Efficient evaluation of the representation formula for boundary element methods

Barbara Fuchs

Born 26th May 1988 in Bad Honnef, Germany

September 25, 2012

Master's Thesis Mathematics

Advisor: Prof. Dr. Mario Bebendorf

Institute for Numerical Simulation

Mathematisch-Naturwissenschaftliche Fakultät der

Rheinischen Friedrich-Wilhelms-Universität Bonn

Contents

Introduction

In the area of acoustics or electromagnetics for instance, the simulation of physical phenomena leads to the problem of solving elliptic partial differential equations. Usually, such problems cannot be solved explicitly, so their solution needs to be determined numerically in finite dimensional spaces. Two common methods are the *finite element method* (FEM) and the *boundary element method* (BEM). Both methods have different advantages and disadvantages. In the three-dimensional case we have to discretize the volume of the computational domain Ω in order to use the FEM whereas the BEM only needs the discretization of the area $\partial\Omega$. Obviously, the resulting degree of freedom N using BEM is significantly smaller than by using FEM. A serious drawback of BEM are the non-symmetric and fully populated system matrices in contrast to the sparse and symmetric system matrices of FEM. Thus the complexity for solving elliptic partial differential equations via FEM or BEM needs $\mathcal{O}(N)$ and $\mathcal{O}(N^2)$ operations respectively. With some techniques like Panel-Clustering (cf. [4]) the BEM only needs $\mathcal{O}(N \log N)$ operations. The most important advantage of BEM arises if we want to solve the exterior boundary value problem on unbounded domains. Since BEM leads to boundary integral equations we do not need to discretize the unbounded domain Ω, only the small boundary $\partial\Omega$. The solution of such boundary integral equations automatically fulfills the radiation condition $u(x) \to 0$ for $|x| \to \infty$. Using FEM it is not clear how to handle this condition. Because of this reason BEM is the preferred method to solve exterior boundary value problems in acoustics or field theory.

The principle of BEM consists of reformulating elliptic differential equations to boundary integral equations. Solving these equations we obtain a solution on the boundary. Green's formula represents the solution at any point outside the boundary by boundary integrals. Since the evaluation of these integrals via Gauss quadrature is neither efficient nor stable near the boundary we will introduce a new method. In the first chapter of this master's thesis elliptic partial differential equations and the resulting boundary integral equations are considered in addition to the theoretical background of completing the boundary data. Since kernel functions form the main part of Green's representation formula, they are discussed in detail in chapter two. Properties of kernel functions such as asymptotic smoothness are considered as well as possibilities to approximate them by degenerate kernels. These degenerate kernels can be computed by Taylor expansion or adaptive cross approximation (ACA). For the latter a fast algorithm is presented. The advantage of this algorithm is that neither derivatives must be computed nor the required

rank needs to be known in advance. In chapter three we introduce a concept to partition the boundary in an efficient way using so-called cluster-trees. Furthermore, the number of needed clusters is estimated. The next both chapters deal with error and complexity estimates of the introduced algorithm which are established in chapter six.

Chapter 1

Problem

The aim of this master's thesis is to find an efficient way to evaluate the solution of boundary integral equations at several points. Hence, we solve the problem

$$\begin{array}{rcll} \mathscr{L}u & = & f & \text{in } \Omega \text{ (or } \Omega^c), \\ \gamma_0 u & = & g_D & \text{on } \Gamma_D, \\ \gamma_1 u & = & g_N & \text{on } \Gamma_N \end{array} \tag{1.1}$$

on bounded Lipschitz domains $\Omega \subset \mathbb{R}^d$ or its complement $\Omega^c := \mathbb{R}^d \setminus \overline{\Omega}$. The considered operator $\mathscr{L}$ is a second order partial differential operator. $\mathscr{L}$ can be scalar or a system of m operators

$$(\mathscr{L}u)_k = -\sum_{i,j=1}^{d} \sum_{l=1}^{m} \partial_i (c_{ij}^{kl} \partial_j) u_l + \delta^{kl} u_l, \quad k = 1, \ldots, m, \tag{1.2}$$

with coefficient functions c_{ij}^{kl} and δ^{kl}, $i, j = 1, \ldots, d$, $k, l = 1, \ldots, m$. Furthermore f, the Dirichlet data g_D and the Neumann data g_N are given on parts Γ_D and Γ_N of the boundary $\partial\Omega =: \Gamma = \overline{\Gamma}_D \cup \overline{\Gamma}_N$. In (1.1), we denote the Dirichlet trace by γ_0. Let $\nu(x)$ be the outer normal at the point $x \in \Gamma_N$. Then the co-normal derivative is defined by

$$(\gamma_1 u)_k := \sum_{i,j=1}^{d} \sum_{l=1}^{m} \nu_i \, c_{ij}^{kl} \, \partial_j u_l \quad \text{on } \Gamma_N.$$

.

1.1 Preliminaries

In the following chapters we assume that the differential operator $\mathscr{L}$ is uniform elliptic. That means the operator $\mathscr{L}$ fulfills

$$\sum_{i,j=1}^{d} \sum_{k,l=1}^{m} c_{ij}^{kl} \, v_i w_k v_j w_l \geq \lambda_{\mathscr{L}} \|v\|^2 \|w\|^2 \quad \text{for all } v \in \mathbb{R}^d, w \in \mathbb{R}^m, \tag{1.3}$$

the so called **Legendre-Hadamard condition**. In (1.3), $\|\cdot\|$ denotes the Euclidean norm and $\lambda_{\mathscr{L}}$ is a constant with $\lambda_{\mathscr{L}} > 0$. In addition, we assume that c_{ij}^{kl} is bounded, thus

$$\max_{x\in\Omega} |c_{ij}^{kl}(x)| \leq \Lambda_{\mathscr{L}}, \quad i,j = 1,\ldots,d, \quad k,l = 1,\ldots,m.$$

The solution of (1.1) and its components, respectively, is searched in **Sobolev spaces**

$$W^{k,p}(\Omega) := \{u \in L^p(\Omega) : \partial^\alpha u \in L^p(\Omega) \text{ for all } |\alpha| \leq k\}, \quad k \in \mathbb{N}_0,\ p \in \mathbb{N},$$

where we denote by ∂^α the weak derivative

$$\partial^\alpha = \left(\frac{\partial}{\partial_{x_1}}\right)^{\alpha_1} \left(\frac{\partial}{\partial_{x_2}}\right)^{\alpha_2} \cdots \left(\frac{\partial}{\partial_{x_d}}\right)^{\alpha_d}$$

with the multi-index $\alpha \in \mathbb{N}_0$. For any multi-index $\alpha \in \mathbb{N}_0$ we define $|\alpha| := \alpha_1+\alpha_2+\ldots+\alpha_d$, $x^\alpha := x_1^{\alpha_1} \cdot x_2^{\alpha_2} \cdot \ldots \cdot x_d^{\alpha_d}$ and $\alpha! := \alpha_1! \cdot \alpha_2! \cdot \ldots \cdot \alpha_d!$. With respect to the Sobolev space $W^{k,p}$ we define the Sobolev norm

$$\|u\|_{W^{k,p}(\Omega)} := \left(\sum_{|\alpha|\leq k} \|\partial^\alpha u\|_{L^p(\Omega)}^p\right)^{\frac{1}{p}}.$$

Let supp $u := \overline{\{x \in \Omega : u(x) \neq 0\}}$ denote the support of u in Ω, then we can define the set $W_0^{k,p}(\Omega)$ as the closure of the set

$$C_0^\infty(\Omega) := \{u \in C^\infty(\Omega) : \text{supp } u \subset \Omega\}$$

in $W_{k,p}(\Omega)$ with respect to the norm $\|\cdot\|_{W^{k,p}(\Omega)}$. For the case $p = 2$ the Sobolev spaces are in addition **Hilbert spaces**, denoted by $H^k(\Omega) := W^{k,2}(\Omega)$ and $H_0^k(\Omega) := W_0^{k,2}(\Omega)$ with the scalar product

$$(u,v)_{H^k(\Omega)} := \sum_{|\alpha|\leq k} \int_\Omega \partial^\alpha u\, \partial^\alpha v \ \mathrm{d}x.$$

The Sobolev space $H^{-k}(\Omega)$ of negative order is defined as the dual space of $H_0^k(\Omega)$.

On the boundary, we can define Sobolev spaces $H^s(\Gamma)$, $s \in \mathbb{R}$ by using parameterizations of Γ. Therefore, we require that the boundary Γ is in $C^{k-1,1}$. For a part $\Gamma_0 \subset \Gamma$ of the boundary Γ the Sobolev spaces $H^s(\Gamma_0)$ and $\widetilde{H}^s(\Gamma_0)$, $s \geq 0$ are defined by

$$H^s(\Gamma_0) := \{u|_{\Gamma_0} : u \in H^s(\Gamma)\}$$
$$\widetilde{H}^s(\Gamma_0) := \{u|_{\Gamma_0} : u \in H^s(\Gamma),\ \text{supp } u \subset \overline{\Gamma}_0\}$$

with the norm

$$\|u\|_{H^s(\Gamma_0)} := \inf\{\|\widetilde{u}\|_{H^s(\Gamma)} : \widetilde{u} \in H^s(\Gamma),\ \widetilde{u}|_{\Gamma_0} = u\}.$$

Negative Sobolev spaces on the part Γ_0 of the boundary are defined again by duality

$$H^{-s}(\Gamma_0) := [\widetilde{H}^s(\Gamma_0)]'$$
$$\widetilde{H}^{-s}(\Gamma_0) := [H^s(\Gamma_0)]'.$$

1.2 Green's Representation Formula

Assume that $g_D \in H^{\frac{1}{2}}(\Gamma_D)$ and $g_N \in H^{-\frac{1}{2}}(\Gamma_N)$. Then the solution u of (1.1) is uniquely defined by conditions on the boundary Γ supposed that the Dirichlet part has positive measure. If additional constraints are imposed, then also pure Neumann problems can be treated. On these conditions, we can reformulate the boundary value problem (1.1) with $f = 0$ as integral equations on the boundary Γ. For simplicity, we consider operators

$$(\mathscr{L}u)_k = -\sum_{i,j=1}^{d}\sum_{l=1}^{m}\partial_i(c_{ij}^{kl}\partial_j)u_l, \quad k = 1,\dots,m.$$

Thus we restrict ourselves to the leading part of the operator $\mathscr{L}$.

Let δ denote Dirac's δ. We assume that for $\mathscr{L}$ a **singularity function** S can be found, i.e. an $m \times m$ matrix of functions satisfying

$$\mathscr{L}S = \delta I_m \quad \in \mathbb{R}^d.$$

At least for operators with constant coefficients the existence of S can be guaranteed. We need to know S explicitly, since S will appear as part of the kernel function of the resulting integral operators. To simplify matters we show how the boundary integral equations are derived if $\mathscr{L} = -\Delta$ is the Laplacian. For this operator, the co-normal derivative γ_1 coincides with the normal derivative ∂_ν.

Theorem 1.1. *The solution u of (1.1) can be computed in Ω or its exterior Ω^c with* ***Green's representation formula***

$$\pm u(x) = (\mathcal{V}t)(x) - (\mathcal{K}u)(x), \quad x \in \Omega \ (x \in \Omega^c), \tag{1.4}$$

by the Dirichlet data $u(x)$ and the Neumann data $t(x) := \partial_\nu u(x)$ for $x \in \Gamma$. For the exterior boundary value problem, the assumption

$$u(x) \to 0, \quad \text{for } \|x\| \to \infty,$$

is needed in addition.

In (1.4), $\mathcal{V}$ denotes the **single-layer potential operator**

$$(\mathcal{V}w)(x) := \int_\Gamma S(y-x)w(y)\,\mathrm{d}s_y, \quad x \in \mathbb{R}^d, \tag{1.5}$$

acting on w on the boundary $\Gamma = \Gamma_D \cup \Gamma_N$. $\mathcal{K}$ is the **double-layer potential operator**

$$(\mathcal{K}w)(x) := \int_\Gamma w(y)\partial_{\nu_y}S(y-x)\,\mathrm{d}s_y, \quad x \in \mathbb{R}^d, \tag{1.6}$$

and

$$S(x) = \begin{cases} -\frac{1}{2}|x|, & d = 1 \\ -\frac{1}{2\pi} \ln \|x\|, & d = 2 \\ \frac{1}{(d-1)\omega_d'} \|x\|^{2-d}, & d \geq 3 \end{cases} \tag{1.7}$$

denotes the singularity function of the Laplacian, where ω_d' is the surface measure of the unit sphere in $\mathbb{R}^d$. Hence $\pm u(x)$ can be written as

$$\pm u(x) = \int_\Gamma S(y-x) \partial_{\nu_y} u(y) \, \mathrm{d}s_y - \int_\Gamma u(y) \partial_{\nu_y} S(y-x) \, \mathrm{d}s_y.$$

Proof. (cf. [5]). Without loss of generality we consider the interior boundary value problem. The above representation follows from Green's first identity

$$\int_\Omega \operatorname{grad} w \cdot \operatorname{grad} u \, \mathrm{d}x = \int_\Gamma w \, \partial_\nu u \, \mathrm{d}s - \int_\Omega w \Delta u \, \mathrm{d}x,$$

and Green's second identity

$$\int_\Omega (w \Delta u - u \Delta w) \, \mathrm{d}x = \int_\Gamma (w \, \partial_\nu u - u \, \partial_\nu w) \, \mathrm{d}s.$$

Using the second identity with $w(y) = S(y-x)$, we obtain Green's third identity

$$\begin{aligned} u(x) &= \int_\Omega S(y-x) \underbrace{\Delta_y u(y)}_{0} - u(y) \underbrace{\Delta_y S(y-x)}_{-\delta(x)} \, \mathrm{d}y \\ &= \int_\Gamma S(y-x) \, \partial_{\nu_y} u(y) - u(y) \, \partial_{\nu_y} S(y-x) \, \mathrm{d}s_y. \end{aligned}$$

□

1.3 Symmetric Boundary Integral Formulation

In order to evaluate the representation formula (1.4) we need to know u and $\partial_\nu u$ on the whole boundary Γ. In this chapter we will describe how the Cauchy data $[\gamma_0 u, \gamma_1 u]$ can be completed, since u is only known on Γ_D and $\partial_\nu u$ is only known on Γ_N.

Let

$$(\mathcal{K}' w)(y) := \int_\Gamma w(x) \partial_{\nu_y} S(x-y) \, \mathrm{d}s_x, \quad y \in \Gamma$$

denote the adjoint of $\mathcal{K}$ and $\mathcal{D}$ be the **hypersingular operator** obtained by applying the negative Neumann trace γ_1 to the double-layer potential operator (1.6). If we apply the trace operators γ_0 and γ_1 to Green's formula (1.4) together with the **jump relations**

$$\begin{aligned}\partial_\nu(\mathcal{V}w)(y) &\to (\mathcal{K}'w)(y_0) \pm \frac{1}{2}w(y_0),\\ (\mathcal{K}w)(y) &\to (\mathcal{K}w)(y_0) \mp \frac{1}{2}w(y_0),\end{aligned}$$

which map any $y \in \Omega$ ($y \in \Omega^c$) to a $y_0 \in \Gamma$, we obtain

$$\begin{aligned}\gamma_0 u &= \gamma_0(\mathcal{V}\partial_\nu u - \mathcal{K}u)\\ &= \mathcal{V}\gamma_1 u - \mathcal{K}\gamma_0 u \pm \frac{1}{2}\gamma_0 u\end{aligned}$$

and

$$\begin{aligned}\gamma_1 u &= \gamma_1(\mathcal{V}\partial_\nu u - \mathcal{K}u)\\ &= \mathcal{K}'\gamma_1 u \pm \frac{1}{2}\gamma_1 u - \mathcal{K}\gamma_1 u\\ &= \mathcal{K}'\gamma_1 u \pm \frac{1}{2}\gamma_1 u + \mathcal{D}\gamma_0 u.\end{aligned}$$

Hence we get the following system of boundary integral equations on Γ

$$\begin{bmatrix} \gamma_0 u \\ \gamma_1 u \end{bmatrix} = \begin{bmatrix} \pm\frac{1}{2}\mathcal{I} - \mathcal{K} & \mathcal{V} \\ \mathcal{D} & \pm\frac{1}{2}\mathcal{I} + \mathcal{K}' \end{bmatrix} \begin{bmatrix} \gamma_0 u \\ \gamma_1 u \end{bmatrix}. \tag{1.8}$$

Next, we will introduce some properties of the single-layer potential, double-layer potential and hypersingular operator (cf. [5] or [7]). The single-layer potential operator $\mathcal{V} : \widetilde{H}^{-\frac{1}{2}}(\Gamma_D) \to H^{\frac{1}{2}}(\Gamma_D)$ is continuous and $\widetilde{H}^{-\frac{1}{2}}(\Gamma_D)$-**coercive**, that means

$$\langle \mathcal{V}w, w\rangle_{L^2(\Gamma_D)} \geq c_{\mathcal{V}}\|w\|^2_{\widetilde{H}^{-\frac{1}{2}}(\Gamma_D)} \qquad \text{for all } w \in \widetilde{H}^{-\frac{1}{2}}(\Gamma_D).$$

Moreover, the hypersingular operator $\mathcal{D} : \widetilde{H}^{\frac{1}{2}}(\Gamma_N) \to H^{-\frac{1}{2}}(\Gamma_N)$ is continuous and $\widetilde{H}^{\frac{1}{2}}(\Gamma_N)$-coercive, thus

$$\langle \mathcal{D}w, w\rangle_{L^2(\Gamma_N)} \geq c_{\mathcal{D}}\|w\|^2_{\widetilde{H}^{\frac{1}{2}}(\Gamma_N)} \qquad \text{for all } w \in \widetilde{H}^{\frac{1}{2}}(\Gamma_N).$$

The double-layer potential operator $\mathcal{K} : H^{\frac{1}{2}}(\Gamma) \to H^{\frac{1}{2}}(\Gamma)$ is continuous, i.e.

$$\langle \mathcal{K}v, w\rangle_{L^2(\Gamma)} \leq c_{\mathcal{K}}\|v\|_{H^{\frac{1}{2}}(\Gamma)}\|w\|_{H^{\frac{1}{2}}(\Gamma)} \qquad \text{for all } v, w \in H^{\frac{1}{2}}(\Gamma).$$

In order to complete the Cauchy data $[\gamma_0 u, \gamma_1 u]$ let $\widetilde{g}_D$ and $\widetilde{g}_N$ denote the canonical extensions of g_D and g_N to Γ. We set

$$\begin{aligned}\widetilde{u} &:= u - \widetilde{g}_D,\\ \widetilde{t} &:= t - \widetilde{g}_N,\end{aligned}$$

where $t(x) = \partial_\nu u(x)$. With this definition we have to compute $\widetilde{u} \in \widetilde{H}^{\frac{1}{2}}(\Gamma_N)$ and $\widetilde{t} \in \widetilde{H}^{-\frac{1}{2}}(\Gamma_D)$. Obviously $\widetilde{u} = 0$ on Γ_D and $\widetilde{t} = 0$ on Γ_N, thus we obtain from (1.8)

$$\begin{aligned}\widetilde{g}_D &= \frac{1}{2}\widetilde{g}_D - \mathcal{K}(\widetilde{u} + \widetilde{g}_D) + \mathcal{V}(\widetilde{t} + \widetilde{g}_N) \quad \text{on } \Gamma_D,\\ \widetilde{g}_N &= \mathcal{D}(\widetilde{u} + \widetilde{g}_D) + \frac{1}{2}\widetilde{g}_N + \mathcal{K}'(\widetilde{t} + \widetilde{g}_N) \quad \text{on } \Gamma_N\end{aligned}$$

and hence

$$\begin{aligned}-\mathcal{V}\widetilde{t} + \mathcal{K}\widetilde{u} &= \mathcal{V}\widetilde{g}_N - \left(\frac{1}{2}\mathcal{I} + \mathcal{K}\right)\widetilde{g}_D \quad \text{on } \Gamma_D,\\ \mathcal{K}'\widetilde{t} + \mathcal{D}\widetilde{u} &= \left(\frac{1}{2}\mathcal{I} - \mathcal{K}'\right)\widetilde{g}_N - \mathcal{D}\widetilde{g}_D \quad \text{on } \Gamma_N\end{aligned} \tag{1.9}$$

for the inner boundary value problem. The previous system of integral equations (1.9) is referred to as the **symmetric boundary integral formulation** of the mixed boundary value problem (1.1). If the Dirichlet boundary Γ_D does not vanish, this system of equations is uniquely solvable.

1.4 Boundary Data using Galerkin's Method

After having approximated the manifold Γ by triangles, each operator $\lambda\mathcal{I} + \mathcal{A}$ with $(\mathcal{A}v)(y) := \int_\Gamma \kappa(x,y)v(x)\,\mathrm{d}s_x$ of the symmetric boundary integral formulation (1.9) is discretized as $\lambda M + A$, where M denotes the mass matrix and A the stiffness matrix. Let the piecewise linears ϕ_j, $j \in J$, be a basis of the finite-dimensional ansatz space $V_h \subset V$; i.e. we search a solution u_h of the form $u_h = \sum_{j\in J} u_j\phi_j$. The finite-dimensional trial space $W_h \subset V'$ is spanned by the piecewise constants ψ_i, $i \in I$. We use the Galerkin method to test $(\lambda\mathcal{I} + \mathcal{A})u_h = g$ in variational form

$$\int_\Gamma \lambda u_h\psi_i + (\mathcal{A}u_h)\psi_i\,\mathrm{d}s = \int_\Gamma g\psi_i\,\mathrm{d}s, \quad i \in I.$$

Thus, the mass matrix M takes the form

$$m_{ij} = \int_\Gamma \phi_j(x)\psi_i(x)\,\mathrm{d}s, \quad i \in I, j \in J,$$

and the stiffness matrix A has the form

$$a_{ij} = \int_\Gamma\int_\Gamma \kappa(x,y)\psi_i(y)\phi_j(x)\,\mathrm{d}s_x\,\mathrm{d}s_y, \quad i \in I, j \in J.$$

The mass matrix M is sparse and does not cause any numerical problems. Since M vanishes on admissible blocks $t \times s$, i.e. blocks which satisfy

$$\min\{\operatorname{diam} X_t, \operatorname{diam} X_s\} \leq \eta \operatorname{dist}(X_s, X_t),$$

we can add the entries of M to the non-admissible blocks of an approximant of A. In our chosen way of discretization, we have $I \neq J$ for the discretization A of operators $\mathcal{A}$. Let $t \subset I$ and $s \subset J$, then we can define the following linear operators $\Lambda_{1,t} : L^2(\Gamma) \to \mathbb{R}^t$ and $\Lambda_{2,s} : L^2(\Gamma) \to \mathbb{R}^s$ by

$$\begin{aligned}(\Lambda_{1,t} f)_i &:= \int_\Gamma f(x)\psi_i(x)\,\mathrm{d}s_x, \qquad \text{for } i \in t,\\ (\Lambda_{2,s} f)_j &:= \int_\Gamma f(x)\phi_j(x)\,\mathrm{d}s_x, \qquad \text{for } j \in s.\end{aligned}$$

We define the adjoint $\Lambda_{2,s}^* \mathbb{R}^s \to L^2(\Gamma)$ of $\Lambda_{2,s} : L^2(\Gamma) \to \mathbb{R}^s$ by

$$(\Lambda_{2,s}^* z, f)_{L^2(\Gamma)} = z^T(\Lambda_{2,s} f) \quad \text{for all } z \in \mathbb{R}^s,\ f \in L^2(\Gamma).$$

Using this notation, we can write each block A_{ts} of the stiffness matrix $A \in \mathbb{R}^{I \times J}$ as

$$A_{ts} = \Lambda_{1,t}\, \mathcal{A}\, \Lambda_{2,s}^*.$$

Next, we need to define the support of $\Lambda : L^2(\Gamma) \to \mathbb{R}^t$. The support is given by

$$\operatorname{supp}\ \Lambda = \Gamma \setminus G,$$

where G is the largest open set such that $\Lambda\phi = 0$ for all ϕ with $\operatorname{supp}\ \phi \subset G$. With this definition, we set

$$\begin{aligned}Y_i &= \operatorname{supp}\ \Lambda_{1,i}, \quad i \in I,\\ X_j &= \operatorname{supp}\ \Lambda_{2,j}, \quad j \in J.\end{aligned}$$

In order to compute the entries a_{ij} of the stiffness matrix A, we need to evaluate the kernel function κ. The operators $\Lambda_{1,i}$ and $\Lambda_{2,j}$ guarantee that the kernel function κ is evaluated on $X_j \times Y_i$. Hence, for any sub-block A_{ts} of the matrix A we have to evaluate κ on $X_s := \bigcup_{j \in s} X_j$ and $Y_t = \bigcup_{i \in t} Y_i$.

Now we can turn to the discrete variational formulation of (1.9). The solution (u_h, t_h) is searched of the form

$$\begin{aligned}u_h &= \sum_{j \in J} u_j \phi_j,\\ t_h &= \sum_{i \in I} t_i \psi_i,\end{aligned}$$

and thus we obtain the following algebraic system of equations for the unknown coefficients $u \in \mathbb{R}^{|J|}$ and $t \in \mathbb{R}^{|I|}$ of u_h and t_h

$$\begin{bmatrix} -V & K \\ K^T & D \end{bmatrix} \begin{bmatrix} t \\ u \end{bmatrix} = \begin{bmatrix} V & -\frac{1}{2}M - K \\ -\frac{1}{2}M - K^T & -D \end{bmatrix} \begin{bmatrix} \widetilde{g}_N \\ \widetilde{g}_D \end{bmatrix} =: \begin{bmatrix} f_N \\ f_D \end{bmatrix}.$$

The discretization of the single-layer potential operator $\mathcal{V}$, the double-layer potential operator $\mathcal{K}$ and the hypersingular operator $\mathcal{D}$ are calculated by

$$\begin{aligned} V_{kl} &= (\mathcal{V}\psi_l, \psi_k)_{L^2}, \\ K_{kj} &= (\mathcal{K}\phi_j, \psi_k)_{L^2}, \\ D_{ij} &= (\mathcal{D}\phi_j, \phi_i)_{L^2}, \end{aligned}$$

where $k, l = 1, \ldots, |I|$ and $i, j = 1 \ldots |J|$.

To describe the convergence of the above discretization method, we need a generalization of finite element analysis. Let $(\widetilde{u}, \widetilde{h}) \in H^2(\Gamma_N) \times H^1(\Gamma_D)$, be the solution of (1.9). Using Céa's lemma, we can show that

$$\|\widetilde{u} - u_h\|^2_{H^{\frac{1}{2}}(\Gamma_N)} + \|\widetilde{t} - t_h\|^2_{H^{-\frac{1}{2}}(\Gamma_D)} \leq ch^3 \left(\|\widetilde{u}\|^2_{H^2(\Gamma_N)} + \|\widetilde{t}\|^2_{H^1(\Gamma_D)} \right).$$

From this estimate, we see that the discrete solution (u_h, t_h) converges for decreasing mesh size $h \to 0$ against the continuous solution $(\widetilde{u}, \widetilde{t})$ of (1.9); cf. [5].

Chapter 2

Kernel Functions

In this chapter we discuss the same theoretical background as in Chapters 3.2-3.4 of [2].

2.1 Properties of Kernel Functions

In this section we will introduce some properties of kernel functions of systems of partial differential operators

$$(\mathscr{L}u)_k = -\sum_{i,j=1}^{d}\sum_{l=1}^{m}\partial_i(c_{ij}^{kl}\partial_j)u_l + \delta u_k, \qquad k = 1,\dots,m \tag{2.1}$$

with constant coefficients c_{ij}^{kl} and δ satisfying the Legendre-Hadamard condition (1.3). We will need these properties to prove that the kernel functions are asymptotically smooth.

Definition 2.1. *A function $\kappa : \mathbb{R}^d \times \Omega \to \mathbb{R}$ satisfying $\kappa(\cdot, y) \in C^\infty(\mathbb{R}^d \setminus \{y\})$ for all $y \in \Omega$ is called **asymptotically smooth** in Ω with respect to x if there are constants c and γ such that for all $y \in \Omega$ and all $\alpha \in \mathbb{N}_0^d$*

$$|\partial_x^\alpha \kappa(x,y)| \le cp!\gamma^p \frac{|\kappa(x,y)|}{\|x-y\|^p} \text{ for all } x \in \mathbb{R}^d \setminus \{y\}, \tag{2.2}$$

where $p = |\alpha|$.

Instead of (2.2) sometimes another condition is used for the definition of asymptotic smoothness. Alternatively we can use the condition

$$|\partial_x^\alpha \kappa(x,y)| \le cp!\gamma^p \|x-y\|^{-s-p} \text{ for all } y \ne x, \tag{2.3}$$

on the derivatives of κ with some $s \in \mathbb{R}$. Conditions (2.2) and (2.3) are equivalent if κ has an algebraic singularity for $y = x$.

Definition 2.2. *The **Fourier transform** $\mathfrak{F} : L^2(\Omega) \to L^2(\Omega)$ is defined by*

$$(\mathfrak{F}v)(x) = \frac{1}{(2\pi)^{d/2}} \int_{\mathbb{R}^d} e^{-ix\cdot y} v(y)\,\mathrm{d}y,$$

and normalized such that $\mathfrak{F}^* = \mathfrak{F}^{-1}$.

Lemma 2.3. *For $u \in [H_0^1(\Omega)]^m$ satisfying the Legendre-Hadamard condition (1.3) it holds that*

$$\lambda_{\mathscr{L}} \|\mathfrak{J}(u)\|_{L^2}^2 \le \sum_{i,j=1}^{d} \sum_{k,l=1}^{m} \int_\Omega c_{ij}^{kl}\, \partial_i u_k\, \partial_j u_l \,\mathrm{d}x.$$

Proof. Using $\mathfrak{F}[\partial^\alpha u](\xi) = \xi^\alpha (2\pi i)^{|\alpha|} \mathfrak{F}u(\xi)$, it follows that

$$-\partial_i c_{ij}^{kl}\, \partial_j u_l = -\mathfrak{F}^*\mathfrak{F}(\partial_i c_{ij}^{kl}\, \partial_j u_l) = (2\pi)^2 \mathfrak{F}^*(c_{ij}^{kl}\, \xi_i\, \xi_j\, \mathfrak{F}u_l).$$

Together with (1.3) and $\|\mathfrak{F}u\|_{L^2(\Omega)} = \|u\|_{L^2(\Omega)}^2$ we obtain

$$\begin{aligned}
\sum_{i,j=1}^{d} \sum_{k,l=1}^{m} \int_\Omega c_{ij}^{kl}\, \partial_i u_k\, \partial_j u_l \,\mathrm{d}x &= (2\pi)^2 \sum_{i,j=1}^{d} \sum_{k,l=1}^{m} \int_\Omega c_{ij}^{kl}\, \xi_i\, \xi_j\, \mathfrak{F}u_k\, \mathfrak{F}u_l \,\mathrm{d}x \\
&\ge (2\pi)^2 \lambda_{\mathscr{L}} \sum_{i,j=1}^{d} \sum_{k,l=1}^{m} \int_\Omega |\xi_i\, \mathfrak{F}u_l|^2 \,\mathrm{d}x \\
&= \lambda_{\mathscr{L}} \sum_{i,j=1}^{d} \sum_{k,l=1}^{m} \int_\Omega |\mathfrak{F}(\partial_i u_l)|^2 \,\mathrm{d}x \\
&= \lambda_{\mathscr{L}} \sum_{i,j=1}^{d} \sum_{k,l=1}^{m} \|\partial_i u_l\|_{L^2}^2 \\
&= \lambda_{\mathscr{L}} \|\mathfrak{J}(u)\|_{L^2}^2,
\end{aligned}$$

where $\mathfrak{J}(u) \in \mathbb{R}^{m\times d}$ denotes the Jacobian of u. □

Note that the previous estimate only holds for constant coefficients c_{ij}^{kl}.

Lemma 2.4. *Let $D \subset \mathbb{R}^d$ be a domain having an intersection with Ω that has positive measure. Assume that $u \in \left[H^1(D)\right]^m$ is a weak solution of $\mathscr{L}u = 0$ in $D \cap \Omega$ and $u = 0$*

in $D \setminus \Omega$. Then for any compact set $K \subset D$ it holds that

$$\|\mathfrak{J}(u)\|_{L^2(K)} \leq \frac{c_{\mathscr{L}}}{\sigma}\|u\|_{L^2(D)},$$

where

$$c_{\mathscr{L}} = \sqrt{8d^2m\frac{\Lambda_{\mathscr{L}}}{\lambda_{\mathscr{L}}}\left(1+2dm\frac{\Lambda_{\mathscr{L}}}{\lambda_{\mathscr{L}}}\right)+2\frac{\sigma^2}{\lambda_{\mathscr{L}}}|\delta|} \quad \textit{and} \quad \sigma = \operatorname{dist}(K,\partial D).$$

Proof. Let $\eta \in C^1(D)$ be a cut-off function with respect to (K,σ). Then η satisfies $0 \leq \eta \leq 1$, $\eta = 1$ in K, $\eta = 0$ in a neighborhood of ∂D. We can choose η such that $|\partial_i \eta| \leq \frac{2}{\sigma}$, $i = 1,\dots,d$ in D. Since $u \in \left[H^1(\Omega)\right]^m$ it follows that $\eta^2 u \in \left[H_0^1(D\cap\Omega)\right]^m$. From

$$\begin{aligned}
&\partial_i(\eta u_k)\,\partial_j(\eta u_l) + u_k\,\partial_i\eta\,\partial_j(\eta u_l)\\
&\quad = u_l\,\partial_i(\eta u_k)\,\partial_j\eta + u_k\,\eta\,\partial_i\eta\,\partial_j u_l + \eta^2\,\partial_i u_k\,\partial_j u_l + u_k\,u_l\,\partial_i\eta\,\partial_j\eta + u_k\,\eta\,\partial_i\eta\,\partial_j u_l\\
&\quad = 2\,u_k\,\eta\,\partial_i\eta\,\partial_j u_l + \eta^2\,\partial_i u_k\,\partial_j u_l + u_l\,\partial_i(\eta u_k)\,\partial_j\eta + u_k\,u_l\,\partial_i\eta\,\partial_j\eta\\
&\quad = \partial_i(\eta^2 u_k)\,\partial_j u_l + u_l\,\partial_i(\eta u_k)\,\partial_j\eta + u_k\,u_l\,\partial_i\eta\,\partial_j\eta
\end{aligned}$$

we obtain

$$\partial_i(\eta u_k)\,\partial_j(\eta u_l) = \partial_i(\eta^2 u_k)\,\partial_j u_l + u_l\,\partial_i(\eta u_k)\,\partial_j\eta + u_k\,u_l\,\partial_i\eta\,\partial_j\eta - u_k\,\partial_i\eta\,\partial_j(\eta u_l). \quad (2.4)$$

Using $\displaystyle\int_D \eta^2 u_k(\mathscr{L}u)_l\,\mathrm{d}x = 0$ we get

$$\begin{aligned}
0 &= \sum_{l=0}^{m}\int_D \eta^2 u_k(\mathscr{L}u)_l\,\mathrm{d}x\\
&= \sum_{l=0}^{m}\int_D \eta^2 u_k\left(\sum_{i,j=1}^{d}\sum_{k=1}^{m} -\partial_i(c_{ij}^{kl}\partial_j)u_k + \delta u_l\right)\mathrm{d}x \qquad (2.5)\\
&\overset{(P.I.)}{=} \sum_{i,j=1}^{d}\sum_{k,l=1}^{m}\int_D \partial_i(\eta^2 u_k)\,c_{ij}^{kl}\,\partial_j u_k + \delta\eta^2 u_k u_l\,\mathrm{d}x.
\end{aligned}$$

Both together leads for any $\varepsilon > 0$ to

$$\begin{aligned}
&\sum_{i,j=1}^{d}\sum_{k,l=1}^{m}\int_D c_{ij}^{kl}\,\partial_i(\eta u_k)\,\partial_j(\eta u_l) + \delta\eta^2 u_k u_l \,\mathrm{d}x \\
&\quad\overset{(2.4)}{=} \sum_{i,j=1}^{d}\sum_{k,l=1}^{m}\int_D c_{ij}^{kl}\left(\partial_i(\eta^2 u_k)\,\partial_j u_l + u_l\,\partial_i(\eta u_k)\,\partial_j\eta + u_k\,u_l\,\partial_i\eta\,\partial_j\eta - u_k\,\partial_i\eta\,\partial_j(\eta u_l)\right) \\
&\qquad + \delta\eta^2 u_k u_l \,\mathrm{d}x \\
&\quad\overset{(2.5)}{=} \sum_{i,j=1}^{d}\sum_{k,l=1}^{m}\int_D c_{ij}^{kl}\left(u_l\,\partial_i(\eta u_k)\,\partial_j\eta + u_k\,u_l\,\partial_i\eta\,\partial_j\eta - u_k\,\partial_i\eta\,\partial_j(\eta u_l)\right)\,\mathrm{d}x \\
&\quad\le \Lambda_{\mathscr{L}}\sum_{i,j=1}^{d}\sum_{k,l=1}^{m}\int_D |u_k|\,|u_l|\,|\partial_i\eta|\,|\partial_j\eta| + 2\,|u_k|\,|\partial_i\eta|\,|\partial_j(\eta u_l)|\,\mathrm{d}x \\
&\quad\le 4\Lambda_{\mathscr{L}}\frac{d}{\sigma}\sum_{i,j=1}^{d}\sum_{k,l=1}^{m}\int_D \frac{1}{\sigma}|u_k|\,|u_l| + |u_k|\,|\partial_j(\eta u_l)|\,\mathrm{d}x \\
&\quad\le 4\Lambda_{\mathscr{L}}\frac{d}{\sigma}\left(m\frac{d}{\sigma}\|u\|_{L^2(D)} + \sum_{i,j=1}^{d}\sum_{k,l=1}^{m}\left(\int_D |u_k|^2\,\mathrm{d}x\right)^{1/2}\left(\int_D |\partial_j(\eta u_l)|^2\,\mathrm{d}x\right)^{1/2}\right) \\
&\quad\overset{(*)}{\le} 2\Lambda_{\mathscr{L}}\frac{dm}{\sigma}\left(2\frac{d}{\sigma}\|u\|^2_{L^2(D)} + \frac{d}{\varepsilon}\sum_{k=1}^{m}\int_D |u_k|^2\,\mathrm{d}x + \varepsilon\sum_{j=1}^{d}\sum_{l=1}^{m}\int_D |\partial_j(\eta u_l)|^2\,\mathrm{d}x\right) \\
&\quad= 2\Lambda_{\mathscr{L}}\frac{d^2 m}{\sigma^2}\left(2+\frac{\sigma}{\varepsilon}\right)\|u\|^2_{L^2(D)} + 2\Lambda_{\mathscr{L}}\frac{dm}{\sigma}\varepsilon\int_D \|\mathfrak{J}(\eta u)\|_F^2\,\mathrm{d}x,
\end{aligned}$$

where we have used at $(*)$ that $2ab \le a^2/\varepsilon + \varepsilon b^2$ for all $a, b \in \mathbb{R}$. From Lemma 2.3 we obtain

$$\lambda_{\mathscr{L}}\int_D \|\mathfrak{J}(\eta u)\|_F^2\,\mathrm{d}x \le \left(2\frac{d^2 m\,\Lambda_{\mathscr{L}}}{\sigma^2}\left(2+\frac{\sigma}{\varepsilon}\right) + |\delta|\right)\|u\|^2_{L^2(D)} + 2\frac{dm\,\Lambda_{\mathscr{L}}}{\sigma}\varepsilon\int_D \|\mathfrak{J}(\eta u)\|_F^2\,\mathrm{d}x.$$

In the end we get

$$\begin{aligned}
\|\mathfrak{J}(u)\|^2_{L^2(K)} &\le \|\mathfrak{J}(\eta u)\|^2_{L^2(D)} \\
&\le \frac{1}{\sigma^2}\frac{2\,d^2 m\,\lambda_{\mathscr{L}}(2+\sigma/\varepsilon) + \sigma^2|\delta|}{\lambda_L - 2\,dm\,\Lambda_{\mathscr{L}}\,\varepsilon/\sigma}\|u\|^2_{L^2(D)},
\end{aligned}$$

and by choosing $\varepsilon = \frac{\lambda_{\mathscr{L}}\sigma}{4dm\lambda_{\mathscr{L}}}$ the result. □

Remark 2.5. The previous proof shows that non-negative δ do not enter the constant $c_{\mathscr{L}}$.

Next, we want to derive pointwise estimates which we need to prove the asymptotic smoothness of the singularity function. We can apply Lemma 2.4 iteratively on a sequence

of balls $B_{r_l}(x)$, $l = 1, \dots, k$ to derive the following estimate for u satisfying $\mathscr{L}u = 0$ in $B_r(x) \subset \mathbb{R}^d$ and $k \in \mathbb{N}$

$$\|u\|_{H^k(B_\rho(x))} \le c(k, \rho, r)\|u\|_{L^2(B_r(x))} \quad \text{for all } 0 < \rho < r, \tag{2.6}$$

where c depends on the coefficients of $\mathscr{L}$. Because of the Sobolev embedding theorem, (2.6) implies that $\mathscr{L}$-harmonic functions are locally C^∞. If we choose $k = d+1$, we obtain from (2.6)

$$\sup_{B_\rho(x)} |u| \le c\|u\|_{H^{d+1}(B_\rho(x))} \le c'(\rho, r)\|u\|_{\mathscr{L}^2(B_r(x))}.$$

Hence, we use a rescaling argument and obtain for $x \in \Omega$ and $0 \le r \le \operatorname{dist}(x, \partial\Omega)$

$$\sup_{B_\rho(x)} |u| \le c_R\, r^{-\frac{d}{2}} \|u\|_{L^2(B_r(x))}, \quad 0 < \rho < r, \tag{2.7}$$

with a constant $c_R > 0$ independent of ρ and r.

Theorem 2.6. *The entries of the singularity matrix $S(x-y)$ of $\mathscr{L}$ are asymptotically smooth in $\mathbb{R}^d$ with respect to x.*

Proof. Choose a point $y \in \mathbb{R}^d$ which is fixed. For $x \in \mathbb{R}^d \setminus \{y\}$ let $R = \|x - y\|/2$. We assume that a function u is $\mathscr{L}$-harmonic in $B_r(x)$, that means $\mathscr{L}u = 0$ in $B_r(x)$, $0 < r < R$. Choosing $0 < \rho < r$ and $\rho' := (r+\rho)/2$, we obtain from (2.7) and the previous Lemma 2.4 that

$$\begin{aligned}
\sup_{z \in B_\rho(x)} |\partial_{z_i} u(z)|^2 &\overset{(2.7)}{\le} \frac{c_R^2}{\rho'^d} \int_{B_{\rho'}(x)} |\partial_{z_i} u(z)|^2 \,\mathrm{d}z \\
&\overset{2.4}{\le} \frac{c_R^2\, c_{\mathscr{L}}^2}{\rho'^d (r-\rho')^2} \int_{B_{\rho'}(x)} |u(z)|^2 \,\mathrm{d}z \\
&\le c_R^2\, c_{\mathscr{L}}^2 \frac{2^d}{(r+\rho)^d} \frac{2^2}{(r-\rho)^2}\, \omega_d\, r^d \sup_{z \in B_r(x)} |u(z)|^2 \\
&= 2^{d+2} \frac{\omega_d\, r^d}{(r+\rho)^d} \frac{c_R^2\, c_{\mathscr{L}}^2}{(r-\rho)^2} \sup_{z \in B_r(x)} |u(z)|^2,
\end{aligned} \tag{2.8}$$

where ω_d denotes the volume of the unit ball in $\mathbb{R}^d$.
Let $\alpha \in \mathbb{N}_0^d$ be a multi-index and $p = |\alpha|$. We define a nested sequence of balls

$$B_k = \left\{ z \in \mathbb{R}^d : \|x - z\| < \frac{Rk}{p+1} \right\}, \quad k = 1, \dots, p+1,$$

centered at x. Then $B_k \subset B_R(x) \subset \mathbb{R}^d \setminus \{y\}$ and $\operatorname{dist}(B_k, \partial B_{k+1}) = \frac{R}{p+1}$. Using estimate (2.8) with $\rho = \frac{Rk}{p+1}$ and $r = \frac{R(k+1)}{p+1}$ yields

$$\begin{aligned}\sup_{z\in B_k} |\partial_{z_i} u(z)| &\leq 2^{\frac{d}{2}+1} \left(\frac{k+1}{2k+1}\right)^{\frac{d}{2}} \frac{c_R\, c_{\mathscr{L}}\sqrt{\omega_d}}{R}(p+1) \sup_{z\in B_{k+1}} |u(z)| \\ &= c'_{\mathscr{L}} \frac{p+1}{R} \left(\frac{2k+2}{2k+1}\right)^{\frac{d}{2}} \sup_{z\in B_{k+1}} |u(z)|, \quad k+1,\dots,p,\end{aligned}$$

where $c'_{\mathscr{L}} := 2\, c_R\, c_{\mathscr{L}}\sqrt{\omega_d}$. Since each entry $S_{ij}(\cdot - y)$ of the singularity matrix and each of its derivatives $\partial_x^\alpha S(x-y)$ is $\mathscr{L}$-harmonic in $B_R(x) \subset \mathbb{R}^d$ for arbitrary $\alpha \in \mathbb{N}_0^d$, we can apply the previous estimate successively to the p partial derivatives of the function $S_{ij}(\cdot - y)$ and obtain

$$\sup_{z\in B_1} |\partial_z^\alpha S_{ij}(z-y)| \leq (p+1)^{\frac{d}{4}} \left(\frac{c'_{\mathscr{L}}(p+1)}{R}\right)^p \sup_{z\in B_{p+1}} |S_{ij}(z-y)|,$$

since $\prod_{k=1}^p \frac{2k+2}{2k+1} \leq \sqrt{p+1}$. Using Stirling's approximation

$$\sqrt{2\pi(p+1)} \left(\frac{p+1}{e}\right)^{p+1} < (p+1)!,$$

we end up with

$$\begin{aligned}|\partial_x^\alpha S_{ij}(x-y)| &\leq (p+1)^{\frac{d}{4}-1} \left(\frac{c'_{\mathscr{L}}}{R}\right)^p \frac{(p+1)!\, e^{p+1}}{\sqrt{2\pi(p+1)}} \sup_{z\in B_R(x)} |S_{ij}(z-y)| \\ &= \frac{e}{\sqrt{2\pi}}(p+1)^{\frac{d}{4}-\frac{1}{2}} p! \left(\frac{c'_{\mathscr{L}}\, e}{R}\right)^p \sup_{z\in B_R(x)} |S_{ij}(z-y)| \\ &\leq \frac{e}{\sqrt{2\pi}}(2^{p+1})^{\frac{d}{4}-\frac{1}{2}} p! \left(\frac{c'_{\mathscr{L}}\, e}{R}\right)^p \sup_{z\in B_R(x)} |S_{ij}(z-y)| \\ &= \frac{e}{\sqrt{2\pi}} 2^{\frac{d}{4}-\frac{1}{2}} p! \left(2^{\frac{d}{4}-\frac{1}{2}} \frac{c'_{\mathscr{L}}\, e}{R}\right)^p \sup_{z\in B_R(x)} |S_{ij}(z-y)| \\ &\leq \frac{e\, c_H}{\sqrt{2\pi}} 2^{\frac{d}{4}-\frac{1}{2}} p! \left(2^{\frac{d}{4}-\frac{1}{2}} \frac{c'_{\mathscr{L}}\, e}{R}\right)^p |S_{ij}(x-y)| \\ &= \underbrace{\frac{e\, c_H}{\sqrt{2\pi}} 2^{\frac{d}{4}-\frac{1}{2}}}_{=:c}\, p! \underbrace{\left(2^{\frac{d}{4}+\frac{1}{2}} c'_{\mathscr{L}}\, e\right)^p}_{=:\gamma^p} \frac{|S_{ij}(x-y)|}{\|x-y\|^p}\end{aligned}$$

due to $p \leq 2^p$ and Harnack's inequality $\sup_{z\in B_R(x)} |S_{ij}(z-y)| \leq c_H S_{ij}(x-y)$, which can be used since $S_{ij}(\cdot - y)$ is $\mathscr{L}$-harmonic in $B_R(x)$. □

The previous lemma shows that the singularity function S of any elliptic operator is asymptotically smooth. Analogously, we can show that S is asymptotically smooth with respect to y. Thus, the kernel function of the double-layer operator (1.6) of the Laplacian in $\mathbb{R}^3$ is asymptotically smooth on Γ with respect to x. Using this fact, we can prove in Subsection 2.3 the convergence of the ACA algorithm.

2.2 Degenerate Kernel Approximation by Taylor Expansion

As in [2], we want to show that the kernel functions of the single-layer operator $\mathcal{V}$ and the double-layer operator $\mathcal{K}$ can be approximated by a small sum of functions with separated variables, if some assumptions, such as asymptotic smoothness, are fulfilled.

Definition 2.7. *Let $D_X, D_Y \subset \mathbb{R}^d$ be two domains. A kernel function $\kappa : D_X \times D_Y \to \mathbb{R}$ is called **degenerate** if $k \in \mathbb{N}$ and functions $u_l : D_X \to \mathbb{R}$ and $v_l : D_Y \to \mathbb{R}$, $l = 1, \ldots, k$ exist such that*

$$\kappa(x, y) = \sum_{l=1}^{k} u_l(x)\, v_l(y),$$

*$x \in D_X$, $y \in D_Y$. The number k is called **degree of degeneracy**.*

Since the singularity function S of the Laplacian is asymptotically smooth with respect to x, the kernel function $\kappa(x, y) := S(y - x)$ of the single-layer operator and the kernel function $\kappa(x, y) := \partial_{\nu_y} S(y-x)$ of the double-layer operator are asymptotically smooth on Γ with respect to x. Now we will use this property to show the existence of an exponentially convergent approximation of asymptotically smooth kernels. To this end let D_X be a cube with sides of length a and center ξ_{D_X} and let D_Y be a convex set. κ has a Taylor expansion

$$\begin{aligned}\kappa(x, y) \;&=\; \sum_{|\alpha|<p} \frac{1}{\alpha!}\partial_x^\alpha \kappa(\xi_{D_X}, y)(x - \xi_{D_X})^\alpha + \sum_{|\alpha|\geq p} \frac{1}{\alpha!}\partial_x^\alpha \kappa(\xi_{D_X}, y)(x - \xi_{D_X})^\alpha \\ &=: T_p[\kappa](x, y) + R_p(x, y),\end{aligned}$$

where $T_p[\kappa](x, y)$ is a kernel approximation and $R_p(x, y)$ denotes the remainder of the expansion.

Theorem 2.8. *Assume that $\eta \operatorname{dist}(\xi_{D_X}, D_Y) \geq a$ holds with $\eta > 0$ satisfying $\gamma d\eta < 1$. If κ is asymptotically smooth on the cube D_X with respect to x, then it holds that*

$$|\kappa(x, y) - T_p[\kappa](x, y)| \leq c\frac{(\gamma d\eta)^p}{1 - \gamma d\eta}|\kappa(\xi_{D_X}, y)| \tag{2.9}$$

for all $x \in D_X$ and $y \in D_Y$.

Proof. Since $\|x - \xi_{D_X}\| \leq \sqrt{d}a$ and $\|\xi_{D_X} - y\| \geq \operatorname{dist}(\xi_{D_X}, D_Y)$, it follows that

$$\begin{aligned}|R_p(x - y)| &\leq \sum_{|\alpha|\geq p} \frac{1}{\alpha!}|\partial_x^\alpha \kappa(\xi_{D_X}, y)||(x - \xi_{D_X})^\alpha| \\ &\leq c\,|\kappa(\xi_{D_X}, y)| \sum_{|\alpha|\geq p} \frac{\gamma^{|\alpha|}|\alpha|!}{\alpha!\|\xi_{D_X} - y\|^{|\alpha|}}|(x - \xi_{D_X})^\alpha|\end{aligned}$$

$$
\begin{aligned}
&= c\,|\kappa(\xi_{D_X}, y)| \sum_{l=p}^{\infty} \left(\frac{\gamma}{\|\xi_{D_X} - y\|} \right)^l \sum_{|\alpha|=l} \binom{l}{\alpha} |(x - \xi_{D_X})^\alpha| \\
&\leq c\,|\kappa(\xi_{D_X}, y)| \sum_{l=p}^{\infty} \left(\gamma\sqrt{d} \frac{\|x - \xi_{D_X}\|}{\|\xi_{D_X} - y\|} \right)^l \\
&\leq c\,|\kappa(\xi_{D_X}, y)| \sum_{l=p}^{\infty} (\gamma d \eta)^l \\
&\leq c\,\frac{(\gamma d \eta)^p}{1 - \gamma d \eta} |\kappa(\xi_{D_X}, y)|.
\end{aligned}
$$

In step 4 we have used that $\sum_{|\alpha|=l} \binom{l}{\alpha} |\xi^\alpha| = \left(\sum_{i=1}^d |\xi_i| \right)^l \leq \sqrt{d}\|\xi\|^l$ for all $\xi \in \mathbb{R}^d$. □

The previous theorem shows that the Taylor expansion converges exponentially with convergence rate $\gamma d \eta < 1$ if the kernel is asymptotically smooth. To achieve a given approximation accuracy $\varepsilon > 0$, it must hold $p \sim |\log \varepsilon|$. Since $T_p[\kappa](\cdot, y)$ is a d-variate polynomial of order at most $p-1$, it follows that the degree of degeneracy $k = \dim(\Pi_{p-1}^d) \leq p^d$ scales like

$$k \sim |\log \varepsilon|^d. \tag{2.10}$$

2.3 Degenerate Kernel Approximation by Adaptive Cross Approximation

Since we need the computation of derivatives for the truncated Taylor expansion, this has only theoretical meaning. Instead, we use the in [2] introduced adaptive cross approximation (ACA) to find an approximation of the kernel functions on domains D_X, D_Y satisfying the assumptions of Theorem 2.8. ACA iteratively finds an interpolation of $\kappa(x, y)$ by using restrictions of it as approximation basis. First we consider the function

$$\widetilde{\kappa}(x, y) := \frac{\kappa(x, y_0)\,\kappa(x_0, y)}{\kappa(x_0, y_0)},$$

where fixed $x_0 \in D_X$ and $y_0 \in D_Y$ are close to x and y, respectively. Note that $\kappa(x_0, y_0) \neq 0$ has to hold in order that $\widetilde{\kappa}$ is well-defined. Due to the above definition, the degree of degeneracy of $\widetilde{\kappa}$ is one. In addition, it holds that

$$
\begin{aligned}
\widetilde{\kappa}(x_0, y) &= \kappa(x_0, y) \quad \text{for all } y \in D_Y, \\
\widetilde{\kappa}(x, y_0) &= \kappa(x, y_0) \quad \text{for all } x \in D_X.
\end{aligned}
$$

Thus, we see that $\widetilde{\kappa}$ is an interpolation of κ on whole domains. The approximation error can be estimated by

$$\begin{aligned}|\kappa(x,y)-\widetilde{\kappa}(x,y)| &= \left|\kappa(x,y)-\frac{\kappa(x,y_0)\kappa(x_0,y)}{\kappa(x_0,y_0)}\right| \\ &= \left|\kappa(x,y)-\kappa(x,y_0)-\frac{\kappa(x,y_0)}{\kappa(x_0,y_0)}\left(\kappa(x_0,y)-\kappa(x_0,y_0)\right)\right| \\ &\leq |\kappa(x,y)-\kappa(x,y_0)|+\frac{|\kappa(x,y_0)|}{|\kappa(x_0,y_0)|}|\kappa(x_0,y)-\kappa(x_0,y_0)|.\end{aligned}$$

Assume we choose x_0 such that $|\kappa(x,y_0)| \leq |\kappa(x_0,y_0)|$ for all $x \in D_X$, then

$$|\kappa(x,y)-\widetilde{\kappa}(x,y)| \leq 2 \max_{z\in D_X} |\kappa(z,y)-\kappa(z,y_0)|.$$

In order to find a better approximation of higher order, we will generate a sequence of degenerate kernels which will be shown to converge exponentially to κ. For simplicity let

$$\kappa(x,[y]_k) = \begin{bmatrix} \kappa(x,y_{j_1}) \\ \vdots \\ \kappa(x,y_{j_k}) \end{bmatrix} \in \mathbb{R}^k \quad \text{and} \quad \kappa([x]_k,y) = \begin{bmatrix} \kappa(x_{i_1},y) \\ \vdots \\ \kappa(x_{i_k},y) \end{bmatrix} \in \mathbb{R}^k$$

with points $x_{i_l} \in D_X$ and $y_{j_l} \in D_Y$, $l = 1,\ldots,k$. With this notation, we can derive degenerate approximations of the form

$$\kappa(x,y) = \kappa(x,[y]_k)^T W_k^{-1} \kappa([x]_k,y) + r_k(x,y), \tag{2.11}$$

where the $k \times k$ matrix W_k is defined by

$$W_k = \begin{bmatrix} \kappa(x_{i_1},y_{j_1}) & \ldots & \kappa(x_{i_1},y_{j_k}) \\ \vdots & & \vdots \\ \kappa(x_{i_k},y_{j_1}) & \ldots & \kappa(x_{i_k},y_{j_k}) \end{bmatrix}.$$

We need these results later on to construct an iterative algorithm for approximating matrices by low-rank matrices without knowing the rank of approximation in advance.

First we consider the analytic problem of approximating a general asymptotically smooth kernel by a degenerate kernel. We define sequences $\{s_k\}$, $\{r_k\}$ for the approximation of κ by the following rule

$$r_0(x,y) = \kappa(x,y), \quad s_0(x,y) = 0,$$

and for $k = 0,1,\ldots$

$$\begin{aligned} r_{k+1}(x,y) &:= r_k(x,y) - \frac{r_k(x,y_{j_{k+1}})\, r_k(x_{i_{k+1}},y)}{r_k(x_{i_{k+1}},y_{j_{k+1}})}, \\ s_{k+1}(x,y) &:= s_k(x,y) + \frac{r_k(x,y_{j_{k+1}})\, r_k(x_{i_{k+1}},y)}{r_k(x_{i_{k+1}},y_{j_{k+1}})} \end{aligned} \tag{2.12}$$

with $x_{i_{k+1}} \in D_X$ and $y_{j_{k+1}} \in D_Y$ chosen such that $r_k(x_{i_{k+1}},y_{j_{k+1}}) \neq 0$.

Lemma 2.9. *For $1 \leq l \leq k$ it holds that $r_k(x, y_{j_l}) = 0$ for all $x \in D_X$ and $r_k(x_{i_l}, y) = 0$ for all $y \in D_Y$.*

Proof. We prove the lemma by induction over k. We have seen that the lemma is true for $k = 1$. Assume it holds for $k-1$, so we have $r_{k-1}(x, y_{j_l}) = 0$ for all $x \in D_X$ and all $1 \leq l < k$. Using (2.12), we obtain

$$r_k(x, y_{j_l}) = r_{k-1}(x, y_{j_l}) - \frac{r_{k-1}(x, y_{j_k})\, r_{k-1}(x_{i_k}, y_{j_l})}{r_{k-1}(x_{i_k}, y_{j_k})} = 0$$

for all $1 \leq l < k$. Obviously, the lemma holds true for $l = k$ since

$$r_k(x, y_{j_k}) = r_{k-1}(x, y_{j_k}) - \frac{r_{k-1}(x, y_{j_k})\, r_{k-1}(x_{i_k}, y_{j_k})}{r_{k-1}(x_{i_k}, y_{j_k})} = 0.$$

Interchanging the roles of x and y, we also can show that $r_k(x_{i_l}, y) = 0$ for $1 \leq l \leq k$ and all $y \in D_Y$. □

The previous lemma shows that the functions r_k accumulate zeros. Hence, s_k successively interpolates κ and we can approximate

$$\begin{aligned}\kappa(x, y) \approx\ & s_k(x, y) \\ =\ & \sum_{l=1}^{k} r_{l-1}(x, y_{j_l}) \frac{r_{l-1}(x_{i_l}, y)}{r_{l-1}(x_{i_l}, y_{j_l})} \\ =:\ & \sum_{l=1}^{k} u_l(x)\, v_l(y)\end{aligned}$$

by a sum of functions with separated variables.

Denote by $W_k^{(l)}(x) \in \mathbb{R}^{k \times k}$ the matrix which results from replacing the lth row of W_k by the vector $\kappa(x, [y]_k)$. The determinant of $W_k^{(l)}(x)$ can be computed by the following recursion formula.

Lemma 2.10. *For $1 \leq l < k$ it holds that*

$$\det W_k^{(l)}(x) = r_{k-1}(x_{i_k}, y_{j_k}) \det W_{k-1}^{(l)}(x) - r_{k-1}(x, y_{j_k}) \det W_{k-1}^{(l)}(x_{i_k})$$

and

$$\begin{aligned}\det W_1^{(1)}(x) &= r_0(x, y_{j_1}), \\ \det W_k^{(k)}(x) &= r_{k-1}(x, y_{j_k}) \det W_{k-1}, \quad k > 1.\end{aligned}$$

In particular, we have

$$\det W_k = r_0(x_{i_1}, y_{j_1}) \cdot \ldots \cdot r_{k-1}(x_{i_k}, y_{j_k}).$$

Proof. From (2.12) we can easily verify that there are coefficients $\alpha_\nu^{(k-1)}$, $\nu = 1, \dots, k-1$, so that for all $x \in D_X$

$$r_{k-1}(x, y_{j_k}) = \kappa(x, y_{j_k}) - \sum_{\nu=1}^{k-1} \alpha_\nu^{(k-1)} \kappa(x, y_{j_\nu}).$$

Thus, it is possible to replace each entry $\kappa(\cdot, y_{j_k})$ in the last column of $W_k^{(l)}(x)$ by $r_{k-1}(\cdot, y_{j_k})$ and obtain $\widetilde{W}_k^{(l)}(x)$ without changing the determinant, because we have only subtracted multiples of columns of $W_k^{(l)}(x)$ from the last column of it. Since $r_{k-1}(x_{i_l}, y_{j_l}) = 0$, $1 \leq l < k$ by the previous lemma, only the lth and the kth entry of the last column of $\widetilde{W}_k^{(l)}$ do not vanish. Using Laplace's theorem yields the claim. □

Since we choose i_k, j_k such that each $r_{k-1}(x_{i_k}, y_{j_k}) \neq 0$, the previous lemma guarantees the non-singularity of W_k. Now, we can prove that the decomposition of κ into s_k and r_k has the form (2.11).

Lemma 2.11. *For the generated sequences s_k and r_k, $k \geq 0$ it holds that*

$$s_k(x, y) + r_k(x, y) = \kappa(x, y),$$

where for $k \geq 1$

$$s_k(x, y) = \kappa(x, [y]_k)^T W_k^{-1} \kappa([x]_k, y).$$

Proof. We prove the lemma by induction over k. Obviously, the lemma holds for $k = 1$. From the definition of r_k and s_k we can see that

$$\begin{aligned} s_k(x, y) + r_k(x, y) &= s_{k-1}(x, y) + r_{k-1}(x, y) \\ &= \kappa(x, y). \end{aligned}$$

To simplify matters we set

$$\begin{aligned} a_k &= W_{k-1}^{-1} \kappa([x]_{k-1}, y_{j_k}), \\ b_k &= W_{k-1}^{-T} \kappa(x_{i_k}, [y]_{k-1}) \quad \text{and} \\ \gamma_k &= (r_{k-1}(x_{i_k}, y_{j_k}))^{-1}. \end{aligned}$$

Due to the induction we have

$$\begin{aligned}
s_k(x,y) &= s_{k-1}(x,y) + \gamma_k r_{k-1}(x,y_{j_k}) r_{k-1}(x_{i_k},y) \\
&= \kappa(x,[y]_{k-1})^T W_{k-1}^{-1} \kappa([x]_{k-1},y) + \gamma_k r_{k-1}(x,y_{j_k}) r_{k-1}(x_{i_k},y) \\
&= \kappa(x,[y]_{k-1})^T W_{k-1}^{-1} \kappa([x]_{k-1},y) \\
&\quad + \gamma_k (s_{k-1}(x,y_{j_k}) - \kappa(x,y_{j_k}))(s_{k-1}(x_{i_k},y) - \kappa(x_{i_k},y)) \\
&= \kappa(x,[y]_{k-1})^T W_{k-1}^{-1} \kappa([x]_{k-1},y) \\
&\quad + \gamma_k (\kappa(x,[y]_{k-1}) a_k - \kappa(x,y_{j_k}))(b_k^T \kappa([x]_{k-1},y) - \kappa(x_{i_k},y)) \\
&= \kappa(x,[y]_{k-1})^T (W_{k-1}^{-1} + \gamma_k a_k b_k^T) \kappa([x]_{k-1},y) - \kappa(x,[y]_{k-1}) \gamma_k a_k \kappa(x_{i_k},y) \\
&\quad - \kappa(x,y_{j_k}) \gamma_k b_k^T \kappa([x]_{k-1},y) + \kappa(x,y_{j_k}) \gamma_k \kappa(x_{i_k},y) \\
&= \begin{bmatrix} \kappa(x,[y]_{k-1}) \\ \kappa(x,y_{j_k}) \end{bmatrix}^T \begin{bmatrix} W_{k-1}^{-1} + \gamma_k a_k b_k^T & -\gamma_k a_k \\ -\gamma_k b_k^T & \gamma_k \end{bmatrix} \begin{bmatrix} \kappa([x]_{k-1},y) \\ \kappa(x_{i_k},y) \end{bmatrix}
\end{aligned}$$

and

$$\begin{aligned}
& W_k \begin{bmatrix} W_{k-1}^{-1} + \gamma_k a_k b_k^T & -\gamma_k a_k \\ -\gamma_k b_k^T & \gamma_k \end{bmatrix} \\
&= \begin{bmatrix} W_{k-1} & \kappa([x]_{k-1},y_{j_k}) \\ \kappa(x_{i_k},[y]_{k-1})^T & \kappa(x_{i_k},y_{j_k}) \end{bmatrix} \begin{bmatrix} W_{k-1}^{-1} + \gamma_k a_k b_k^T & -\gamma_k a_k \\ -\gamma_k b_k^T & \gamma_k \end{bmatrix} \\
&= \begin{bmatrix} I_{k-1} + (W_{k-1} a_k - \kappa([x],y_{j_k})) \gamma_k b_k^T & \gamma_k (\kappa([x]_{k-1},y_{j_k}) - W_{k-1} a_k) \\ \kappa(x_{i_k},[y]_{k-1})^T W_{k-1}^{-1} + (s_{k-1}(x_{i_k},y_{j_k}) - \kappa(x_{i_k},y_{j_k})) \gamma_k b_k^T & \gamma_k (\kappa(x_{i_k},y_{j_k}) - \kappa(x_{i_k},[y]_{k-1})^T a_k) \end{bmatrix} \\
&= \begin{bmatrix} I_{k-1} & 0 \\ (1 + \gamma_k (s_{k-1}(x_{i_k},y_{j_k}) - \kappa(x_{i_k},[y]_{k-1})^T)) b_k^T & \gamma_k r_{k-1}(x_{i_k},y_{j_k}) \end{bmatrix} \\
&= \begin{bmatrix} I_{k-1} & 0 \\ 0 & 1 \end{bmatrix} \\
&= I_k.
\end{aligned}$$

From this we obtain the representation

$$s_k(x,y) = \kappa(x,[y]_k)^T W_k^{-1} \kappa([x]_k,y)$$

also for s_k. □

In contrast to the one-dimensional space $\mathbb{R}$, the polynomial interpolation in multidimensional space $\mathbb{R}^d$, $d \geq 2$ is not unique in general. If the interpolation points lie on a hyperface of degree p, there is no unique interpolation polynomial in $\prod_p^d$. Thus, the uniqueness depends on the configuration of the points.

Corollary 2.12. *The function $s_k(x,y)$ is the uniquely defined interpolant of $\kappa(x,y)$ at the nodes y_{j_l} in the span of the functions $\kappa(x_{i_l},y)$, $l=1,\dots,k$.*

Proof. Using Cramer's rule we can determine $W_k^{-1}\kappa([x]_k,y)$ by

$$\left(W_k^{-1}\kappa\left([x]_k,y\right)\right)_l = \frac{\det V_k^{(l)}(y)}{\det W_k}, \quad l=1,\dots,k, \tag{2.13}$$

where the matrix $V_k^{(l)}(y)$ arises from W_k by replacing the lth column by $\kappa([x]_k,y)$. The function

$$L_l(y) := \frac{\det V_k^{(l)}(y)}{\det W_k} \in \operatorname{span}\{\kappa(x_{i_\nu},y),\ \nu=1,\dots,k\}$$

satisfies $L_\mu(y_{j_\nu}) = \delta_{\mu\nu}$, $1\le\mu,\nu\le k$. Thus $L_l(y)$ is the lth Lagrange function for the interpolation system $\{\kappa(x_{i_\nu},y),\ \nu=1,\dots,k\}$. □

2.3.1 Error Analysis

Next, we will show that the remainder $r_k(x,y)$ can be estimated by the remainder of the best approximation in any system $\Xi=\{\xi_1,\dots,\xi_k\}$ of functions. For instance, we consider the approximation by polynomials. Assume that the matrix $(\xi_\mu(y_{j_\nu}))_{\mu,\nu}$ is non-singular so that the interpolation in this system is unique.

Denote by

$$\|\mathcal{I}_k^\Xi\| := \max\{\|\mathcal{I}_k^\Xi\|_{\infty,D_Y}/\|f\|_{\infty,D_Y} : f\in C(D_Y)\}$$

the Lebesgue constant of the interpolation operator $\mathcal{I}_k^\Xi$ defined by

$$\mathcal{I}_k^\Xi f := \sum_{l=1}^k f(y_{j_l})\, L_l^\Xi,$$

with $L_l^\Xi, l=1,\dots,k$ being the Lagrange functions for ξ_l and y_{j_l}, $l=1,\dots,k$. From

$$f-\mathcal{I}_k^\Xi(f) = f-p+\mathcal{I}_k^\Xi(p-f) \quad \text{for all } p\in\operatorname{span}\Xi,$$

we obtain that, up to constants, the interpolation error $E_k^\Xi(f) := f-\mathcal{I}_k^\Xi f$ is bounded by the error of the best approximation

$$\|E_k^\Xi(f)\|_{\infty,D_Y} \le (1+\|\mathcal{I}_k^\Xi\|)\inf_{p\in\operatorname{span}\Xi}\|f-p\|_{\infty,D_Y}. \tag{2.14}$$

Lemma 2.13. *Assume in each step we choose the pivots x_{i_k} of ACA such that*

$$|r_{k-1}(x_{i_k}, y_{j_k})| \geq |r_{k-1}(x, y_{j_k})| \quad \text{for all } x \in D_X.$$

Then for $1 \leq l \leq k$ it holds that

$$\sup_{x \in D_X} \frac{|\det W_k^{(l)}(x)|}{|\det W_k|} \leq 2^{k-l}.$$

Proof. From Lemma 2.10 we obtain for $1 \leq l < k$

$$\frac{\det W_k^{(l)}(x)}{\det W_k} = \frac{\det W_{k-1}^{(l)}(x)}{\det W_{k-1}} - \frac{r_{k-1}(x, y_{j_k})}{r_{k-1}(x_{i_k}, y_{j_k})} \frac{\det W_{k-1}^{(l)}(x_{i_k})}{\det W_{k-1}}$$

and for $l = k$

$$\frac{\det W_k^{(k)}(x)}{\det W_k} = \frac{r_{k-1}(x, y_{j_k})}{r_{k-1}(x_{i_k}, y_{j_k})}.$$

Since we have $\frac{r_{k-1}(x, y_{j_k})}{r_{k-1}(x_{i_k}, y_{j_k})} \leq 1$ by assumption, we get for $1 \leq l < k$

$$\sup_{x \in D_X} \frac{|\det W_k^{(l)}(x)|}{\det W_k} \leq 2 \sup_{x \in D_X} \frac{|\det W_{k-1}^{(l)}(x)|}{\det W_{k-1}}$$

from what the assertion follows. □

Define $\kappa_x : D_Y \to \mathbb{R}$ by $\kappa_x(y) := \kappa(x, y)$ for $y \in D_Y$ and fixed $x \in D_X$, hence it is enough to estimate r_k by the error $E_k^{\Xi}(\kappa_x)$ of the interpolation in Ξ if we want to estimate r_k by the best approximation error in Ξ.

Lemma 2.14. *For $x \in D_X$ and $y \in D_Y$ it holds that*

$$r_k(x, y) = E_k^{\Xi}(\kappa_x)(y) - \sum_{l=1}^{k} \frac{\det W_k^{(l)}(x)}{\det W_k} E_k^{\Xi}(\kappa_{x_{i_l}})(y).$$

Proof. We denote the vector of the Lagrange functions L_l^{Ξ}, $l = 1, \ldots, k$, to the points $y_{j_1}, \ldots, y_{j_k}$ by

$$L^{\Xi}(y) = \begin{bmatrix} L_1^{\Xi}(y) \\ \vdots \\ L_k^{\Xi}(y) \end{bmatrix}.$$

Using Lemma 2.11 and (2.13) we obtain

$$\begin{aligned} r_k(x,y) &\overset{2.11}{=} \kappa(x,y) - \kappa(x,[y]_k)^T W_k^{-1} \kappa([x]_k, y) \\ &= \kappa(x,y) - \kappa(x,[y]_k)^T L^\Xi(y) - \kappa(x,[y]_k)^T W_k^{-1} \left(\kappa([x]_k,y) - W_k L^\Xi(y)\right) \\ &= E_k^\Xi(\kappa_x)(y) - \sum_{l=1}^k \left(\kappa(x,[y]_k)^T W_k^{-1}\right)_l E_k^\Xi(\kappa_{x_{i_l}})(y) \\ &\overset{(2.13)}{=} E_k^\Xi(\kappa_x)(y) - \sum_{l=1}^k \frac{\det W_k^{(l)}(x)}{\det W_k} E_k^\Xi(\kappa_{x_{i_l}})(y). \end{aligned}$$

□

Combining both two previous lemmas we get

$$|r_k(x,y)| \leq 2^k \sup_{z\in\{x,x_{i_1},\dots,x_{i_k}\}} |E_k^\Xi(\kappa_z)(y)| \tag{2.15}$$

$$\leq 2^k (1 + \|\mathcal{I}_k^\Xi\|) \sup_{z\in\{x,x_{i_1},\dots,x_{i_k}\}} \inf_{p\in \operatorname{span}\Xi} \|\kappa(z,\cdot) - p\|_{\infty,D_Y}, \tag{2.16}$$

due to (2.14). With this estimate, we have shown that, up to constants, the approximation error r_k is smaller than the approximation error associated with any system of functions $\Xi = \{\xi_1,\dots,\xi_k\}$. Hence ACA yields quasi-optimal results and both approximations lead to the same degree of degeneracy. The exponentially growing factor 2^k is a worst-case estimate. The topic of current research is to prove this.

The next theorem is due to Sauer and Xu. It estimates the error of multivariate polynomial interpolation. The notation will be the same as in [6].

Theorem 2.15. *Let the Lagrange interpolation in the points $\boldsymbol{x}^0,\dots,\boldsymbol{x}^n$ be unique. For $f \in C^{n+1}(\mathbb{R}^d)$ and $x \in \mathbb{R}^d$ it holds that*

$$|f(x) - L^n(f)(x)| \leq \sum_{\mu\in\Lambda_n} \frac{1}{(n+1)!} |p_{\mu_n}^{[n]}(x)\pi_\mu(\boldsymbol{x}^\mu)| \cdot \|D_{x-x_{\mu_n}^{(n)}} D_{\boldsymbol{x}^\mu}^n f\|_\infty, \tag{2.17}$$

where $L^n(f)$ denotes the interpolation polynomial to f of degree n. It suffices to take the supremum over the convex hull of $\{\boldsymbol{x}^0,\dots,\boldsymbol{x}^n,x\}$.

Now we can use this expression for the error of Lagrange interpolation to estimate the error of ACA as in [1].

Theorem 2.16. *Assume we choose x_{i_l}, $l = 1, \dots, k$ such that*

$$|r_{l-1}(x_{i_l}, y_{j_l})| \geq |r_{l-1}(x, y_{j_l})| \quad \text{for all } x \in D_X,$$

and let κ be an asymptotically smooth function with

$$|\partial_y^\alpha \kappa(x, y)| \leq cp!\gamma^p \|x - y\|^{-s-p}, \quad \text{for all } x \neq y,$$

with $p = |\alpha|$. Then the remainder of the approximation $s_k(x, y) \approx \kappa(x, y)$ can be estimated by

$$|r_k(x, y)| \leq c_p \operatorname{dist}^{-s}(D_X, D_Y)\eta^p, \tag{2.18}$$

where $k = \dim \Pi_{p-1}^d$ and c_p does not depend on η but only on the points $y_1, \dots, y_k$.

Proof. To prove this theorem, we will apply the Sauer-Xu formula (2.17) to $\kappa_x(y)$. Since κ is asymptotically smooth with respect to y, it holds

$$\begin{aligned} |D_{y - y_{\mu_{p-1}}^{(p-1)}} D_{\boldsymbol{y}^\mu}^{p-1} \kappa_x(y)| &\leq \operatorname{diam}^p(D_Y) d^p cp!\gamma^p \operatorname{dist}^{-s-p}(D_X, D_Y) \\ &\leq cp!(\gamma d\eta)^p \operatorname{dist}^{-s}(D_X, D_Y), \end{aligned}$$

for $x \in D_X, y \in D_Y$. Hence, we can estimate the error of Lagrange interpolation by

$$\begin{aligned} |E_k(\kappa_x)(y)| &= |\kappa_x(y) - L^{p-1}(\kappa_x)(y)| \\ &\leq c(\gamma d\eta)^p \operatorname{dist}^{-s}(D_X, D_Y) \sum_{\mu \in \Lambda_n} |p_{\mu_{p-1}}^{[p-1]}(y)\pi_\mu(\boldsymbol{y}^\mu)|. \end{aligned}$$

Using (2.15) we obtain

$$|r_k(x, y)| \leq c_p \operatorname{dist}^{-s}(D_X, D_Y)\eta^p,$$

where

$$c_p = c(\gamma d)^p (1 + 2^k) \sup_{y \in D_Y} \sum_{\mu \in \Lambda_n} |p_{\mu_{p-1}}^{[p-1]}(y)\pi_\mu(\boldsymbol{y}^\mu)|.$$

Note that the expression $p_{\mu_{p-1}}^{[p-1]}(y)\pi_\mu(\boldsymbol{y}^\mu)$ does not depend on κ_x but on the points $y_1, \dots, y_k$. □

2.3.2 Algorithm

In this section we describe an algebraic version of the construction of the sequences (2.12). This is analogous to approximate the matrix

$$A = \begin{bmatrix} \kappa(x_1, y_1) & \kappa(x_1, y_2) & \cdots & \kappa(x_1, y_m) \\ \kappa(x_2, y_1) & \kappa(x_2, y_2) & \cdots & \kappa(x_2, y_m) \\ \vdots & \vdots & \ddots & \vdots \\ \kappa(x_n, y_1) & \kappa(x_n, y_2) & \cdots & \kappa(x_n, y_m) \end{bmatrix} \in \mathbb{R}^{n \times m},$$

with $x_i \in D_X$, $i = 1, \ldots, n$ and $y_j \in D_Y$, $j = 1, \ldots, m$. The algorithm works as follows. We start with the matrix $R_0 = A$. Then, in each step we search a nonzero pivot (i_k, j_k) in R_k and subtract a scaled outer product of the i_kth row and the j_kth column. Thus, we obtain the matrix R_{k+1} by

$$R_{k+1} = R_k - \frac{(R_k)_{1:n,j_k}(R_k)_{i_k,1:m}}{(R_k)_{i_k j_k}}, \tag{2.19}$$

where $(R_k)_{i,1:m}$ and $(R_k)_{1:n,j}$ denote the ith row and the jth column of R_k respectively. Due to the assumption of Lemma 2.13, we choose i_k the maximum element in modulus of the j_kth column; i.e.,

$$|(R_{k-1})_{i_k j_k}| = \max_{i=1,\ldots,n} |(R_{k-1})_{i j_k}|.$$

Example 2.17. We apply three steps of the algorithm to the following matrix R_0. The green entries are the chosen pivots.

$$R_0 = \begin{bmatrix} 0.70711 & 0.68599 & 0.94281 & 0.68599 & 0.56569 \\ 0.68599 & 0.70711 & 0.89443 & 0.63246 & 0.55470 \\ 0.56569 & 0.55470 & 0.70711 & 0.55470 & 0.47140 \\ 0.68599 & 0.63246 & 0.89443 & 0.70711 & 0.55470 \\ 0.94281 & 0.89443 & 1.41420 & 0.89443 & 0.70711 \end{bmatrix}$$

$$R_1 = R_0 - \frac{1}{0.94281} \begin{bmatrix} 0.70711 \\ 0.68599 \\ 0.56569 \\ 0.68599 \\ 0.94281 \end{bmatrix} \begin{bmatrix} 0.94281 \\ 0.89443 \\ 1.41420 \\ 0.89443 \\ 0.70711 \end{bmatrix}^T$$

$$= \begin{bmatrix} 0 & 0.01517 & -0.11784 & 0.01517 & 0.03536 \\ 0 & 0.05632 & -0.13454 & -0.01833 & 0.04021 \\ 0 & 0.01804 & -0.14142 & 0.01804 & 0.04713 \\ 0 & -0.01833 & -0.13454 & 0.05632 & 0.04021 \\ 0 & 0 & 0 & 0 & 0 \end{bmatrix}$$

$$R_2 = R_1 - \frac{1}{-0.14142} \begin{bmatrix} -0.11784 \\ -0.13454 \\ -0.14142 \\ -0.13454 \\ 0 \end{bmatrix} \begin{bmatrix} 0 \\ 0.01804 \\ -0.14142 \\ 0.01804 \\ 0.04713 \end{bmatrix}^T$$

$$= \begin{bmatrix} 0 & 0.000134 & 0 & 0.000134 & -0.003919 \\ 0 & 0.039160 & 0 & -0.035490 & -0.004635 \\ 0 & 0 & 0 & 0 & 0 \\ 0 & -0.035490 & 0 & 0.039160 & -0.004635 \\ 0 & 0 & 0 & 0 & 0 \end{bmatrix}$$

$$R_3 = R_2 - \frac{1}{-0.004635} \begin{bmatrix} -0.003919 \\ -0.004635 \\ 0 \\ -0.004635 \\ 0 \end{bmatrix} \begin{bmatrix} 0 \\ -0.035490 \\ 0 \\ 0.039160 \\ -0.004635 \end{bmatrix}^T$$

$$= \begin{bmatrix} 0 & 0.030143 & 0 & -0.032978 & 0 \\ 0 & 0.074650 & 0 & -0.074650 & 0 \\ 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 \end{bmatrix}$$

The algorithm has the advantage that we do not need to compute the whole matrix R_k, since in the kth step only the entries of the i_kth row and j_kth column of R_k are used. Making use of the fact, that only few of the original entries of A have to be computed, leads to the following efficient reformulation of (2.19), where the vectors u_k and $\widetilde{v}_k$ coincide with $(R_{k-1})_{1:n,j_k}$ and $(R_{k-1})^T_{i_k,1:m}$, respectively.

Algorithm 1: Adaptive Cross Approximation (ACA)

Let $k = 1$; $Z = \emptyset$;
repeat
  $i_k := \operatorname{argmax}_{j \in \{1,\dots,n\} \setminus Z} |(u_k)_j|$
  $\widetilde{v}_k := a_{i_k,1:m}$
  for $l = 1, \dots, k-1$ **do**
    $\widetilde{v}_k := \widetilde{v}_k - (u_l)_{i_k} v_l$
  end for
  $Z := Z \cup \{i_k\}$
  if $\widetilde{v}_k$ does not vanish **then**
    $j_k := \operatorname{argmax}_{j \in \{1,\dots,n\}} |(\widetilde{v}_k)_j|$
    $v_k := (\widetilde{v}_k)^{-1}_{j_k} \widetilde{v}_k$
    $u_k := a_{1:n,j_k}$
    for $l = 1, \dots, k-1$ **do**
      $u_k := u_k - (v_l)_{j_k} u_l$
    end for
    $k := k + 1$
  end if
until stopping criterion (2.20) is fulfilled or $Z = \{1, \dots, m\}$

We memorize the vanishing rows by collecting them in the set Z. Since the i_kth row of R_{k+1} will vanish, if we use the i_kth row of R_k as v_k, we add i_k to Z. The matrix A will be approximated by $S_k := \sum_{l=1}^{k} u_l v_l^T$ and it holds $A - S_k = R_k$. Obviously, the rank of S_k cannot be larger than k.

Let $\varepsilon > 0$ be given. As stopping criterion we can use the following condition on k

$$\|u_{k+1}\|_2 \|v_{k+1}\|_2 \leq \frac{\varepsilon(1-\eta)}{1+\varepsilon} \|S_k\|_F. \tag{2.20}$$

We assume that $\|R_{k+1}\|_F$ can be bounded by $\eta |R_k\|_F$ with $\eta = \overline{\eta}$ from (4.1), then we can estimate

$$\begin{aligned} \|R_k\|_F &\leq \|R_{k+1}\|_F + \|u_{k+1} v_{k+1}^T\|_F \\ &\leq \eta \|R_k\|_F + \|u_{k+1}\|_2 \|v_{k+1}\|_2, \end{aligned}$$

and hence

$$\begin{aligned} \|R_k\|_F &\leq \frac{1}{1-\eta} \|u_{k+1}\|_2 \|v_{k+1}\|_2 \\ &\overset{(2.20)}{\leq} \frac{\varepsilon}{1+\varepsilon} \|S_k\|_F \\ &\leq \frac{\varepsilon}{1+\varepsilon} (\|A\|_F + \|R_k\|_F). \end{aligned}$$

The previous estimate is equivalent to

$$\|R_k\|_F \leq \varepsilon \|A\|_F,$$

and thus condition (2.20) guarantees a relative approximation error ε. Using this condition, the rank required to guarantee a prescribed accuracy ε can be found adaptively and needs not to be known in advance.

Remark 2.18. There are configurations of domains where the choice of rows as in Algorithm 1 does not work. Other possibilities to choose them are described in [2].

Chapter 3

Panel-Clustering

The boundary Γ is discretized with small triangles, so called panels. In order to find an efficient way to evaluate Green's representation formula (1.4) we need to partition the boundary. Each part of the partition is a cluster of panels. Since it is too expensive to search an optimal partition in the set of all partitions, we restrict ourselves to the set arising by recursive subdivision of the boundary.

3.1 Cluster Trees

In this section we introduce the concept of clusters and cluster trees, which we will need to find an appropriate partition $\Gamma_1, \ldots, \Gamma_n$ of the boundary,

Definition 3.1. *A **cluster** τ is a subset such that $\emptyset \neq \tau \subset I$, for any set $I \subset \mathbb{N}$.*

Let $\mathcal{T}_h := \{\pi_1, \ldots, \pi_m\}$ be a triangulation of the boundary Γ, then we identify by a cluster τ the nonempty union of panels $\bigcup_{i \in \tau} \pi_i$. Now we will define a tree, whose vertices consist of clusters τ.

Definition 3.2. *A tree $T_I = (V, E)$ with vertices V and edges E is called **cluster tree** for a set $I = \{1, \ldots, m\} \subset \mathbb{N}$, if the following conditions are satisfied*

1. *I is the root of T_I,*
2. *$\tau = \bigcup_{\sigma \in S(\tau)} \sigma$ for all $\tau \in V \setminus \mathscr{L}(T_I)$,*
3. *there exists a constant C such that the degree $\deg \tau := |S(\tau)| \geq 2$ of each vertex $\tau \in V \setminus \mathscr{L}(T_I)$ is bounded from below by $\deg \tau \leq C$.*

Here, $S(\tau) := \{\sigma \in V : (\tau, \sigma) \in E\}$ denotes the **set of sons** of τ and $\mathscr{L}(T_I) := \{\tau \in V : S(\tau) = \emptyset\}$ the **set of leaves** of T_I. The **level** of a cluster $\tau \in T_I$ is defined as the

distance to the root. The fact that τ is the disjoint union of its sons $S(\tau)$ implies that $\tau \subset I$ for all $\tau \in T_I$ and that each level

$$T_I^{(l)} := \{\tau \in T_l : \text{level } \tau = l\}$$

of T_I contains a partition of I. By $L(T_I) := \max_{\tau \in V(T_I)} \text{level}(\tau) + 1$ we denote the **depth** of the cluster tree T_I.

Next, we want to show that the complexity for storing a cluster tree is linear. To this end we need the following lemma.

Lemma 3.3. *Let $q := \min_{\tau \in T_I \setminus \mathscr{L}(T_I)} \deg \tau \geq 2$. Then for the number of vertices in T_I it holds that*

$$|V(T_I)| \leq \frac{q|\mathscr{L}(T_I)| - 1}{q - 1} \leq 2|\mathscr{L}(T_I)| - 1.$$

Proof. We reduce the tree $T_0 := T_I$ by deleting in k steps one after another the nodes. We start with the fathers of the leaves $\mathscr{L}(T_0)$. Let T_l denote the tree after l steps and q_l the degree of the lth step. Obviously, it holds $|V(T_{l+1})| = |V(T_l)| - q_l$ and $|\mathscr{L}(T_{l+1})| = |\mathscr{L}(T_l)| - q_l + 1$. After k steps we have $|V(T_k)| = 1 = |\mathscr{L}(T_k)|$, where

$$|V(T_k)| = |V(T_0)| - \sum_{l=1}^{k-1} q_l \quad \text{and} \quad |\mathscr{L}(T_k)| = |\mathscr{L}(T_0)| - \sum_{l=1}^{k-1} (q_l - 1).$$

Comparing both equations yields $|V(T_0)| = |\mathscr{L}(T_0)| + (k-1)$, and from $q_k \geq k$ it follows that

$$\begin{aligned} 1 &= |\mathscr{L}(T_k)| \\ &= |\mathscr{L}(T_0)| - \sum_{l=1}^{k-1} (q_l - 1) \\ &\leq |\mathscr{L}(T_0)| - (k-1)(q-1). \end{aligned}$$

Hence we obtain

$$|V(T_0)| \leq \frac{q|\mathscr{L}(T_0)| - 1}{q - 1} \leq 2|\mathscr{L}(T_I)| - 1,$$

since $q \geq 2$ and $|\mathscr{L}(T_I)| \geq 1$. □

If we suppose that each cluster τ has a minimal size $|\tau| \geq n_{min} > 1$, then the number of leaves $|\mathscr{L}(T_I)|$ is bounded by $|I|/n_{min}$. Hence, the complexity for storing a cluster tree is linear, namely $\mathcal{O}(2|\mathscr{L}(T_I)| - 1) = \mathcal{O}(2|I|/n_{min} - 1) = \mathcal{O}(|I|)$.

In the following we will only consider $T = T_I$ with $I = \{1, \ldots, m\}$, so we omit the index I. A sphere around z with radius r is denoted by

$$K_r(z) := \{x \in \mathbb{R}^d : \|x - y\|_2 < r\}.$$

For each cluster $\tau \in V(T)$, there exists a (unique) closed sphere $K = \overline{K(\tau)}$ with minimum radius containing τ. Hence, we denote by z_τ the center and by ρ_τ the radius of the sphere $K(\tau)$, i.e.

$$K(\tau) = K_{\rho_\tau}(z_\tau).$$

In the following we assume that the panels $\pi_i, i \in I = \{1, \ldots, m\}$, are **quasi-uniform**, i.e. there exists a constant $c_U > 0$ such that

$$\max_{i \in I} \mu(\pi_i) \leq c_U \min_{i \in I} \mu(\pi_i), \tag{3.1}$$

and **shape regular**, i.e. there is a constant $c_R > 0$ such that

$$\mu(\pi_i) \geq c_R \, (\rho_{\pi_i})^{d-1}, \quad i \in I. \tag{3.2}$$

With $\mu(M)$ we denote the measure of a $(d-1)$-dimensional manifold $M \subset \mathbb{R}^d$, i.e. the area of M. We assume that the computational domain $\Gamma_m = \bigcup_{i=1}^m \pi_i$ is a $(d-1)$-dimensional manifold, i.e. for all $z \in \mathbb{R}^d$ it holds

$$\mu(\Gamma_m \cap K_r(z)) \leq c_\Gamma \, r^{d-1} \quad \text{for all } r > 0, \tag{3.3}$$

with a constant $c_\Gamma > 0$ depending on the curvature of the hypersurface $\Gamma_m \subset \mathbb{R}^d$.

Definition 3.4. *A cluster tree is called* ***geometrically balanced****, if there are constants $c_g, c_G > 0$ such that for each level $l = 0, \ldots, L(T) - 1$*

a) $\rho_\tau \leq c_g 2^{-l}$, (3.4)

b) $\mu(\tau) \geq 2^{-l}/c_G$, (3.5)

for all $\tau \in V(T)$.

3.2 Coverings of Γ_m by Acceptable Clusters

Analogously to spheres, we can define a bounding box around a cluster τ if we use the l_∞-norm instead of the l_2-norm. An axis parallel **bounding box** around z with radius $r \in \mathbb{R}^d$ is denoted by

$$B_r(z) := \{x \in \mathbb{R}^d : |x_i - z_i| < r_i\}.$$

If $r = (r, \dots, r)$, then the previous definition is equivalent to

$$B_r(z) = \{x \in \mathbb{R}^d : \|x - z\|_\infty < r\}.$$

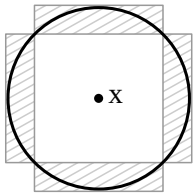
For each cluster $\tau \in V(T)$, there exists a (unique) closed bounding box $B = \overline{B(\tau)}$ with minimum radius containing τ. Hence, we denote by z_τ^B the center and by $\rho_\tau^B \in \mathbb{R}^d$ the radius of the bounding box $B(\tau)$, i.e.

$$B(\tau) = B_{\rho_\tau^B}(z_\tau^B).$$

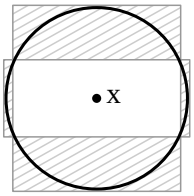
Definition 3.5. *Let $0 < \widetilde{\eta} < 1$. A cluster $\tau \in V(T_I)$ is **acceptable** with respect to a point $x \in \mathbb{R}^d$ if*

$$\operatorname{dist}(x, B(\tau)) \geq \widetilde{\eta} \operatorname{dist}(x, \tau), \tag{3.6}$$

where $\operatorname{dist}(x, \tau)$, $\operatorname{dist}(x, B(\tau))$ denote the distances of x from τ and $B(\tau)$ respectively.



(a) all clusters are acceptable



(b) only right and left cluster are acceptable

Figure 3.1: Two different coverings w.r.t. x and $\widetilde{\eta} = 0.5$.

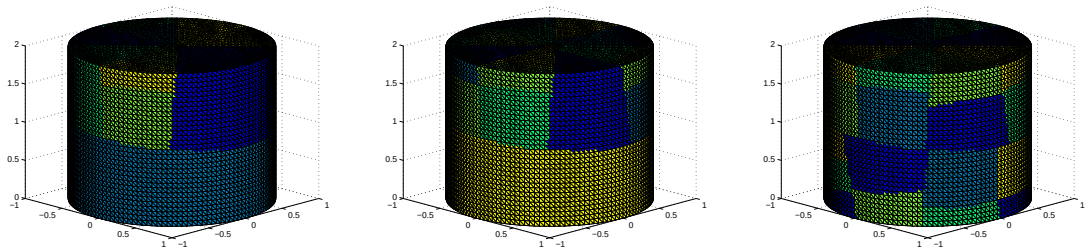
The parameter $\widetilde{\eta}$ controls how much the bounding box will reduce the distance between x and τ. Since error and rank of the approximation of kernel functions depends on the distance between the point x and a cluster τ, this definition avoids that both error and rank become larger as necessary.

Definition 3.6. *We call $\mathcal{C} = \{\tau_1, \dots, \tau_n\} \subset V(T)$ an **acceptable covering** (of Γ_m) with respect to x if*

a) $\Gamma_m = \bigcup_{j=1}^{n} \tau_j$, and

b) either $\tau_j \in \mathscr{L}(T)$ or τ_j is acceptable with respect to x.

If x is near the boundary, it may happen that there is no covering of Γ_m consisting only of acceptable clusters. Condition b) states that the only non-acceptable clusters can be the leaves of T.



(a) $x = (0, 0, 1.9116)$ (b) $x = (0, 0, 1.7027)$ (c) $x = (0, 0, 1)$

Figure 3.2: Acceptable coverings $\mathcal{C}(x)$ with respect to different points x.

Lemma 3.7. *For each $x \in \mathbb{R}^d$ there is a unique acceptable covering $\mathcal{C} = \mathcal{C}(x)$ with respect to x with minimum number $n = n(x) := |\mathcal{C}(x)|$. This covering is called* ***minimum acceptable covering*** *with respect to x.*

Proof. There is at least one admissible covering with respect to x, because we may choose $n = m$ and $\mathcal{C} = \mathscr{L}(T)$. The uniqueness will be proved by contradiction. To this end assume that $\mathcal{C} = \{\tau_1, \dots, \tau_n\}$ and $\mathcal{C}' = \{\tau'_1, \dots, \tau'_n\}$ are two different minimum acceptable coverings with respect to x. As $\mathcal{C} \neq \mathcal{C}'$, there is a cluster $\tau_j \in \mathcal{C}$ with $\tau_j \notin \mathcal{C}'$. Further, there is an index k such that $\tau_j \cap \tau'_k \neq \emptyset$ contains inner points. Due to the construction of T it must hold $\tau_j \subset \tau'_k$ or $\tau_j \supset \tau'_k$. Assume $\tau_j \subset \tau'_k$. Set $j_1 := j$ and let $j_2, \dots, j_l$ be all other indices with $\tau_{j_\nu} \subset \tau'_k$. Since $\tau_j \neq \tau'_k$, τ'_k is the disjoint union of $l \geq 2$ clusters, i.e. $\tau'_k = \bigcup_{1 \leq \nu \leq l} \tau_{j_\nu}$. Hence, the covering obtained from $\mathcal{C}$ by replacing $\{\tau_{j_1}, \dots, \tau_{j_l}\} \subset \mathcal{C}$ by τ'_k is also acceptable and contains only $n + 1 - l < n$ clusters in contradiction to the minimality of $n = |\mathcal{C}|$. □

Since the complexity of our procedure will depend on the number of clusters in a covering, this number should be as small as possible and can be estimated with the same construction as in [4].

Theorem 3.8. *Assume that condition (3.3) holds and that there is a constant C_P such that for all $z \in \mathbb{R}^d$ and $R \geq r > 0$ there is a subset $\mathcal{C} \subset V(T)$ of clusters with*

$$a) \quad \Gamma_m \cap \overline{K_R(z)} \subset \dot{\bigcup_{\tau \in \mathcal{C}}} \tau, \tag{3.7}$$

$$b) \quad \operatorname{diam}(\tau)/2 \leq r \quad \forall \tau \in \mathcal{C} \setminus \mathscr{L}(T), \tag{3.8}$$

$$c) \quad |\mathcal{C}| \leq C_P (R/r)^{d-1}, \tag{3.9}$$

then the number n of clusters in $\mathcal{C}(x)$ can be estimated by

$$n \le C \log\left(\frac{1}{(1-\widetilde{\eta})\operatorname{dist}(x,\Gamma_m)}\right)\left(\frac{1}{1-\widetilde{\eta}}\right)^{d-1}. \tag{3.10}$$

In [4] it is shown (cf. Proposition B.4) that quasi-uniform panels and a geometrically balanced cluster tree will satisfy conditions (3.7)-(3.9).

Proof. The size of $\Gamma_m \subset V(T)$ is $\rho := \rho_{\Gamma_m}$.

1. First we assume that $\sqrt{d}\rho \le (1-\widetilde{\eta})\operatorname{dist}(x,\Gamma_m)$. Let $\tau = \Gamma_m$ be the root of T. Then τ is the cluster containing all panels. It holds $\sqrt{d}\rho_\tau \le (1-\widetilde{\eta})\operatorname{dist}(x,\Gamma_m) = (1-\widetilde{\eta})\operatorname{dist}(x,\tau)$. So we obtain

$$\begin{aligned}\widetilde{\eta}\operatorname{dist}(x,\tau) &= \operatorname{dist}(x,\tau) - (1-\widetilde{\eta})\operatorname{dist}(x,\tau)\\ &\le \operatorname{dist}(x,\tau) - \sqrt{d}\rho_\tau\\ &\le \operatorname{dist}(x,B(\tau)),\end{aligned}$$

   i.e. τ is acceptable with respect to x. Hence, the acceptable covering of Γ_m contains only the cluster τ.
2. Next we consider the case $0 < (1-\widetilde{\eta})\operatorname{dist}(x,\Gamma_m) < \sqrt{d}\rho$. For all $l = 0,1,\ldots$ we apply conditions (3.7)-(3.9) with $z = x$, $R = R_l = 2^{-l}(2 + \frac{1}{1-\widetilde{\eta}})\rho$, $r = r_l = R_l\frac{1-\widetilde{\eta}}{4\sqrt{d}}$, hence there are coverings $\mathcal{C}_l$ with

$$\Gamma_m \cap \overline{K_{R_l}(x)} \subset \dot{\bigcup_{\tau^l\in\mathcal{C}_l}} \tau^l,$$

$$|\mathcal{C}_l| \le C_P\left(\frac{R_l}{r_l}\right)^{d-1} = C_P\left(\frac{4\sqrt{d}}{1-\widetilde{\eta}}\right)^{d-1},$$

   $l = 0,1,\ldots$ Let

$$K^l := \overline{K_{R_l}(x)} \setminus K_{R_{l+1}}(x),$$

   then we define $\mathcal{C}_l' \subset \mathcal{C}_l$ by

$$\mathcal{C}_l' := \{\tau \in \mathcal{C}_l : \tau \cap K^l \ne \emptyset\}.$$

   If $\tau \in \mathcal{C}_l'$ is not a leaf of T, it fulfills $\rho_\tau \le r_l = R_l\frac{1-\widetilde{\eta}}{4\sqrt{d}}$ (3.8). Since $\|y-x\|_2 \ge \frac{R_l}{2}$ for

any $y \in \tau \cap K^l \neq \emptyset$, we can conclude

$$\begin{aligned}\operatorname{dist}(x,\tau) &= \inf_{\xi\in\tau} \|x-\xi\|_2 \geq \inf_{\xi\in\tau}(\|x-y\|_2 - \|y-\xi\|_2)\\ &\geq \frac{R_l}{2} - r_l = \frac{R_l}{2} - R_l\frac{1-\widetilde{\eta}}{4}\\ &> \frac{R_l}{2} - \frac{R_l}{4} = \frac{R_l}{4} = \frac{\sqrt{d}r_l}{1-\widetilde{\eta}}\\ &\geq \frac{\sqrt{d}\rho_\tau}{1-\widetilde{\eta}}. \end{aligned} \tag{3.11}$$

Thus we obtain

$$\begin{aligned}\widetilde{\eta}\operatorname{dist}(x,\tau) &= \operatorname{dist}(x,\tau) - (1-\widetilde{\eta})\operatorname{dist}(x,\tau)\\ &\leq \operatorname{dist}(x,\tau) - \sqrt{d}\rho_\tau\\ &\leq \operatorname{dist}(x,B(\tau)),\end{aligned}$$

i.e. τ is acceptable with respect to x. Hence, $\mathcal{C}_l'$ is an acceptable covering of K^l with respect to x and it fulfills

$$\begin{aligned}&K^l \cap \Gamma_m \subset \dot{\bigcup_{\tau\in\mathcal{C}_l}} \tau, \quad \tau \in \mathcal{C}_l' \setminus \mathscr{L}(T) \text{ acceptable with respect to } x,\\ &|\mathcal{C}_l'| \leq |\mathcal{C}_l| \leq C_P\left(\frac{4\sqrt{d}}{1-\widetilde{\eta}}\right)^{d-1}.\end{aligned}$$

Let $L \geq 0$ be the first integer with

$$2^{-L}\left(2+\frac{1}{1-\widetilde{\eta}}\right)\rho = R_L < \operatorname{dist}(x,\Gamma_m).$$

Set $\mathcal{C}' := \mathcal{C}_0' \cup \mathcal{C}_1' \cup \ldots \cup \mathcal{C}_{L-1}'$. Since the clusters of $\mathcal{C}'$ are not disjoint, we restrict $\mathcal{C}'$ to $\mathcal{C} := \{\tau' \in \mathcal{C}' : \text{ there is no } \tau \in \mathcal{C}' \text{ with } \tau' \subset \tau\}$. $\mathcal{C}$ satisfies

$$\begin{aligned}\Gamma_m &= \Gamma_m \cap \left(\overline{K_{(2+\frac{1}{1-\widetilde{\eta}})\rho}(x)} \setminus K_{R_L}(x)\right) = \Gamma_m \cap \dot{\bigcup_{l=0}^{L-1}} K^l\\ &\subset \bigcup_{l=0}^{L-1}\left(\dot{\bigcup_{\tau\in\mathcal{C}_l'}}\tau\right) = \bigcup_{\tau\in\mathcal{C}'}\tau = \dot{\bigcup_{\tau\in\mathcal{C}}}\tau,\end{aligned}$$

i.e. $\mathcal{C}$ is a covering of Γ_m. Note that $\mathcal{C}$ is acceptable. The number of clusters in $\mathcal{C}$

can be estimated by

$$\begin{aligned}
|\mathcal{C}| \le |\mathcal{C}'| &\le \sum_{l=0}^{L-1} |\mathcal{C}'_l| \le \sum_{l=0}^{L-1} |\mathcal{C}_l| \le \sum_{l=0}^{L-1} C_p \left(\frac{4\sqrt{d}}{1-\widetilde{\eta}} \right)^{d-1} \\
&= L\, C_p \left(\frac{4\sqrt{d}}{1-\widetilde{\eta}} \right)^{d-1} \\
&\le \left(\log_2 \left(\left(2 + \frac{1}{1-\widetilde{\eta}} \right) \frac{\rho}{\operatorname{dist}(x, \Gamma_m)} \right) + 1 \right) C_p \left(\frac{4\sqrt{d}}{1-\widetilde{\eta}} \right)^{d-1} \\
&\le C \log \left(\frac{1}{(1-\widetilde{\eta}) \operatorname{dist}(x, \Gamma_m)} \right) \left(\frac{1}{1-\widetilde{\eta}} \right)^{d-1}.
\end{aligned}$$

□

Remark 3.9. This estimate is only a worst-case estimate. Let our computational domain be an axis parallel cuboid. If we consider the exterior boundary value problem we have only one cluster, independent of $\operatorname{dist}(x, \Gamma_m)$. Let a_{min} be the shortest side length of any bounding box $B(\tau)$, $\tau \in V(T)$. If once $\operatorname{dist}(x, \Gamma_m) < a_{min}$ the number of clusters will not increase. So the number of clusters is bounded by

$$|\mathcal{C}| \le C \log \left(\frac{2}{(1-\widetilde{\eta}) a_{min}} \right) \left(\frac{1}{1-\widetilde{\eta}} \right)^{d-1}.$$

The number n' of non-acceptable clusters in $\mathcal{C}(x)$ can be estimated with the following theorem.

Theorem 3.10. *Assume that condition (3.3) holds. Let T be a geometrically balanced cluster tree. Then the number n' of non-acceptable clusters in $\mathcal{C}(x)$ can be estimated by*

$$n' \le C \left(\frac{1}{1-\widetilde{\eta}} \right)^{d-1}. \tag{3.12}$$

Proof. The number n' of non-acceptable clusters is maximal if we choose $\mathcal{C}(x) = \mathscr{L}(T)$ as acceptable covering. Define $\rho_{max} := \max\{\rho_\tau : \tau \in \mathscr{L}(T)\}$ and set $r = \frac{2+\sqrt{d}}{1-\widetilde{\eta}} \rho_{max}$, then all τ not completely contained in $K_r(x)$ ($\Rightarrow r \le \operatorname{dist}(x, \tau) + 2\rho_\tau$) are acceptable with respect to x. This can be seen from

$$\begin{aligned}
\rho_\tau \le \rho_{max} &= \frac{1-\widetilde{\eta}}{2+\sqrt{d}}\, r \\
&\le \frac{1-\widetilde{\eta}}{2+\sqrt{d}} (\operatorname{dist}(x, \tau) + 2\rho_\tau),
\end{aligned}$$

$$
\begin{aligned}
\Leftrightarrow \quad & \left(1 - \frac{2(1-\widetilde{\eta})}{2+\sqrt{d}}\right)\rho_\tau && \leq \frac{1-\widetilde{\eta}}{2+\sqrt{d}}\,\mathrm{dist}(x,\tau) \\
\Leftrightarrow \quad & (\sqrt{d}+2\widetilde{\eta})\rho_\tau && \leq (1-\widetilde{\eta})\,\mathrm{dist}(x,\tau) \\
\Rightarrow \quad & \sqrt{d}\rho_\tau && \leq (1-\widetilde{\eta})\,\mathrm{dist}(x,\tau) \\
\Rightarrow \quad & \widetilde{\eta}\,\mathrm{dist}(x,\tau) && = \mathrm{dist}(x,B(\tau)).
\end{aligned}
$$

Therefore, $n' \leq |\mathcal{C}'|$ for $\mathcal{C}' := \{\tau \in \mathscr{L}(T) : \tau \subset K_r(x)\}$. Using (3.3) and the properties (3.4), (3.5) of a geometrically balanced cluster tree we can estimate

$$
\begin{aligned}
n' \frac{2^{-(L(T)-1)}}{c_G} &\leq \sum_{\tau\in\mathcal{C}'} \mu(\tau) = \mu\left(\bigcup_{\tau\in\mathcal{C}'} \tau\right) \\
&\leq (K_r(x) \cap \Gamma_m) \leq c_\Gamma\, r^{d-1},
\end{aligned}
$$

and hence

$$
\begin{aligned}
n' &\leq c_G\, c_\Gamma\, 2^{-(L(T)-1)}\, r^{d-1} \\
&\leq c_G\, c_\Gamma\, 2^{-(L(T)-1)} \left(\frac{(2+\sqrt{d})\rho_{max}}{1-\widetilde{\eta}}\right)^{d-1} \\
&\leq c_g\, c_G\, c_\Gamma\, 2^{d-1} \left(\frac{1}{1-\widetilde{\eta}}\right)^{d-1} \\
&\leq C \left(\frac{1}{1-\widetilde{\eta}}\right)^{d-1}.
\end{aligned}
$$

□

The previous Theorems 3.8 and 3.10 show that both the number of acceptable and the number of non-acceptable clusters of a covering $\mathcal{C}(x)$ can be estimated by constants independent of the number m of panels.

Chapter 4

Complexity

4.1 Computation of an Acceptable Covering

In the first part of the implementation, we find a partition of the boundary Γ such that the assumptions of Theorem 2.8 are satisfied. To this end we discretize the boundary Γ with small triangles $\{\pi_1, \ldots, \pi_m\}$, so-called panels. Depending on the distance to the evaluation point $x \in \Omega$, we divide the boundary Γ up into disjoint clusters $\Gamma_i, i = 1, 2, \ldots, n$ consisting of p_i panels respectively. For this purpose, we need to construct a geometrically balanced cluster tree $T = T_I$ with $I = \{1, \ldots, m\}$. If the panels π_i, $i \in I$, are quasi-uniform, this can be done in $\mathcal{O}(m \log m)$ operations (cf. Theorem 1.27 in [2]).

The minimum acceptable covering $\mathcal{C}(x)$ with respect to x will be computed by the following recursive procedure.

Algorithm 2: Acceptable Covering

$\mathcal{C} := \emptyset$
Divide(Γ_m, $\mathcal{C}$)

procedure DIVIDE(τ, $\mathcal{C}$)
    if τ is acceptable w.r.t. x **then** $\mathcal{C} := \mathcal{C} \cup \{\tau\}$
    else if $\tau \in \mathscr{L}(T)$ **then** $\mathcal{C} := \mathcal{C} \cup \{\tau\}$
    else
        for all $\sigma \in S(\tau)$ **do** Divide(σ, $\mathcal{C}$)
        end for
    end if
end procedure

First, the distance from x to the discretized boundary Γ_m has to be computed in $\mathcal{O}(m)$. In order to check whether a cluster τ is acceptable or not, the bounding box $B(\tau)$ must be determined. All bounding boxes in one level l of the cluster tree T can be computed in $\mathcal{O}(m)$. Since the cluster tree has a depth of $L(T) = \mathcal{O}(\log m)$, the total effort for all

bounding boxes is of order $\mathcal{O}(m \log m)$. The distance from x to each of the $\mathcal{O}(m)$ bounding boxes can be calculated in constant time. Thus we need $\mathcal{O}(m \log m)$ operations to find an acceptable covering of Γ_m with respect to x.

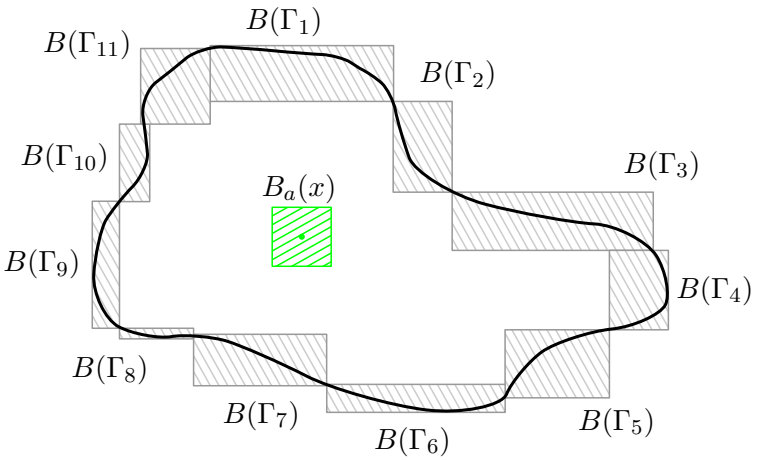


Figure 4.1: Bounding boxes around the clusters $\Gamma_1, \ldots, \Gamma_{11}$.

4.2 Approximation of the Kernel Functions

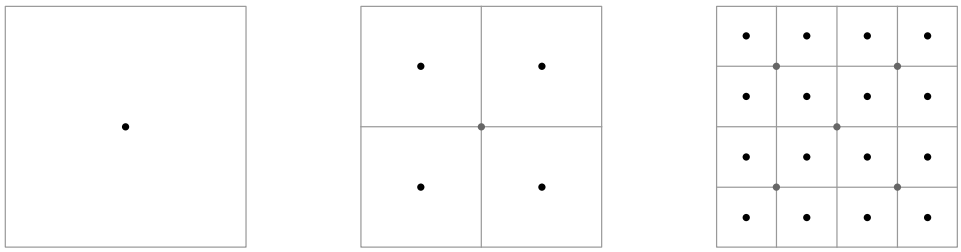
If we have found an $\widetilde{\eta}$-acceptable covering of Γ_m, we choose the length $a = \eta \min_i \operatorname{dist}(x, B(\Gamma_i))$ of the box $B_a(x)$ with center x such that the assumption $\eta \operatorname{dist}(x, B(\Gamma_i)) \geq a$ of Theorem 2.8 is satisfied for all acceptable clusters Γ_i, $i = 1, 2, \ldots, n$. The larger we choose $\widetilde{\eta}$ the larger $\operatorname{dist}(x, B(\Gamma_i))$ will be and the larger we can choose a. If the length a is larger, perhaps more evaluation points can be covered with one single box $B_a(x)$. Hence $\widetilde{\eta}$ avoids that we do not choose a too small.

With this choice of a, we guarantee that any pair $(B_a(x),\ B(\Gamma_i))$ is **admissible** in the usual sense, i.e.

$$\min\{\operatorname{diam}(B_a(x)), \operatorname{diam}(B(\Gamma_i))\} \leq \overline{\eta} \operatorname{dist}(B_a(x), B(\Gamma_i)), \tag{4.1}$$

with $\overline{\eta} = 2\sqrt{d}\eta/(2 - \sqrt{d}\eta)$. This can be seen from

$$\begin{aligned}
& \operatorname{diam}(B_a(x)) && = \sqrt{d}a \leq \sqrt{d}\eta \operatorname{dist}(x, B(\Gamma_i)) \\
& && \leq \sqrt{d}\eta(\operatorname{dist}(B_a(x), B(\Gamma_i)) + 0.5 \operatorname{diam}(B_a(x))) \\
\Leftrightarrow\ & (1 - 0.5\sqrt{d}\eta) \operatorname{diam}(B_a(x)) && \leq \sqrt{d}\eta \operatorname{dist}(B_a(x), B(\Gamma_i)) \\
\Leftrightarrow\ & \operatorname{diam}(B_a(x)) && \leq \frac{2\sqrt{d}\eta}{2 - \sqrt{d}\eta} \operatorname{dist}(B_a(x), B(\Gamma_i)).
\end{aligned}$$



(a) first order (b) second order (c) third order

Figure 4.2: Hierarchical mesh of different orders.

In the next chapter we will see, that $\overline{\eta}$ controls the approximation error. The concept of acceptable coverings has the advantage, that we can choose η small without influencing the number of clusters in the covering $\mathcal{C}(x)$. Thus we can control both error and number of clusters independently of each other. Since we choose a such that any pair $(B_a(x),\, B(\Gamma_i))$ is admissible, the required rank and the approximation error are independent of $\widetilde{\eta}$.

In the next step, we place a hierarchical mesh in the boxes $B_a(x)$, $B(\Gamma_1)$, $B(\Gamma_2), \ldots,$ $B(\Gamma_n)$. The mesh of order L consists of

$$\sum_{l=0}^{L-1} \left(2^d\right)^l = \frac{\left(2^d\right)^L - 1}{2^d - 1}$$

points.

In these sets of points, ACA searches its pivots x_l^i and y_l^i, $l = 1, \ldots, k_i$ for calculating the approximation of $\kappa(x, y)$ on each domain $B_a(x) \times B(\Gamma_i)$, $i = 1, \ldots, n$. The degree of degeneracy k_i is chosen adaptively until a given accuracy is achieved for all pairs of nodes in the boxes $B_a(x)$ and $B(\Gamma_i)$. Since we need the outer normal ν_y for calculating the kernel function $\kappa(x, y)$ of the double-layer potential operator

$$\kappa(x, y) = \partial_{\nu_y} S(y - x) = -\frac{\nu_y \cdot (y - x)}{4\pi \|y - x\|^3},$$

only the part

$$-\frac{1}{4\pi \|y - x\|^3}$$

is approximated by ACA. In particular we calculate the vectors u_l^i and v_l^i, $l = 1, \ldots, k_i$ using Algorithm 1. This can be done in $\mathcal{O}(k_i^2(n_x + n_y))$ operations, where n_x and n_y denote the number of points in the hierarchical mesh in the boxes $B_a(x)$ and $B(\Gamma_i)$ respectively. It will turn out that we can choose n_x and n_y of order $\mathcal{O}(k_i)$. Thus the vectors u_l^i and v_l^i, $l = 1, \ldots, k_i$ can be computed in $\mathcal{O}(k_i^3)$ operations per cluster Γ_i. Next, we compute the approximations $\widetilde{\kappa_S}$ and $\widetilde{\kappa_D}$ of

$$\widetilde{\kappa_S} \approx \kappa_S(x, y) = S(y - x) \quad \text{and} \quad \widetilde{\kappa_D} \approx \kappa_D(x, y) = -\frac{1}{4\pi \|y - x\|^3}$$

at the quadrature points $y_1^{i,j}, \ldots, y_q^{i,j}$ for each panel π_j, $j = 1, \ldots, p_i$ of the cluster Γ_i. Actually we have to compute the vectors $v(x) \in \mathbb{R}^k$ and $u(y_q^{i,j}) \in \mathbb{R}^k$ of

$$\kappa(x, y_q^{i,j}) \approx \sum_{l=0}^{k_i} v_l(x) u_l(y_q^{i,j}).$$

These computations have a complexity of $\mathcal{O}(k_i^2)$ per cluster and $\mathcal{O}(k_i^2)$ per quadrature point $y_q^{i,j}$ respectively.

4.3 Evaluation for Several Points

In the last step, we put all information together to evaluate the solution u at the point $x \in \Omega$.

$$\begin{aligned}
u(x) \approx & \sum_{i=1}^{n} \sum_{j=1}^{p_i} \sum_{l=1}^{q} \left(\omega_l \, \widetilde{\kappa_S}(y_l^{i,j} - x) \, g_N(y_l^{i,j}) - \omega_l \, g_D(y_l^{i,j}) \left(\nu^{i,j} \cdot (y_l^{i,j} - x) \right) \widetilde{\kappa_D}(y_l^{i,j} - x) \right) \\
& + \sum_{i=n+1}^{n+n'} \sum_{j=1}^{p_i} \sum_{l=1}^{q} \left(\omega_l \, \kappa_S(y_l^{i,j} - x) \, g_N(y_l^{i,j}) - \omega_l \, g_D(y_l^{i,j}) \left(\nu^{i,j} \cdot (y_l^{i,j} - x) \right) \kappa_D(y_l^{i,j} - x) \right) \\
= & \sum_{i=1}^{n} \sum_{j=1}^{p_i} \sum_{l=1}^{q} \left(\sum_{m=1}^{k_i^1} \omega_l \, u_m^i(x) \, v_m^i(y_l^{i,j}) \, g_N(y_l^{i,j}) \right. \\
& \qquad \left. - \sum_{m=1}^{k_i^2} \omega_l \, g_D(y_l^{i,j}) \left(\nu^{i,j} \cdot (y_l^{i,j} - x) \right) w_m^i(x) \, z_m^i(y_l^{i,j}) \right) \\
& + \sum_{i=n+1}^{n+n'} \sum_{j=1}^{p_i} \sum_{l=1}^{q} \left(\omega_l \, \kappa_S(y_l^{i,j} - x) \, g_N(y_l^{i,j}) - \omega_l \, g_D(y_l^{i,j}) \left(\nu^{i,j} \cdot (y_l^{i,j} - x) \right) \kappa_D(y_l^{i,j} - x) \right) \\
= & \sum_{i=1}^{n} \left(\sum_{m=1}^{k_i^1} u_m^i(x) \sum_{j=1}^{p_i} \sum_{l=1}^{q} \omega_l \, v_m^i(y_l^{i,j}) \, g_N(y_l^{i,j}) \right. \\
& \qquad - \sum_{m=1}^{k_i^2} w_m^i(x) \sum_{j=1}^{p_i} \sum_{l=1}^{q} \omega_l \, g_D(y_l^{i,j}) \left(\nu^{i,j} \cdot y_l^{i,j} \right) z_m^i(y_l^{i,j}) \\
& \qquad \left. + \sum_{m=1}^{k_i^1} \sum_{t=1}^{d} w_m^i(x) \, x_t \sum_{j=1}^{p_i} \sum_{l=1}^{q} \omega_l \, g_D(y_l^{i,j}) \, z_m^i(y_l^{i,j}) \, \nu_t^{i,j} \right) \\
& + \sum_{i=n+1}^{n+n'} \sum_{j=1}^{p_i} \sum_{l=1}^{q} \left(\omega_l \, \kappa_S(y_l^{i,j} - x) \, g_N(y_l^{i,j}) - \omega_l \, g_D(y_l^{i,j}) \left(\nu^{i,j} \cdot (y_l^{i,j} - x) \right) \kappa_D(y_l^{i,j} - x) \right)
\end{aligned}$$

where ω_l denotes the quadrature weight of the node y_l and ν_j^i the outer normal of the panel π_j of the cluster Γ_i. Since

$$\sum_{j=1}^{p_i}\sum_{l=1}^{q}\omega_l\, v_m^i(y_l^{i,j})\, g_N(y_l^{i,j}),$$
$$\sum_{j=1}^{p_i}\sum_{l=1}^{q}\omega_l\, g_D(y_l^{i,j})(\nu_j^i\cdot y_l^{i,j})z_m^i(y_l^{i,j}),$$
$$\sum_{j=1}^{p_i}\sum_{l=1}^{q}\omega_l\, g_D(y_l^{i,j})\, z_m^i(y_l^{i,j})\, \nu_t^{i,j}$$

are independent of x, we can store the results of these sums to save computation time by evaluating the solution at some other point $\widetilde{x}\in D_X$. If we choose $\widetilde{x}\notin D_X$, we have to calculate a new covering of Γ with clusters Γ_i and thus a new approximation of κ on each of these clusters.

Let N be the number of evaluation points. For the evaluation of the single-layer operator on acceptable clusters we need to compute the sum $C_S^i := \sum_{j=1}^{p_i}\sum_{l=1}^{q}\omega_l v_m^i(y_l^{i,j})g_N(y_l^{i,j})$ once. This can be done in $\mathcal{O}(nm)$ operations. For each evaluation point x the sum

$$\sum_{i=1}^{n}\sum_{m=1}^{k_i^1} u_m^i(x)\, C_S^i$$

will be computed in time proportional to $\mathcal{O}(nk_i)$. Due to (2.10), k_i is of order $|\log\varepsilon|^d$. On non-acceptable clusters the kernel function will not be approximated but evaluated exactly since for a good approximation we had to choose a too small. If a cluster τ is non-acceptable it must be a leaf of T. Since T is a geometrically balanced cluster tree, the number of panels in τ is bounded. So we need $\mathcal{O}(n')$ operations per evaluation point for the exact evaluation on non-acceptable clusters.

Hence we obtain a total complexity of

$$\begin{aligned}&\mathcal{O}(m\log(m)+m\log(m)+k^3n+k^2nN+k^2m+mn+knN+n'N)\\&\quad=\mathcal{O}(m\log(m)+k^3n+k^2nN+k^2m+nm+n'N)\\&\quad=\mathcal{O}(m\log(m)+|\log\varepsilon|^{2d}m+nm+|\log\varepsilon|^{3d}n+|\log\varepsilon|^{2d}nN+n'N)\end{aligned}$$

for the evaluation of the single-layer potential operator at N points. Note that the number n of clusters was independent of m and N, but dependent on the distance from the evaluation points to the boundary Γ_m and the control parameter $\widetilde{\eta}$. The number n' of non-acceptable clusters only depends on $\widetilde{\eta}$.

Now we consider the evaluation of the double-layer potential operator. For the first part we need to compute the sum $C_{D,1}^i := \sum_{j=1}^{p_i}\sum_{l=1}^{q}\omega_l\, g_D(y_l^{i,j})(\nu_j^i\cdot y_l^{i,j})\, z_m^i(y_l^{i,j})$. Again,

this can be done in time proportional to $\mathcal{O}(nm)$. For each evaluation point x the sum

$$-\sum_{i=1}^{n}\sum_{m=1}^{k_i^2} w_m^i(x)\, C_{D,1}^i$$

will be computed with $\mathcal{O}(nk_i)$ operations. For the second part the sum $C_{D,2}^{i,t} := \sum_{j=1}^{p_i}\sum_{l=1}^{q} \omega_l\, g_D(y_l^{i,j})\, z_m^i(y_l^{i,j})\, \nu_t^{i,j}$ will be computed in $\mathcal{O}(nm)$ time. After this, the sum

$$\sum_{i=1}^{n}\sum_{m=1}^{k_i^1}\sum_{t=1}^{d} w_m^i(x)\, x_t\, C_{D,2}^{i,t}$$

must be evaluated for each evaluation point. This can be done in $\mathcal{O}(dk_in)$ operations. Analogous to the one of the single-layer potential operator, the kernel function of the double-layer potential operator will be evaluated exactly.

Hence we obtain a total complexity of

$$\begin{aligned}
&\mathcal{O}(m\log(m) + m\log(m) + k^3n + k^2nN + k^2m + mn + knN + mn + dknN + n'N)\\
&\quad = \mathcal{O}(m\log(m) + k^3n + k^2nN + k^2m + nm + n'N)\\
&\quad = \mathcal{O}(m\log(m) + |\log\varepsilon|^{2d}m + nm + |\log\varepsilon|^{3d}n + |\log\varepsilon|^{2d}nN + n'N)
\end{aligned}$$

for the evaluation of the double-layer potential operator at N points.

Assume that ε, $\widetilde{\eta}$ and the minimal distance from any evaluation point to the boundary Γ_m are fixed. If m and N are of the same order the complexity scales like $N\log(N)$. This is an improvement of the complexity $\mathcal{O}(N^2)$ by exact evaluation.

Chapter 5

Error Estimates

In this chapter we want to estimate the error arising by evaluating any operator $\mathcal{A}$ of the form

$$u(x) := (\mathcal{A}v)(x) = \int_\Gamma \kappa(x,y)\, v(y)\, \mathrm{d}s_y.$$

Let $\widetilde{u}(x)$ denote the approximation of $u(x)$ and $\widetilde{v}(y)$ the approximation of $v(y)$ obtained by the in Section 1.4 described Galerkin method. Then we can estimate

$$\begin{aligned} |u(x) - \widetilde{u}(x)| &= \left| \int_\Gamma \kappa(x,y)\, v(y)\, \mathrm{d}s_y - \mathrm{Q}\left[s_k(x,\cdot)\, \widetilde{v}(\cdot)\right] \right| \\ &\leq \left| \int_\Gamma \kappa(x,y)\, v(y)\, \mathrm{d}s_y - Q\left[\kappa(x,\cdot)\, v(\cdot)\right] \right| \\ &\quad + \left| \mathrm{Q}\left[\kappa(x,\cdot)\, v(\cdot) - s_k(x,\cdot)\, \widetilde{v}(\cdot)\right] \right|, \\ &=: \varepsilon_q + \varepsilon_a \end{aligned}$$

where $\mathrm{Q}[f]$ denotes a quadrature of $f(y)$ by interpolation over Γ_m. The quadrature error ε_q can be estimated by the following theorem.

Theorem 5.1. *Let $\mathcal{T}_h$ be a quasi-uniform triangulation of Γ. The interpolation by piecewise polynomials of degree $t-1$ fulfills*

$$\|u - \mathcal{I}_h u\|_{m,h} \leq c\, h^{t-m} |u|_{t,\Gamma} \quad \text{for } u \in H^t(\Gamma), \quad 0 \leq m \leq t,$$

where c is a constant depending on Γ, c_U and t.

Proof. cf. [3] □

Thus we will only consider the approximation error ε_a. The error fulfills

$$\begin{aligned}
\varepsilon_a &= |\mathrm{Q}\left[\kappa(x,\cdot)\, v(\cdot) - s_k(x,\cdot)\,\widetilde{v}(\cdot)\right]| \\
&\leq |\Gamma_m| \sup_{y\in\Gamma_m} |\kappa(x,y)\, v(y) - s_k(x,y)\,\widetilde{v}(y)| \\
&\leq |\Gamma_m| \left(\sup_{y\in\Gamma_m} \left|\kappa(x,y)\,\left(v(y)-\widetilde{v}(y)\right)\right| + \sup_{y\in\Gamma_m} \left|\left(\kappa(x,y)-s_k(x,y)\right) v(y)\right| \right. \\
&\qquad \left. + \sup_{y\in\Gamma_m} \left|\left(\kappa(x,y)-s_k(x,y)\right)\left(v(y)-\widetilde{v}(y)\right)\right| \right),
\end{aligned}$$

where we have used that $ab - cd = a(b-d) + (a-c)b - (a-c)(b-d)$. We have

$$\begin{aligned}
\sup_{y\in\Gamma_m} \left|\kappa(x,y)\,\left(v(y)-\widetilde{v}(y)\right)\right| &\leq c_v \sup_{y\in\Gamma_m} |v(y)|\,|\kappa(x,y)| \\
&\leq c_v\, \mathrm{dist}(x,\Gamma_m)^{-s} \sup_{y\in\Gamma_m} |v(y)|.
\end{aligned}$$

Since we have partitioned the boundary such that any pair $(B_a(x), B(\Gamma_i))$ is admissible and since κ is asymptotically smooth with respect to x we can use (2.18) to estimate the second summand for all $x \in D_X \subset B_a(x)$ by

$$\begin{aligned}
\sup_{y\in\Gamma_m} \left|\left(\kappa(x,y)-s_k(x,y)\right)v(y)\right| &= \sup_{y\in\Gamma_m} |r_k(x,y)v(y)| \\
&\leq c_p\,\overline{\eta}^p \left(\min_i \mathrm{dist}(B_a(x), B(\Gamma_i))\right)^{-s} \sup_{y\in\Gamma_m} |v(y)|.
\end{aligned}$$

Combining the estimates for the first and second summand, we obtain for the third summand

$$\begin{aligned}
&\sup_{y\in\Gamma_m} \left|\left(\kappa(x,y)-s_k(x,y)\right)\left(v(y)-\widetilde{v}(y)\right)\right| \\
&\qquad \leq c_v\, c_p\,\overline{\eta}^p \left(\min_i \mathrm{dist}(B_a(x), B(\Gamma_i))\right)^{-s} \sup_{y\in\Gamma_m} |v(y)|,
\end{aligned}$$

and hence

$$\begin{aligned}
&|Q\left[\kappa(x,\cdot)v(\cdot) - s_k(x,\cdot)\widetilde{v}(\cdot)\right]| \\
&\quad \leq |\Gamma_m|\, c_v\, \mathrm{dist}(x,\Gamma)^{-s} \sup_{y\in\Gamma} |v(y)| \\
&\qquad + |\Gamma_m|\, c_p\,\overline{\eta}^p \left(\min_i \mathrm{dist}(B_a(x), B(\Gamma_i))\right)^{-s} \sup_{y\in\Gamma_m} |v(y)| \\
&\qquad + |\Gamma_m|\, c_v\, c_p\,\overline{\eta}^p \left(\min_i \mathrm{dist}(B_a(x), B(\Gamma_i))\right)^{-s} \sup_{y\in\Gamma_m} |v(y)| \\
&\quad \leq |\Gamma_m|\, (c_v + c_p\,\overline{\eta}^p + c_v\, c_p\,\overline{\eta}^p) \left(\min_i \mathrm{dist}(B_a(x), B(\Gamma_i))\right)^{-s} \sup_{y\in\Gamma_m} |v(y)|.
\end{aligned}$$

Using the previous estimate for Green's representation formula (1.4), we obtain the error bound

$$\begin{aligned}
&|u(x) - \widetilde{u}(x)| \\
&\quad = \left| \int_\Gamma S(y-x)t(y) - \partial_\nu^y S(y-x)u(y)\,\mathrm{d}s_y - \int_\Gamma s_k^1(x,y)\widetilde{t}(y) - s_k^2(x,y)\widetilde{u}(y)\,\mathrm{d}s_y \right| \\
&\quad \leq \left| \int_\Gamma S(y-x)t(y) - s_k^1(x,y)\widetilde{t}(y)\,\mathrm{d}s_y \right| + \left| \int_\Gamma \partial_\nu^y S(y-x)u(y) - s_k^2(x,y)\widetilde{u}(y)\,\mathrm{d}s_y \right| \\
&\quad \leq \varepsilon_q^1 + |\Gamma_m|\,(c_t + c_{p_1}\,\overline{\eta}^{p_1} + c_t\,c_{p_1}\,\overline{\eta}^{p_1}) \left(\min_i \operatorname{dist}(B_a(x), B(\Gamma_i)) \right)^{-s_1} \sup_{y\in\Gamma_m} |t(y)| \\
&\qquad + \varepsilon_q^2 + |\Gamma_m|\,(c_u + c_{p_2}\,\overline{\eta}^{p_2} + c_u\,c_{p_2}\,\overline{\eta}^{p_2}) \left(\min_i \operatorname{dist}(B_a(x), B(\Gamma_i)) \right)^{-s_2} \sup_{y\in\Gamma_m} |u(y)|.
\end{aligned}$$

If the Dirichlet data u and Neumann data t is given on the boundary Γ_m, the previous estimate can be simplified to

$$\begin{aligned}
&|u(x) - \widetilde{u}(x)| \\
&\quad = \left| \int_\Gamma S(y-x)t(y) - \partial_\nu^y S(y-x)u(y)\,\mathrm{d}s_y - \int_\Gamma s_k^1(x,y)\widetilde{t}(y) - s_k^2(x,y)\widetilde{u}(y)\,\mathrm{d}s_y \right| \\
&\quad \leq \varepsilon_q^1 + |\Gamma_m|\,c_{p_1}\,\overline{\eta}^{p_1} \left(\min_i \operatorname{dist}(B_a(x), B(\Gamma_i)) \right)^{-s_1} \sup_{y\in\Gamma_m} |t(y)| \\
&\qquad + \varepsilon_q^2 + |\Gamma_m|\,c_{p_2}\,\overline{\eta}^{p_2} \left(\min_i \operatorname{dist}(B_a(x), B(\Gamma_i)) \right)^{-s_2} \sup_{y\in\Gamma_m} |u(y)|.
\end{aligned}$$

Chapter 6

Numerical Results

All of the following computations are made on an Intel Xeon processor with 2.53 GHz.

6.1 Influence of Control Parameters η and ε.

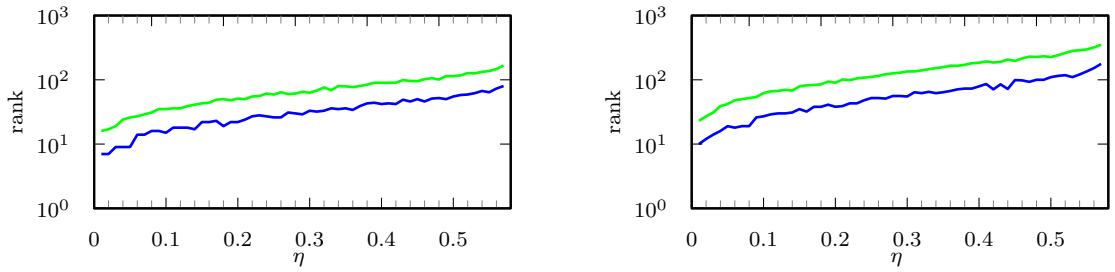
First, we want to analyze the dependency of the algorithm on the control parameter η. For this we test the algorithm for the exterior boundary value problem on the surface of a cube ($[0,8]^3$) with side length 8. The surface is discretized with 12288 panels and the solution is evaluated at the point $x = (4,4,12)$ for the exact boundary data

$$g_D(y) = \frac{1}{4\pi \|y - y_0\|}, \qquad g_N(y) = \partial_\nu g_D(y),$$

with $y_0 = (4,4,4)$ located at the center. Since we need for the convergence of ACA

$$0 < \overline{\eta} = \frac{2\sqrt{d}\eta}{2 - \sqrt{d}\eta} < 2 \qquad \Leftrightarrow \qquad 0 < \eta < \frac{1}{\sqrt{d}} \approx 0.577,$$

we have chosen $\eta = 0.01, 0.02, \ldots, 0.57$. In Theorem 2.8 we have seen that $k \sim \log(\varepsilon)/\log(\overline{\eta})$. Figure 6.1 shows that the algorithm has the same behavior.



(a) maximal rank single-layer operator

(b) maximal rank double-layer operator

Figure 6.1: Required rank of ACA to achieve a relative error of $\varepsilon = 10^{-9}$ (green) and $\varepsilon = 10^{-6}$ (blue) with meshes of order 5 (4681 points).

In Figure 6.2 it is shown that the accuracy of the solution is of the same order as the stopping criterion ε of ACA, independent of η.

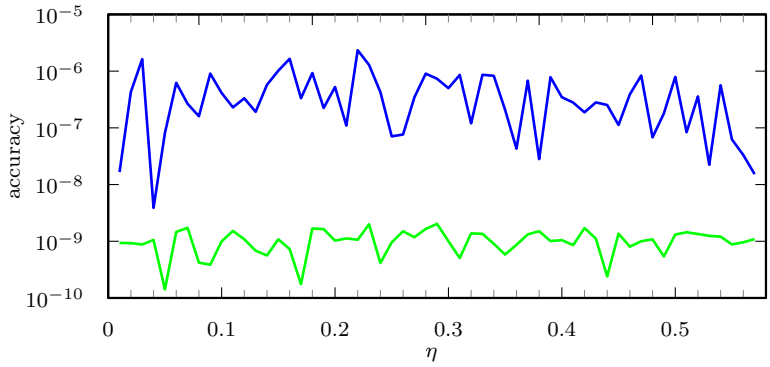


Figure 6.2: Accuracy of the solution with stopping criterion $\varepsilon = 10^{-9}$ (green) and $\varepsilon = 10^{-6}$ (blue) of ACA (4681 points).

Next we establish that the maximum rank k increases potentially in $|log(\varepsilon)|$, where ε denotes the accuracy of ACA. For this we evaluate the solution at $x = (6, 4, 4)$ with $\eta = 0.2$ and $\widetilde{\eta} = 0.5$. The meshes in $B(x)$ and $B(\Gamma_i)$ are both of order five (4681 points). The results can be found in Figure 6.3. In all cases the accuracy of the solution is of the same order as ε.

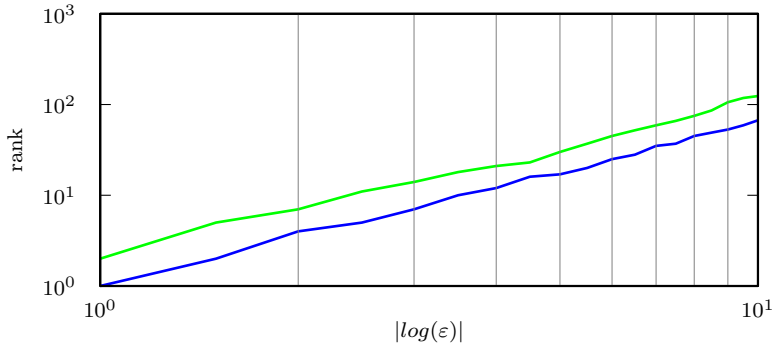


Figure 6.3: Maximum rank of single-layer potential operator (blue) and double-layer potential operator (green).

6.2 Influence of dist(x, Γ_m)

In order to establish that the number of clusters scales like $|\mathcal{C}| \sim \log(1/\operatorname{dist}(x, \Gamma_m))$, we test the algorithm on the surface of a prism shown in Figure 6.4. The evaluation points are located on the red line.

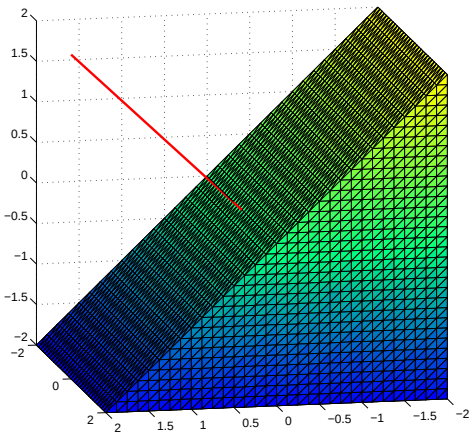
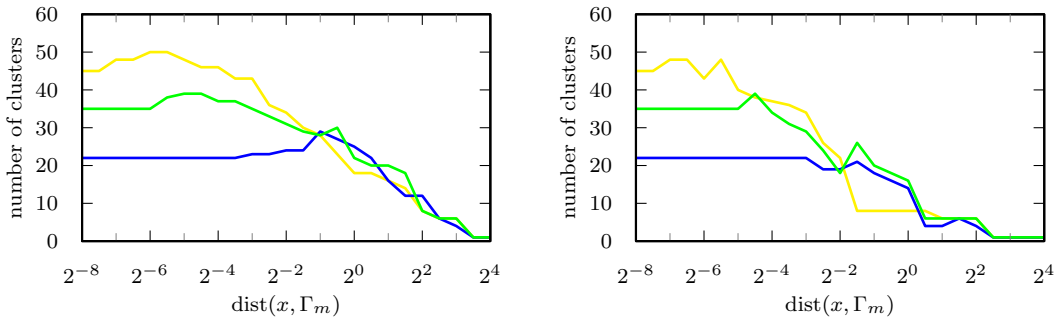


Figure 6.4: Prism (8192 panels).

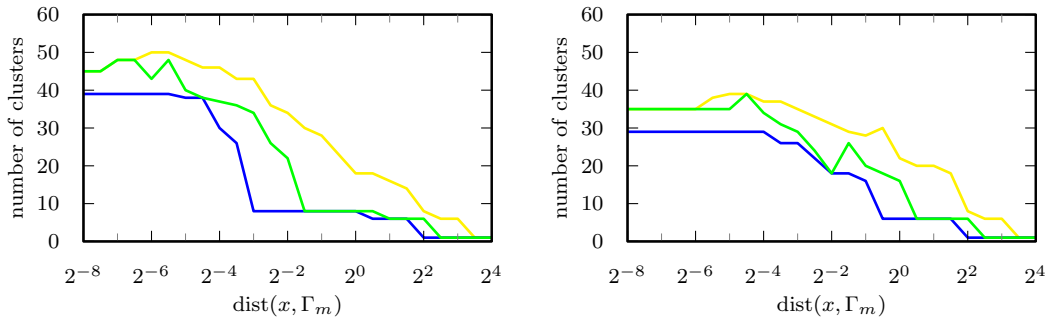
In Figure 6.5 the number of clusters are plotted against dist(x, Γ_m) for different parameters $\widetilde{\eta}$ and different orders of refinement of the surface. The number of clusters grows logarithmically with the distance of x to the boundary Γ_m until a barrier is reached. This barrier depends on the discretization, it grows with a refinement of the discretization of the boundary. Thus we can conclude that the number of clusters grows logarithmically for the limit of refinements.



(a) $\widetilde{\eta} = 0.75$ (b) $\widetilde{\eta} = 0.5$

Figure 6.5: Number of clusters for different orders of refinement: 32768 panels (blue), 131072 panels (green), 524288 panels (yellow).

If we compare the number of clusters for different parameters $\widetilde{\eta}$ we can see, that the larger $\widetilde{\eta}$ the larger this number (cf. Figure 6.6). Hence, we can establish the estimate (3.10).



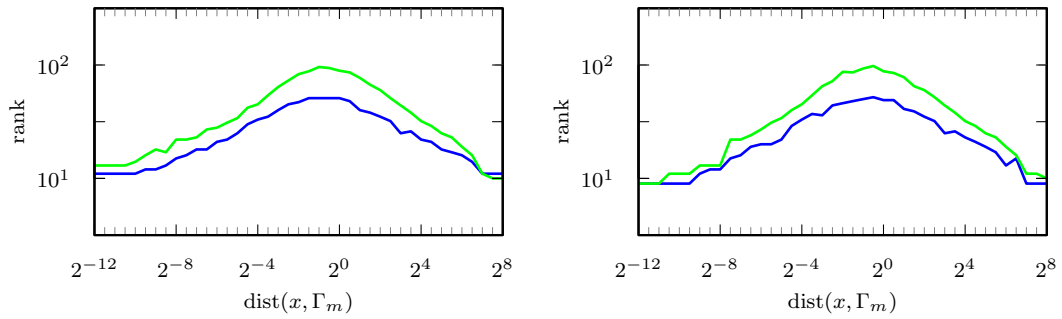
(a) 32768 panels (b) 131072 panels

Figure 6.6: Number of clusters for $\widetilde{\eta} = 0.25$ (blue), $\widetilde{\eta} = 0.5$ (green), $\widetilde{\eta} = 0.75$ (yellow).

In our next test we analyze how the maximum rank changes if we reduce the distance to the boundary. As computational domains we choose a sphere with radius 1 and a cube with side length 2, both centered at the origin. The sphere is discretized with 5120 panels with a minimum side length of 0.0691 and the cube is discretized with 12288 panels with a minimum side length of 0.0625. In both cases we choose the exact boundary data

$$g_D(y) = \frac{1}{4\pi \|y\|}, \qquad g_N(y) = \partial_\nu g_D(y),$$

$\varepsilon = 10^{-9}$, $\eta = 0.2$, $\widetilde{\eta} = 0.5$ and meshes of order four and five in the bounding boxes around the evaluation points $x = (1 + \mathrm{dist}(x, \Gamma_m), 0, 0)$ and the clusters Γ_i, respectively. With this choice of x the boundary Γ_m consists of only one cluster. In Figure 6.7 we can see that for both computational domains the rank first increases and later decreases if we halve $\mathrm{dist}(x, \Gamma_m)$. In the next section we will see that the point of change coincides with the point where the accuracy begins to decrease.

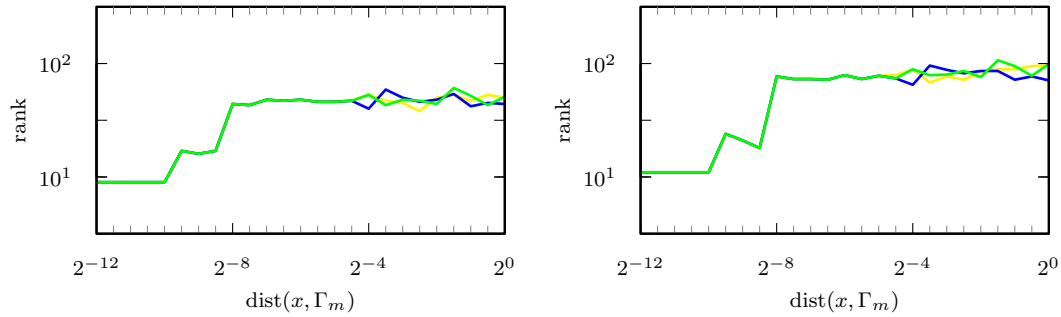


(a) sphere (b) cube

Figure 6.7: Maximum rank of single-layer potential operator (blue) and double-layer potential operator (green).

If we choose instead the points $x = (1 - \mathrm{dist}(x, \Gamma_m), 0, 0)$ in the interior of our computational domain Ω the number of clusters depends on the distance again. The maximum

rank increases (cf. Figure 6.8) as for the exterior boundary value problem. For points in the interior as well as for points at the exterior, the maximum ranks are of the same order. As we can see, the rank is also independent of the parameter $\widetilde{\eta}$.



(a) single-layer operator, sphere

(b) double-layer operator, sphere

(c) single-layer operator, cube

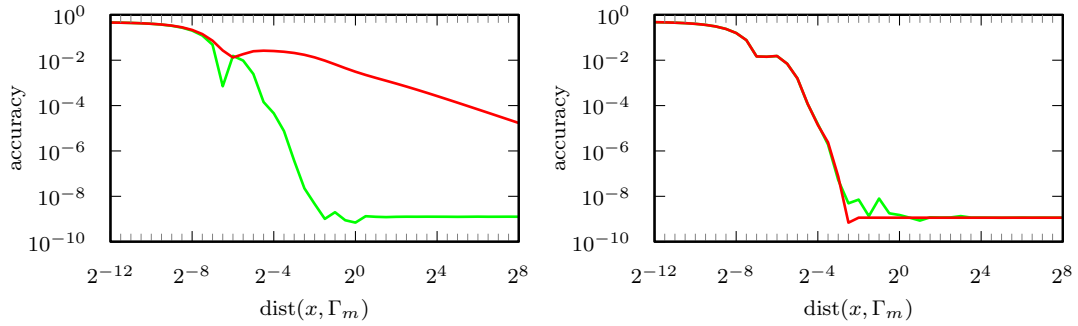
(d) double-layer operator, cube

Figure 6.8: Maximum rank of single-layer potential operator and double-layer potential operator with $\widetilde{\eta} = 0.75$ (blue), $\widetilde{\eta} = 0.5$ (green) and $\widetilde{\eta} = 0.25$ (yellow).

6.3 Comparison with Gauss Quadrature

In the previous test (cf. Figure 6.7) we have compared in addition our accuracy to the accuracy of Gauss quadrature with the same number of panels and quadrature points. In the case of a non-curved surface all quadrature points lie on the surface and thus usual quadrature provides good results (cf. Figure 6.9.b). With our method we can reach an accuracy of the same order. If the surface is curved, Gauss quadrature with plane panels does not work as well since the quadrature points are not located on the boundary. In this case, a higher accuracy can be reached with our method (cf. Figure 6.9.a). If the evaluation point x is far away from the boundary, the accuracy ε is constant. If a certain distance is reached, the error increases potentially with smaller distance, independent of the curvature of the surface. This is a typical phenomena of boundary element methods

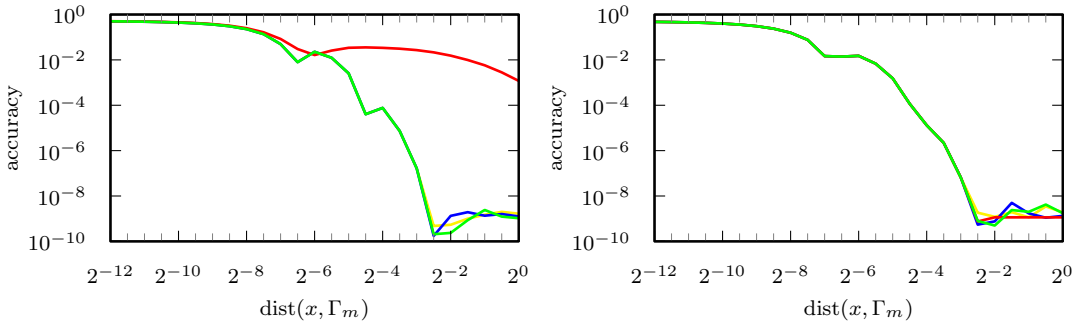
since the derivatives are large near the boundary. If we choose meshes of higher order in the bounding boxes around x and Γ_i the point of change can be moved to the left. For distances smaller than 2^{-8}, our method and Gauss quadrature provide the same results.



(a) sphere (b) cube

Figure 6.9: Accuracy of our method (green) and Gauss quadrature (red).

If we compare the errors for the points in the interior of Ω we can see a behavior similar to them of the points in the exterior (cf. Figure 6.10). Again, Gauss quadrature works better on the non-curved geometry. For evaluation points which are not very closed to the boundary ($\text{dist}(x, \Gamma_m) > 2^{-2}$), the accuracy is constant at the order of $\varepsilon = 10^{-9}$, independent of $\widetilde{\eta}$.



(a) sphere (b) cube

Figure 6.10: Accuracy of our method with $\widetilde{\eta} = 0.75$ (blue), $\widetilde{\eta} = 0.5$ (green), $\widetilde{\eta} = 0.25$ (yellow) and Gauss quadrature (red).

If we do not know the exact boundary data on the whole boundary Γ, we need to complete it as described in Section 1.4. In this case, the relative error at the evaluation point x cannot be smaller than the error made by approximating the boundary data. Thus it suffices to choose the stopping criterion ε for ACA of the same order.

In the previous chapter we have seen that the complexity for evaluating the solution at $N = m$ points is of order $N \log N$ whereas the direct evaluation by Gauss quadrature needs $\mathcal{O}(N^2)$ operations. Again we test the algorithm on the computational domain of a cube with side length 8. We choose $\eta = 0.2$ and $\widetilde{\eta} = 0.5$. The mesh in the bounding box around $x = (3, 3, 7)$ is of order four and the meshes in the bounding boxes around the clusters τ are of order five. ACA is stopped when an accuracy of $\varepsilon = 10^{-9}$ is reached. The resulting runtimes are plotted in Figure 6.11. We see that for large N the slope of the line representing Gauss quadrature is twice the slope of the line representing our method. Thus the complexity results of the previous section are verified.

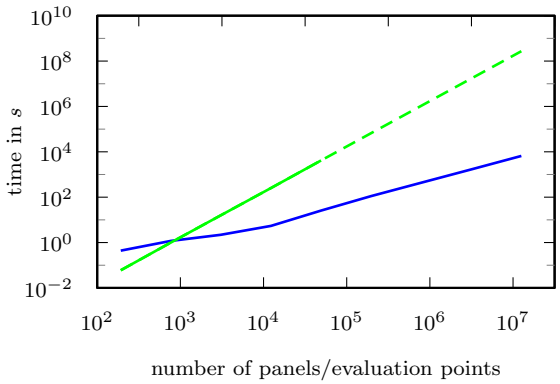


Figure 6.11: Runtime for our algorithm (blue) and Gauss quadrature (green).

Chapter 7

Conclusion

As we have seen in the both previous chapters, the introduced method is an efficient way to evaluate the representation formula for boundary element methods. Accuracy and complexity of Gauss quadrature only are acceptable if we have a few evaluation points far away from the boundary and non-curved geometries. In all other cases our method should be the preferred one. Since the degenerate kernel approximation leads to a separation of variables and large parts can be computed in advance so that the complexity scales like $N \log N$ instead of N^2, our algorithm works faster for more than about 10^3 evaluation points. The numerical experiments performed prove that in addition it is more precise, especially for curved computational domains. Due to large derivatives near the boundary it is not possible to achieve a high accuracy at evaluation points very closed to the boundary. However, this accuracy cannot either be reached by Gauss quadrature. In this case the accuracy of our method and Gauss quadrature are of the same order.

In comparison to the usual panel-clustering method, which has a complexity similar to our modified method, we do neither need to compute any derivatives nor to know in advance the degree of the degenerate kernel approximation. The degree to achieve a desired accuracy can be found adaptively. This is due to the fact that we use the adaptive cross approximation instead of Taylor expansion. Thus the adaptive cross approximation is a suitable alternative for approximating the arising kernels.

References

[1] M. Bebendorf, *Approximation of boundary element matrices*, Numerische Mathematik **86** (2000), no. 4, 565–589.

[2] ———, *Hierarchical Matrices: A Means to Efficiently Solve Elliptic Boundary Value Problems*, Lecture Notes in Computational Science and Engineering (LNCSE), vol. 63, Springer-Verlag, 2008, ISBN 978-3-540-77146-3.

[3] D. Braess, *Finite Elemente: Theorie, schnelle Löser und Anwendungen in der Elastizitätstheorie*, Springer-Lehrbuch Masterclass, Springer, 2010.

[4] W. Hackbusch and Z.P. Nowak, *On the fast matrix multiplication in the boundary element method by panel clustering*, Numerische Mathematik **54** (1989), no. 4, 463–491.

[5] W. McLean, *Strongly Elliptic Systems and Boundary Integral Equations*, Cambridge University Press, 2000.

[6] T. Sauer and Y. Xu, *On multivariate lagrange interpolation*, MATH. COMP **64** (1995), 1147–1170.

[7] S. A. Sauter and C. Schwab, *Boundary element methods*, Springer Series in Computational Mathematics, Springer, 2010.