\, B \in \mathbb{R}^{m\times n}$

Definition 6.2. We define the *set of matrices with rank at most* k (in short: rank-k matrices),

$$\mathbb{R}_k^{m\times n} := \{A \in \mathbb{R}^{m\times n} : \operatorname{rank}(A) \le k\}\,.$$

Attention: $\mathbb{R}_k^{m\times n}$ does *not* form a linear space because addition of two rank-k matrices can increase the rank beyond k.

Lemma 6.3.

$$A \in \mathbb{R}_k^{m\times n} \quad \Longleftrightarrow \quad \exists U \in \mathbb{R}^{m\times k}\,,\ V \in \mathbb{R}^{n\times k} : A = U\,V^\top$$

The above representation $U\,V^\top$ of a rank-k matrix is called *outer product form*. Note that if we have such a representation, the matrix-vector multiplication

$$A\,y \;=\; U\,\underbrace{(V^\top y)}_{\in\mathbb{R}^k}$$

can be computed in $\mathcal{O}(k(m+n))$ operations. Also, the storage amount of U and V is only $k(m+n)$.

Definition 6.4. A matrix $A \in \mathbb{R}_k^{m\times n}$ is said to have *low rank* if

$$k(m+n) \;<\; m\,n\,.$$

Obviously we should represent (in particular store) low-rank matrices in outer product form.

Remark 6.5. Two low-rank matrices can be multiplied and added in low complexity. Also the singular value decomposition (SVD)

$$A \;=\; U\,\Sigma\,V^\top$$

(with $U \in \mathbb{R}^{m\times k}$, $V \in \mathbb{R}^{n\times k}$ orthogonal and $\Sigma \in \mathbb{R}^{k\times k}$ diagonal) of a low-rank matrix can be computed cheaply. Using that one, for A, $B \in \mathbb{R}_k^{m\times n}$, the best approximation C of the sum $A+B$ with respect to the Frobenious norm, i. e,

$$\|A+B-C\|_F \to \min_{C\in\mathbb{R}_k^{m\times n}}\,,$$

can be computed also efficiently. We refer to this approximated addition by *rounded addition*. It is a similar concept to the rounded addition of fixed floating point operations in processors, but here we do not cut the precision of a number but the rank of a matrix. The computational complexity of the rounded addition is $\mathcal{O}(k^2(m+n))$.

6.3 Degenerate kernels

Unfortunately, boundary element matrices *cannot* be approximated by low-rank matrices (but as will turn out certain matrix blocks can). They would, if the kernel of the underlying integral operator had a different form.

Definition 6.6. Let D_1, D_2 be subsets of $\mathbb{R}^d$ or a manifold Γ. An integral kernel $\kappa : D_1 \times D_2 \to \mathbb{R}$ is called *degenerate* if there exists a constant $k \in \mathbb{N}$ and functions $u_\ell : D_1 \to \mathbb{R}$, $v_\ell : D_2 \to \mathbb{R}$ for $\ell = 1, \ldots, k$ such that

$$\kappa(x, y) \;=\; \sum_{\ell=1}^{k} u_\ell(x)\, v_\ell(y) \qquad \forall x \in D_1,\, y \in D_2\,.$$

The number k is called *degree of degeneracy*.

Suppose we have a matrix A defined by

$$A_{ij} \;=\; \int_\Gamma \int_\Gamma \kappa(x, y)\, \psi_j(y)\, \varphi_i(x)\, ds_x\, ds_y$$

and suppose we have index sets I and J and submanifolds D_1, $D_2 \subset \Gamma$ with

$$\operatorname{supp}(\varphi_i) \subset D_1 \quad \forall i \in I\,, \qquad \operatorname{supp}(\psi_j) \subset D_2 \quad \forall j \in J\,.$$

If κ (restricted to $D_1 \times D_2$) is degenerate of degree k then

$$A_{ij} = \sum_{\ell=1}^{k} \int_{D_1} u_\ell(x)\varphi_i(x)\, ds_x \int_{D_1} v_\ell(y)\psi_j(y)\, ds_y \qquad \forall i \in I,\, j \in J\,,$$

and so the block $[A_{ij}]_{i\in I,\, j\in J}$ has rank k.

The kernels appearing in our boundary integral operators are not degenerate. However, we can try to *approximate* them by degenerate kernels.

6.4 Asymptotically smooth kernels

Definition 6.7. An integral kernel $\kappa : D_1 \times \mathbb{R}^d \to \mathbb{R}$ with $\kappa(x, \cdot) \in C^\infty(\mathbb{R}^d \setminus \{x\})$ for all $x \in D_1$ is called *asymptotically smooth* in D_1 with respect to y if there exist constants γ, $c > 0$ such that for all $x \in D_1$ we have

$$\left|\partial_y^\alpha \kappa(x, y)\right| \;\leq\; c\,|\alpha|!\,\gamma^{|\alpha|}\,\frac{|\kappa(x, y)|}{|x - y|^{|\alpha|}} \qquad \forall \text{ multi-indices } \alpha \;\; \forall y \in \mathbb{R}^d \setminus \{x\}\,.$$

Remark 6.8. The kernels $U^*(x,\, y)$ and $\frac{\partial}{\partial n_x} U^*(x,\, y)$ appearing in V and K can be shown to be asymptotically smooth.

We want to exploit this smoothness for a Taylor expansion. However, in the vicinty of the singulary we cannot expect good convergence. Therefore we will assume that x and y are sufficiently far away from each other.

Definition 6.9. For sets D_1, D_2 and $x \in D_1$ we define the distances

$$\operatorname{dist}(x,\, D_2) := \inf_{y \in D_2} |x - y|\,, \qquad \operatorname{dist}(D_1,\, D_2) := \inf_{x \in D_1,\, y \in D_2} |x - y|\,.$$

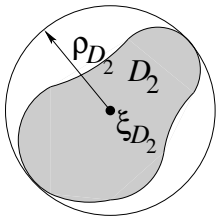
Assume now that a kernel $\kappa : D_1 \times D_2 \to \mathbb{R}$ is analytic with respect to the second argument (y) and assume at least that $\operatorname{dist}(D_1,\, D_2) > 0$. Then by Taylor's expansion we have

$$\kappa(x,\, y) \;=\; \underbrace{\sum_{|\alpha| < p} \frac{1}{\alpha!} \partial_y^\alpha \kappa(x,\, \xi_{D_2})\, (y - \xi_{D_2})^\alpha}_{=: T_p[\kappa](x,\, y)} + R_p(x,\, y)\,,$$

where

$$R_p(x,\, y) \;=\; \sum_{|\alpha| \geq p} \frac{1}{\alpha!} \partial_y^\alpha \kappa(x,\, \xi_{D_2})\, (y - \xi_{D_2})^\alpha$$

and ξ_{D_2} is the *Chebyshev center* of D_2, defined as the center of the ball of minimum radius that contains D_2. We denote the minimum radius by ρ_{D_2}, see below.



The next lemma clarifies how much error we make when cutting the Taylor series.

Lemma 6.10. *Let $\kappa : D_1 \times D_2 \to \mathbb{R}$ an integral kernel which is analytic with respect to y and let $\kappa : D_1 \times \mathbb{R}^d \to \mathbb{R}$ be asymptotically smooth. Furthermore, suppose that the condition*

$$\eta \operatorname{dist}(\xi_{D_1},\, D_2) \;\geq\; \rho_{D_2}$$

holds for some $\eta > 0$ with $2\,\gamma\,\sqrt{d}\,\eta < 1$. Then

$$\big|\kappa(x,\, y) - T_p[\kappa](x,\, y)\big| \;\leq\; \frac{(2\,\gamma\,\sqrt{d}\,\eta)^p}{1 - 2\,\gamma\,\sqrt{d}\,\eta}\, |\kappa(x,\, \xi_{D_2})|\,.$$

The lemma states that if D_1 is sufficiently far away from D_2, we have *exponential convergence* of the Taylor series as $p \to \infty$. I.e. there is hope that we can cut the series for a rather small p (which leads to a low rank representation) and to make only a small error.

Usually, we consider integral kernels which are analytic and asymptotically smooth with respect to both variables x and y. Then we use the symmetric condition

$$\min(\rho_{D_1},\, \rho_{D_2}) \;\leq\; \eta \operatorname{dist}(D_1,\, D_2) \tag{6.1}$$

instead of the condition in Lemma 6.10.

6.5 Admissible blocks

For index sets $I = \{1, \ldots, n\}$ and $J = \{1, \ldots, m\}$ we denote by $t \subset I$, $s \subset J$ *(index) blocks*. Note that the entries need not be contiguous (a block can also look like $\{2,\, 5,\, 7\}$). For $A \in \mathbb{R}^{n\times m} = \mathbb{R}^{I\times J}$ we define

$$A_{t\times s} := [A_{ij}]_{i\in t,\, k\in s}\,,$$

i. e., the restriction to the block $t \times s$. Finally, we denote by $|t|$ the number of indices in the block t.

Definition 6.11. Let $A_{t\times s}$ correspond to

$$\int_{D_1}\int_{D_2} \kappa(x,\, y)\, \psi_j(y)\, \varphi_i(x)\, ds_x\, ds_y \qquad \text{for } i \in t,\, j \in s\,,$$

with $\bigcup_{i\in t} \operatorname{supp}\varphi_i \subset D_1$ and $\bigcup_{j\in s} \operatorname{supp}\psi_j \subset D_2$. Then we call the block $t \times s$ *admissible* if (6.1) is fulfilled.

Lemma 6.12. *For an admissible block $t \times s$ and $\kappa : D_1 \times D_2 \to \mathbb{R}$ analytic and asymptotically smooth in both variables, the matrix block $A_{t\times s}$ (defined as above) can be approximated by a low-rank matrix $\widetilde{A}_{t\times s} \in \mathbb{R}_k^{t\times s}$. Let ε denote the approximation error (with respect to $\|\cdot\|_F$), then*

$$k \leq p^d \simeq |\log\varepsilon|^d\,,$$

where p denotes the order of the Taylor expansion.

The ultimate goal is to find a partition of $I \times J$ into blocks where we can use the Taylor expansion and the low-rank approximation.

Definition 6.13. A set $P \subset \mathcal{P}(I \times J)$ (where $\mathcal{P}(\cdot)$ denotes the power set) is called *partition* of $I \times J$ if

$$I \times J = \bigcup_{b \in P} b\,, \qquad \text{and} \qquad b_1 \neq b_2 \in P \implies b_1 \cap b_2 = \emptyset\,.$$

A block $b = t \times s$ of a partition is called *small* if $\min(|t|, |s|) < n_0$ where n_0 is a positive parameter. Finally, we call a partition P *admissible* if each block $b \in P$ is either admissible or small.

In the next two sections we construct admissible partitions of $I \times J$. There we restrict ourselves to a special class of partitions which are constructed by organizing the index sets I and J separately in a hierarchical tree structure.

6.6 Cluster trees

Definition 6.14. (i) Let $T = (\mathcal{V}, \mathcal{E})$ be a *tree* (i. e., a simple, directed, and connected graph with no cycles). Here $\mathcal{V}$ and $\mathcal{E}$ are the set of vertices and edges of the graph, respectively. For a vertex $t \in \mathcal{V}$ we define the *set of sons*

$$\mathcal{S}(t) := \{t' \in \mathcal{V} : (t, t') \in \mathcal{E}\}\,.$$

The *root* of the tree is a unique vertex which is not a son of any other vertex. We call a vertex a *leaf* if it has no sons. The set of leaves is

$$\mathcal{L}(T) := \{t \in \mathcal{V} : \mathcal{S}(t) = \emptyset\}\,.$$

We define the *level* of a vertex t: if t is the root, $\operatorname{level}(t) := 0$, for all other vertices t, $\operatorname{level}(t)$ is the minimal number of edges connecting t and the root. Finally, the *depth* of the tree is then defined as

$$\operatorname{depth}(T) := \max_{t \in \mathcal{V}} \operatorname{level}(t) + 1\,.$$

(ii) A tree $T_I = (\mathcal{V}, \mathcal{E})$ is called *cluster tree* of a finite index set I if the following conditions hold:

(a) I is the root of T_I,

(b) for each vertex $t \in \mathcal{V}$ we have that t is a non-empty subset of I, its sons are pairwise disjoint, and $t = \bigcup_{t' \in \mathcal{S}(t)} t'$,

(c) all vertices which are not leaves have at least two sons.

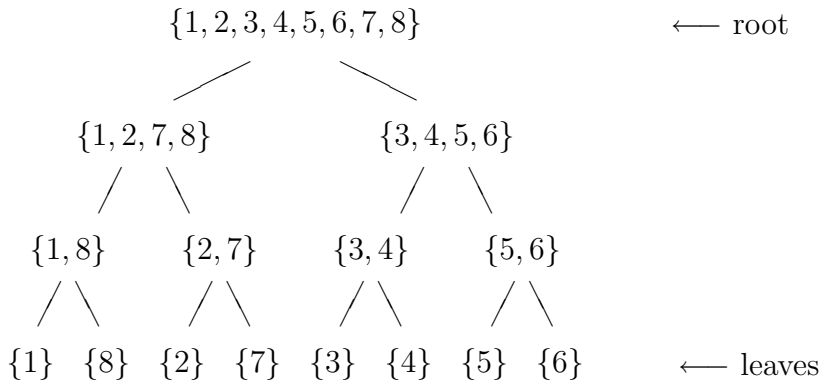


Figure 6.1: Example of a (binary) cluster tree.

Notation: For cluster trees we identify the tree with its vertices and write $t \in T_I$ instead of $t \in \mathcal{V}$.

(iii) We call a cluster tree T_I *balanced* if

$$R := \min_{t \in T_I \setminus \mathcal{L}(T_I)} \min \left\{ \frac{|t_1|}{|t_2|} : t_1,\, t_2 \in \mathcal{S}(t) \right\}$$

is bounded from below by a positive constant, independently of $|I|$.

Figure 6.1 shows an example of a cluster tree for the set $I = \{1, \ldots, 8\}$.

Lemma 6.15. *Let T_I be a balanced cluster tree. Then depth$(T_I) = \mathcal{O}(\log |I|)$. The storage complexity of T_I is then $\mathcal{O}(|I| \log |I|)$.*

For an index set I which represents a collection of elements $\{\tau_i\}_{i \in I}$, we want to generate a cluster tree T_I which will eventually lead to an admissible partition of $I \times I$ (or $I \times J$ for another cluster tree T_J). Here, we use the *principal component analysis* (PCA). To this end we associate to each element τ_i a point y_i (e. g., its center of gravity).

Definition 6.16. Let $t \subset I$ be a block.

- We define the *centroid* $m_t := \sum_{i \in t} \frac{|\tau_i|}{\sum_{j \in t} |\tau_j|}\, y_i$
- A vector $w_t \in \mathbb{R}^d$, $|w_t| = 1$ where the maximum

$$\max_{v \in \mathbb{R}^d,\, |v| = 1} \sum_{i \in t} |v \cdot (y_i - m_t)|^2$$

is attained is called *main direction* of t.

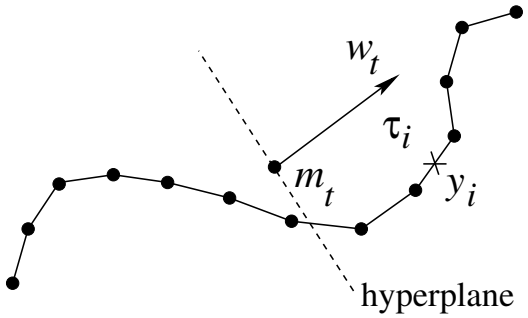


Figure 6.2: Example of block subdivision by the principal component analysis ($d = 2$).

- We define the *covariance matrix* $C_t := \sum_{i \in t} (y_i - m_t)\,(y_i - m_t)^\top \in \mathbb{R}^{d \times d}$.

Obviously, the computation of m_t can be done in linear time. But how to get the main direction? It is rather easy to see that w_t is a main direction of t if and only if $|w_t| = 1$ and w_t is an eigenvector to the maximal eigenvalue of C_t. Thus, in order to compute w_t we can form the covariance matrix C_t (in linear time) and compute its eigensystem.

Having m_t and w_t at our disposal we now subdivide the block t (which represents a collection of elements $\{\tau_i\}_{i \in t}$) using the hyperplane through m_t with normal w_t. We define the sons of t in the cluster tree by

$$\begin{aligned} \mathcal{S}(t) &:= \{t_1, t_2\} \\ t_1 &:= \{i \in t : w_t \cdot (y_1 - m_t) > 0\} \\ t_2 &:= t \setminus t_1\,, \end{aligned}$$

see also Figure 6.2. We apply this recursively to the set I and stop if a block contains less than $n_{\min}$ elements, where $n_{\min}$ is a fixed parameter. This way we get a cluster tree which we call *geometrically balanced*. Recall that we assume a shape-regular and quasi-uniform mesh. Then it can be shown that the cluster tree is also balanced in the sense of Definition 6.14(iii).

Lemma 6.17. *The construction of a cluster tree T_I for a collection of elements $\{\tau_i\}_{i \in I}$ using the principal component analysis as described above requires only $\mathcal{O}(|I| \log |I|)$ operations.*

6.7 Block cluster trees

We now use the cluster trees from the last section to construct an admissible partition for $I \times J$. Let T_I and T_J cluster trees for I and J, respectively, as

constructed above. We define the *block cluster tree* $T_{I\times J}$ by specifying the root to be $I \times J$ and defining for each block $t \times s$ the sons,

$$\mathcal{S}_{I\times J}(t\times s) := \begin{cases} \emptyset & \text{if } t\times s \text{ is admissible} \\ & \text{or } \mathcal{S}_I(t) = \emptyset \text{ or } \mathcal{S}_J(s) = \emptyset\,, \\ \mathcal{S}_I(t)\times\mathcal{S}_J(s) & \text{else.} \end{cases}$$

Above, $\mathcal{S}_{I\times J}$ indicates that the sons are to be understood with respect to the tree $T_{I\times J}$, and $\mathcal{S}_I$ with respect to the tree T_I etc. Obviously, by this construction,

$$\operatorname{depth}(T_{I\times J}) \;\le\; \min\{\operatorname{depth}(T_I), \operatorname{depth}(T_J)\}\,.$$

If T_I and T_J are binary trees (each vertex has two sons or is a leaf), $T_{I\times J}$ is a quadtree (each vertex has four sons or is a leaf).

Most importantly, by this construction the partition generated by the leaves of the block cluster tree $T_{I\times J}$ is admissible. This is because a leaf $t \times s$ is either admissible, or we have that t or s is itself a leaf of T_I or T_J, respectively, which implies that $\min(|t|, |s|) \le n_{\min}$, and so the block is small if we choose $n_{\min}$ accordingly.

A measure for the complexity of a block cluster tree is the so-called *sparsity constant*. Here, we introduce this concept only briefly, as we will just use it once on page 80. For a block $t \in T_I$ we define

$$c_{\text{sp}}^{\text{row}}(T_{I\times J},\, t) := \big|\{s \subset J : t\times s \in T_{I\times J}\}\big|\,,$$

i. e. the number of blocks $t \times s$ in the block cluster tree $T_{I\times J}$ with t being fixed. Similarly, for $s \in T_J$ we define

$$c_{\text{sp}}^{\text{col}}(T_{I\times J},\, s) := \big|\{t \subset I : t\times s \in T_{I\times J}\}\big|\,.$$

Finally, we define the sparsity constant of $T_{I\times J}$ by

$$c_{\text{sp}}(T_{I\times J}) := \max\Big\{ \max_{t\in T_I} c_{\text{sp}}^{\text{row}}(T_{I\times J},\, t)\,,\; \max_{s\in T_J} c_{\text{sp}}^{\text{col}}(T_{I\times J},\, s)\Big\}\,.$$

One can show that if T_I and T_J are geometrically balanced (e. g. constructed by the PCA) and the original mesh is shape-regular and quasi-uniform, the sparsity constant is bounded.

Lemma 6.18. *Let T_I and T_J be balanced cluster trees. Then the construction of the block cluster tree $T_{I\times J}$ as described above requires only $\mathcal{O}(|I|\,\log|I| + |J|\,\log|J|)$ operations.*

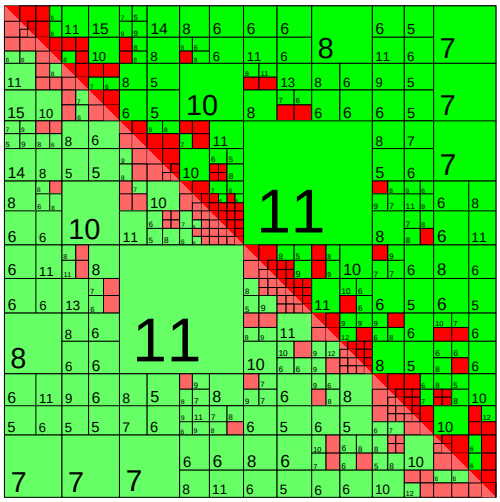


Figure 6.3: Example of a typical $\mathcal{H}$-matrix. Approximation of the single layer potential on a half-sphere discretized by 932 triangles. Green blocks: low-rank blocks (black numbers: local rank used by ACA). Red blocks: dense blocks.

6.8 The set of Hierarchical Matrices

We will now work with the partition generated by our block cluster tree and define a special kind of matrix related to it.

Definition 6.19. The set of *hierarchichal matrices* on the block cluster tree $T_{I\times J}$ with an admissible partition $P = \mathcal{L}(T_{I\times J})$ and block-wise rank k is defined as

$$\mathcal{H}(T_{I\times J},\, k) := \left\{A \in \mathbb{R}^{I\times J} : \operatorname{rank}(A_{t\times s}) \leq k \quad \forall \text{ admissible blocks } t\times s \in P\right\}.$$

In short we call this set the set of $\mathcal{H}$-matrices.

An $\mathcal{H}$-matrix is stored as follows:

- for an admissible block $t \times s$ we use the outer product representation; the storage amount is then $k(|t| + |s|)$,
- for all other blocks we use the conventional entry-wise storate; the storage amount is then bounded by $n_{\min}(|t| + |s|)$.

A typical $\mathcal{H}$-matrix is shown in Figure 6.3 (for the ACA see the next section).

We now sketch how to prove that the total storage amount $N_{\mathrm{st}}(A)$ of an $\mathcal{H}$-matrix $A \in \mathcal{H}(T_{I\times J},\, k)$ fulfills

$$N_{\mathrm{st}} \;=\; \mathcal{O}\big(\max(k,\, n_{\min})\,(|I|\,\log|I| + |J|\,\log|J|)\big)\,.$$

In order to get the storage amount we have to sum up the individual storage amounts of each leave. In fact we will bound this by a sum over *all blocks* in the tree and use the sparsity constant (see page 78):

$$\begin{aligned}
N_{\mathrm{st}} \;&\le \sum_{t\times s\in\mathcal{L}(T_{I\times J})} \max(k,\, n_{\min})\,(|t| + |s|) \;\le \sum_{t\times s\in T_{I\times J}} \max(k,\, n_{\min})\,(|t| + |s|) \\
&\le\; \max(k,\, n_{\min})\,\Big\{ \sum_{t\in T_I} \sum_{s\in T_J : t\times s\in T_{I\times J}} |t| + \sum_{s\in T_J} \sum_{t\in T_I : t\times s\in T_{I\times J}} |s| \Big\} \\
&\le\; c_{\mathrm{sp}}(T_{I\times J})\,\max(k,\, n_{\min})\,\Big\{ \sum_{t\in T_I} |t| + \sum_{s\in T_J} |s| \Big\} \\
&\le\; \widetilde{C}\,\max(k,\, n_{\min})\,(|I|\,\log|I| + |J|\,\log|J|)\big)\,.
\end{aligned}$$

Many algorithms in the context of $\mathcal{H}$-matrices perform the same kind of operations blockwise. The above technique can be used to estimate the total complexity of these algorithms.

Remark 6.20. $\mathcal{H}$-matrices generalize sparse matrices. One can e. g. show that a FEM stiffness matrix can be stored as an $\mathcal{H}$-matrix even with $\mathcal{O}(n)$ storage requirements. In constrast to sparse matrices, we call $\mathcal{H}$-matrices *data-sparse*.

Lemma 6.21. *The computational complexity of the $\mathcal{H}$-matrix by vector multiplication is $\mathcal{O}\big(\max\{k,\, n_{min}\}\big(|I|\,\log|I| + |J|\,\log|J|\big)\big)$.*

This means that we can not only use $\mathcal{H}$-matrices to represent approximations of BEM matrices, but also for iterative solver, as for instance CG, where only the application of the matrix to a vector is required. To get quasi-optimal solvers one needs of course preconditioners, and one can in fact generalize the known multi-level preconditioners for FEM (such as BPX type preconditioners) also for this purpose.

However, we will not discuss that issue, but instead point out that a whole $\mathcal{H}$-arithmetic is available, similar to the floating point arithmetic in processors. E. g. we can add two $\mathcal{H}$-matrices which are defined on the same block cluster tree by using conventional addition in the dense blocks and rounded addition in the low-rank blocks. This way, we obtain again an $\mathcal{H}$-matrix which is an approximation of the exact sum. Multiplication is rather straigtforward and can be based on the multiplication and rounded addition

of low-rank matrices. With the following idea one can even approximate the *inverse* of an $\mathcal{H}$-matrix by an $\mathcal{H}$-matrix. Consider a block t split into two sub-blocks t_1 and t_2 and suppose that

$$A_{tt} = \begin{pmatrix} A_{t_1t_1} & A_{t_1t_2} \\ A_{t_2t_1} & A_{t_2t_2} \end{pmatrix}.$$

Then by block-elimination, we have

$$A_{tt}^{-1} = \begin{pmatrix} A_{t_1t_1}^{-1} + A_{t_1t_1}^{-1} A_{t_1t_2} S^{-1} A_{t_2t_1} A_{t_1t_1}^{-1} & -A_{t_1t_1}^{-1} A_{t_1t_2} S^{-1} \\ -S^{-1} A_{t_2t_1} A_{t_1t_1}^{-1} & S^{-1} \end{pmatrix},$$

with the Schur complement $S := A_{t_2t_2} - A_{t_2t_1} A_{t_1t_1}^{-1} A_{t_1t_2}$. Using rounded addition, multiplication and recursive $\mathcal{H}$-inverse approximations for all the involved operations, one reaches some point where blocks are small and where one can use and form the conventional inverses exactly. With the same idea one can derive an $\mathcal{H}$-*LU* decomposition.

The following lemma summarizes the computational complexities.

Lemma 6.22. *1. Rounded addition of two $\mathcal{H}$-matrices requires*

$$\mathcal{O}(|I| \log |I| + |J| \log |J|)$$

operations.

2. *For $I = J$, rounded multiplication of two $\mathcal{H}$-matrices requires*

$$\mathcal{O}(k^2 |I| \log |I| + k^3 |I|)$$

operations.

3. *For $I = J$, the $\mathcal{H}$-inverse of an $\mathcal{H}$-matrix can be formed in*

$$\mathcal{O}(k^2 |I| \log |I| + k^3 |I|)$$

operations.

4. *For $I = J$, the $\mathcal{H}$-LU decomposition of an $\mathcal{H}$-matrix can be computed in*

$$\mathcal{O}(k^2 |I| \log^2 |I|)$$

operations. Once the decomposition is computed, solving can be done by forward-backward substitution.

6.9 The Adaptive Cross Approximation (ACA)

Prescribing a maximal rank and using the Taylor expansion, on could approximate our BEM matrices by suitable $\mathcal{H}$-matrices. However, (i) an error control is hard to be achieved, and (ii) we have to write new code for the integrals due to the Taylor expansion. In this final section we describe an algorithm where one can reuse existing code and where one has error control.

In order to introduce this technique we formally run the following algorithm for a matrix $A \in \mathbb{R}^{m\times n}$.

$R_0 := A$

For $\ell = 0, 1, \ldots$

Find a non-zero pivot-element (i_ℓ, j_ℓ)

$$R_{\ell+1} := R_\ell - \frac{1}{[R_\ell]_{i_\ell j_\ell}} (R_\ell)_{1:m,j_\ell} (R_\ell)_{i_\ell,1:n}$$

Until ?

Here, $(R_\ell)_{1:m,j_\ell}$ denotes the j_ℓ-th column and $(R_\ell)_{i_\ell,1:n}$ the i_ℓ-th row of R_ℓ.

Example 6.23.

$$R_0 = \begin{bmatrix} 0.431 & 0.345 & \mathbf{0.582} & 0.417 & 0.455 \\ 0.491 & 0.396 & 0.674 & 0.449 & 0.427 \\ 0.446 & 0.358 & 0.583 & 0.413 & 0.441 \\ 0.380 & 0.328 & 0.557 & 0.372 & 0.349 \\ 0.412 & 0.340 & 0.516 & 0.375 & 0.370 \end{bmatrix} \quad \begin{matrix} i_1=1 \\ j_1=3 \\ \rightarrow \end{matrix} \quad \frac{1}{0.582} \begin{bmatrix} 0.582 \\ 0.674 \\ 0.583 \\ 0.557 \\ 0.516 \end{bmatrix} \begin{bmatrix} 0.431 \\ 0.354 \\ 0.582 \\ 0.417 \\ 0.455 \end{bmatrix}^\top$$

$$R_1 = \begin{bmatrix} 0 & 0 & 0 & 0 & 0 \\ -0.008 & -0.014 & 0 & -0.033 & \mathbf{-0.100} \\ 0.014 & 0.003 & 0 & -0.004 & -0.014 \\ -0.032 & -0.011 & 0 & -0.026 & -0.087 \\ 0.029 & 0.025 & 0 & 0.005 & -0.034 \end{bmatrix} \quad \begin{matrix} i_2=2 \\ j_2=5 \\ \rightarrow \end{matrix} \quad \frac{1}{-0.1} \begin{bmatrix} 0 \\ -0.100 \\ -0.014 \\ -0.087 \\ -0.034 \end{bmatrix} \begin{bmatrix} -0.008 \\ -0.014 \\ 0 \\ -0.033 \\ -0.100 \end{bmatrix}^\top$$

$$R_2 = \begin{bmatrix} 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 \\ \mathbf{0.016} & 0.005 & 0 & 0.000 & 0 \\ -0.020 & 0.001 & 0 & 0.002 & 0 \\ 0.032 & 0.030 & 0 & 0.017 & 0 \end{bmatrix} \quad \begin{matrix} i_3=3 \\ j_3=1 \\ \rightarrow \end{matrix} \quad \frac{1}{0.016} \begin{bmatrix} 0 \\ 0 \\ 0.016 \\ -0.020 \\ 0.032 \end{bmatrix} \begin{bmatrix} 0.016 \\ 0.005 \\ 0 \\ 0.000 \\ 0 \end{bmatrix}^\top$$

In the (only illustrative) example we see that we formally subtract a "cross" build by the row and column we have chosen. Also, the absolute values of the remaining matrix entries get smaller and smaller.

Suppose that we stop the iteration after k steps, we have

$$A = S_k + R_k\,, \qquad \text{with} \qquad S_k = \sum_{\ell=1}^{k} u_\ell\, v_\ell^\top\,.$$

The matrix S_k (which is naturally provided in outer-product representation) will be used as an approximation. Obviously, for the computation of S_k we only need to know *some* matrix entries *on demand*, i. e., we can reuse existing code.

The remaining two questions are how to chose the pivot elements and when to stop. We will only answer partially them. There exist algorithms to choose the right pivot elements such that when we use the stopping criterion

$$|u_\ell|\,|v_\ell| \;\leq\; \frac{\varepsilon\,(1-\eta)}{1+\varepsilon}\,\|S_k\|_F$$

for a prescribed tolerance ε and the parameter η from the admissibility condition, we get the guaranteed error bound

$$\|A - S_k\|_F \;\leq\; \varepsilon\,\|A\|_F\,.$$

The total computational complexity of the approximation is

$$\mathcal{O}(n\,\log n\,|\log\varepsilon|^{2d})$$

with $n = |I| \sim |J|$ for building the approximation. The storage amount and the complexity of the matrix-vector multiplication is

$$\mathcal{O}(n\,\log n\,|\log\varepsilon|^{d})\,.$$

The ACA can also used for preconditioning (by choosing ε large, e. g., 0.1). The software package `AHMED` (developed by Mario Bebendorf) implements $\mathcal{H}$-matrices and ACA. $\mathcal{H}$-matrices and alternative approximation techniques can be found in the package `Hlib`, see `www.hlib.org`.

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